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LNCS 14823

Computational Science and Its Applications – ICCSA 2024 Workshops

Hanoi, Vietnam, July 1–4, 2024
Proceedings, Part IX

Springer

Lecture Notes in Computer Science **14823**

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ISSN 0302-9743 ISSN 1611-3349 (electronic)
Lecture Notes in Computer Science
ISBN 978-3-031-65328-5 ISBN 978-3-031-65329-2 (eBook)
https://doi.org/10.1007/978-3-031-65329-2

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Preface

These 11 volumes (LNCS volumes 14815–14825) consist of the peer-reviewed papers from the 55 Workshops of the 2024 International Conference on Computational Science and Its Applications (ICCSA 2024) which took place during July 1–4, 2024 in Hanoi (Vietnam). The peer-reviewed papers of the main conference tracks are published in a separate set consisting of two volumes (LNCS 14813–14814).

The conference was held in a hybrid form, with some participants present in person, hosted in Hanoi, Vietnam, by the Thuy Loi University. We enabled virtual participation for those who were unable to attend the event, due to logistical, political and economic problems, by adopting a technological infrastructure based on open source software (jitsi + riot), and a commercial Cloud infrastructure.

ICCSA 2024 was another successful event in the International Conference on Computational Science and Its Applications (ICCSA) conference series, previously held in Athens, Greece (2023), Malaga, Spain (2022), Cagliari, Italy (hybrid with few participants in presence in 2021 and completely online in 2020), whilst earlier editions took place in Saint Petersburg, Russia (2019), Melbourne, Australia (2018), Trieste, Italy (2017), Beijing. China (2016), Banff, Canada (2015), Guimaraes, Portugal (2014), Ho Chi Minh City, Vietnam (2013), Salvador, Brazil (2012), Santander, Spain (2011), Fukuoka, Japan (2010), Suwon, South Korea (2009), Perugia, Italy (2008), Kuala Lumpur, Malaysia (2007), Glasgow, UK (2006), Singapore (2005), Assisi, Italy (2004), Montreal, Canada (2003), and (as ICCS) Amsterdam, The Netherlands (2002) and San Francisco, USA (2001).

Computational Science is the main pillar of most of the present research, industrial and commercial applications, and plays a unique role in exploiting ICT innovative technologies, and the ICCSA conference series have been providing a venue to researchers and industry practitioners to discuss new ideas, to share complex problems and their solutions, and to shape new trends in Computational Science. As the conference mirrors society from a scientific point of view, this year's undoubtedly dominant theme was the machine learning and artificial intelligence and their applications in the most diverse economic and industrial fields.

The ICCSA 2024 conference is structured in 6 general tracks covering the fields of computational science and its applications: Computational Methods, Algorithms and Scientific Applications – High Performance Computing and Networks – Geometric Modeling, Graphics and Visualization – Advanced and Emerging Applications – Information Systems and Technologies – Urban and Regional Planning. In addition, the conference consisted of 55 workshops, focusing on very topical issues of importance to science, technology and society: from new mathematical approaches for solving complex computational systems, to information and knowledge in the Internet of Things, new statistical and optimization methods, several Artificial Intelligence approaches, sustainability issues, smart cities and related technologies.

In the Workshops proceedings we accepted 281 full papers, 17 short papers and 2 PhD Showcase papers. In the Main Conference Proceedings we accepted 53 full papers, 6 short papers and 3 PhD Showcase papers from 207 submissions to the General Tracks of the conference (acceptance rate 30%). We would like to express our appreciation to the workshops chairs and co-chairs for their hard work and dedication.

The success of the ICCSA conference series in general, and of ICCSA 2024 in particular, vitally depends on the support of many people: authors, presenters, participants, keynote speakers, workshop chairs, session chairs, organizing committee members, student volunteers, Program Committee members, Advisory Committee members, International Liaison chairs, reviewers and others in various roles. We take this opportunity to wholehartedly thank them all.

We also wish to thank our publisher, Springer, for their acceptance to publish the proceedings, for sponsoring part of the best papers awards and for their kind assistance and cooperation during the editing process.

We cordially invite you to visit the ICCSA website https://iccsa.org where you can find all the relevant information about this interesting and exciting event.

July 2024

Osvaldo Gervasi
Beniamino Murgante
Chiara Garau

Welcome Message from Organizers

After the very hard times of COVID, ICCSA continues its successful scientific endeavors in 2024, hosted in Hanoi, Vietnam. This time, ICCSA moved from the Mediterranean Region to Southeast Asia and was held in the metropolitan city of Hanoi, the capital of Vietnam. Hanoi is a vibrant urban environment known for the hospitality of its citizens, its rich history, vibrant culture, and dynamic urban life. Located in the northern part of the country, Hanoi is a bustling metropolis that combines the old with the new, offering a unique blend of ancient traditions and modern development.

ICCSA 2024 took place in a secure environment, allowing for safe and vibrant in-person participation. Combined with the active engagement of the ICCSA 2024 scientific community, this set the stage for highly motivating discussions and interactions regarding the latest developments in computer science and its applications in the real world for improving communities' quality of life.

Thuyloi University, also known as the Water Resources University, is a prominent institution in Hanoi, Vietnam, with a strong reputation in engineering and technical education, particularly in water resources and environmental engineering. In recent years, the University has expanded its academic offerings to include computer science, reflecting the growing importance of technology and digital skills in all sectors. This year, Thuyloi University had the honor of hosting ICCSA 2024. The Local Organizing Committee felt the burden and responsibility of such a demanding task and put all necessary energy into meeting participants' expectations and establishing a friendly, creative, and inspiring scientific and social/cultural environment that allowed for new ideas and perspectives to flourish.

Since all ICCSA participants, whether informatics-oriented or application-driven, realize the tremendous advancements in computer science over the last few decades and the huge potential these advancements offer in coping with the enormous challenges of humanity in a globalized, 'wired,' and highly competitive world, the expectations for ICCSA 2024 were high. The goal was to successfully match computer science progress with communities' aspirations, achieving progress that serves real, place- and people-based needs and paves the way towards a visionary, smart, sustainable, resilient, and inclusive future for both current and future generations.

On behalf of the Local Organizing Committee, I would like to sincerely thank all of you who contributed to ICCSA 2024.

Nguyen Canh Thai

Organization

ICCSA 2024 was organized by Thuyloi University (Vietnam), the University of Perugia (Italy), the University of Basilicata (Italy), Monash University (Australia), Kyushu Sangyo University (Japan), the University of Minho (Portugal), and the University of Cagliari (Italy).

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Sustainable Digital Circular Economy (DiCE 2024)

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Andrea Gallo	University of Trieste, Italy

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Enrico Dagostini	University of Malta, Malta
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Marco Naseddu	University of Cagliari, Italy
Balázs Kulcsaár	University of Debrecen, Hungary
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Maria Ronza	University of Naples, Federico II, Italy
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Evaluating Inner Areas Potentials (EIAP 2024)

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Manuela Rebaudengo	Polytechnic of Turin, Italy
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Econometrics and Multidimensional Evaluation of Urban Environment (EMEUE 2024)

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Maria Somma	University of Naples Federico II, Italy
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Environmental, Social, Governance of Energy Planning (ESGEP 2024)

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Ecosystem Services in Spatial Planning for Resilient Urban and Rural Areas (ESSP 2024)

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Matteo Caglioni	Université Côte d'Azur, France

Ethical AI Applications for a Human-Centered Cyber Society (EthicAI 2024)

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14th International Workshop on Future Computing System Technologies and Applications (FiSTA 2024)

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Kazuaki Tanaka	Kyushu Institute of Technology, Japan
Toshihiro Uchibayashi	Kyushu University, Japan
Toshihiro Yamauchi	Okayama University, Japan
Fenghui Yao	Tennessee State University, USA

Geographical Analysis, Urban Modeling, Spatial Statistics (Geog-An-Mod 2024)

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Andreas Fricke	Hasso-Plattner-Institut für Digital Engineering, Germany
Rodrigo Tapia McClung	Centro de Investigación en Ciencias de Información Geoespacial, Mexico

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Ahinoa Amaro Garcia	University of Las Palmas of Gran Canaria, Spain
Veronica Camerada	University of Sassari, Italy
Maria Attard	University of Malta, Malta
Enrico Dagostini	University of Malta, Malta
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Maria Ronza	University of Naples, Federico II, Italy
Massimiliano Bencardino	University of Salerno, Italy

Geomatics for Resource Monitoring and Management (GRMM 2024)

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Alberico Sonnessa	Polytechnic of Bari, Italy

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International Workshop on Information and Knowledge in the Internet of Things (IKIT 2024)

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Regenerating Brownfields Enhancing Urban Resilience Appeal (INFERENCE 2024)

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Francesca Moraci	Mediterranea University of Reggio Calabria, Italy
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Antonella Versaci	University of Enna Kore, Italy
Celestina Fazia	University of Enna Kore, Italy
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Clarastella Vicari Aversa	Mediterranea University of Reggio Calabria, Italy

International Workshop on Territorial Planning to Integrate Risk and Urban Ontologies (IWPRO 2024)

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Caterina Pietra	University of Pavia, Italy

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MaaS Solutions for Airports, Cities and Regional Connectivity (MaaS 2024)

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Mara Ladu	University of Cagliari, Italy
Martina Sinatra	University of Cagliari, Italy
Ginevra Balletto	University of Cagliari, Italy

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Marco Mazzarino	IUAV Univeristy Venice, Italy
Maria del Mar Munoz Leonisio	University of Cadiz, Spain
Veronica Camerada	Univeristy of Sassari, Italy

Brunella Brundu	Univerisity of Sassari, Italy
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Enrico Dagostini	University of Malta, Malta
Giovanni Mauro	University of Campania Luigi Vanvitelli, Italy
Maria Ronza	University of Naples, Federico II, Italy
Massimiliano Bencardino	University of Salerno, Italy

Development of Urban Mobility Management and Risk Assessment (MAINTAIN 2024)

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Massimo Di Gangi	University of Messina, Italy
Antonio Comi	University of Rome Tor Vergata, Italy
Grigorios Fountas	Aristotle University of Thessaloniki, Greece
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Orlando Belcore	University of Messina, Italy
Marinella Giunta	Mediterranea University of Reggio Calabria, Italy
Borja Alonso	University of Cantabria, Spain
Luigi Dall'Olio	University of Cantabria, Santander, Spain
Kh Md Nahiduzzaman	UBC, Canada

Multidimensional Evolutionary Evaluations for Transformative Approaches (MEETA 2024)

Workshop Organizers

Maria Cerreta	University of Naples Federico II, Italy
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Daniele Cannatella	TU Delft, The Netherlands

Ludovica Larocca	University of Naples Federico II, Italy
Maria Somma	University of Naples Federico II, Italy
Gaia Daldanise	National Research Council, Italy

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Piero Zizzania	University of Naples Federico II, Italy
Stefano Cuntò	University of Naples Federico II, Italy
Sveva Ventre	University of Naples Federico II, Italy
Caterina Loffredo	University of Naples Federico II, Italy
Giuseppe Ciciriello	University of Naples Federico II, Italy
Laura Di Tommaso	University of Naples Federico II, Italy
Benedetta Grieco	University of Naples Federico II, Italy
Simona Panaro	University of Sussex, UK

Building Multi-dimensional Models for Assessing Complex Environmental Systems (MES 2024)

Workshop Organizers

Vanessa Assumma	University of Bologna, Italy
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Federico Dell'Anna	Politechnic of Turin, Italy
Marta Dell'Ovo	Politechnic of Milan, Italy
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Models and Indicators for Assessing and Measuring the Urban Settlement Development in the View of Zero Net Land Take by 2050 (MOVEto0 2024)

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Lucia Saganeiti	University of L'Aquila, Italy
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Angela Pilogallo	University of L'Aquila, Italy
Francesco Zullo	University of L'Aquila, Italy
Alessandro Marucci	University of L'Aquila, Italy

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Ilaria Del Ponte	University of Genoa, Italy
Carmen Guida	University of Naples Federico II, Italy
Chiara Di Dato	University of L'Aquila, Italy

4th Workshop on Privacy in the Cloud/Edge/IoT World (PCEIoT 2024)

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Davide Cerotti	University of Piedmont Oriental, Italy

Scientific Computing Infrastructure (SCI 2024)

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Elena Stankova	St. Petersburg State University, Russia

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Alexander Bogdanov	St. Petersburg State University, Russia
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Downscale Agenda 2030 (SDGscale 2024)

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Salvatore Dore	University of Trieste, Italy
Maria Attard	University of Malta, Malta
Giovanni Mauro	University of Campania Luigi Vanvitelli, Italy
Maria Ronza	University of Naples, Federico II, Italy
Massimiliano Bencardino	University of Salerno, Italy

Socio-Economic and Environmental Models for Land Use Management (SEMLUM 2024)

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Elena Fregonara	Polytechnic of Turin, Italy
Paola Amoruso	LUM, Italy

Ports of the Future - Smartness and Sustainability (SmartPorts 2024)

Workshop Organizers

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Patrizia Serra	University of Cagliari, Italy
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Marco Petrelli	Roma Tre University, Italy

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Veronica Camerada	University of Sassari, Italy
Brunella Brundu	University of Sassari, Italy
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Enrico Dagostini	University of Malta, Malta
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Maria Ronza	University of Naples, Federico II, Italy
Massimiliano Bencardino	University of Salerno, Italy

Smart Transport and Logistics - Smart Supply Chains (SmarTransLog 2024)

Workshop Organizers

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Maria del Mar Munoz Leonisio	University of Cádiz, Spain
Maria Attard	University of Malta, Malta
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Brunella Brundu	University of Sassari, Italy

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Mara Ladu	University of Cagliari, Italy
Martina Sinatra	University of Cagliari, Italy
Francesca Sinatra	University of Trieste, Italy
Salvatore Dore	University of Trieste, Italy
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Marco Mazzarino	IUAV University Venice, Italy
Enrico Dagostini	University of Malta, Malta
Marco Naseddu	University of Cagliari, Italy
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Giovanni Longo	University of Trieste, Italy
Luca Toneatti	University of Trieste, Italy
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Maria Ronza	University of Naples, Federico II, Italy
Massimiliano Bencardino	University of Salerno, Italy

Smart Tourism (SmartTourism 2024)

Workshop Organizers

Silvia Battino	University of Sassari, Italy
Francesca Krasna	University of Trieste, Italy
Maria del Mar Munoz Leonisio	University of Cadiz, Spain

Ginevra Balletto	University of Cagliari, Italy
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Ainhoa Amaro Garcia	University of Las Palmas of Gran Canarias, Spain

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Mara Ladu	University of Cagliari, Italy
Martina Sinatra	University of Cagliari, Italy
Salvatore Dore	University of Trieste, Italy
Veronica Camerada	University of Sassari, Italy
Brunella Brundu	University of Sassari, Italy
Maria Attard	University of Malta, Malta
Tu Anh Trinh	College of Technology and Design for UEH University, Vietnam
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Maria Ronza	University of Naples, Federico II, Italy
Massimiliano Bencardino	University of Salerno, Italy

Sustainable Evolution of Long-Distance Freight Passenger Transport (SOLIDEST 2024)

Workshop Organizers

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Antonio Comi	University of Rome Tor Vergata, Italy
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Luigi Dall'Olio	University of Cantabria, Spain
Antonio Russo	University of Enna Kore, Italy

Sustainability Performance Assessment: Models, Approaches, and Applications Toward Interdisciplinary and Integrated Solutions (SPA 2024)

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ICCSA 2024 took place on the main campus of Thuyloi University in Hanoi, Vietnam.

Plenary Lectures

Harnessing Artificial Intelligence for Enhanced Spatial Analysis of Natural Hazard Assessments

Prof. Dr. Biswajeet Pradhan

Director - Centre for Advanced Modelling and Geospatial Information Systems (CAMGIS), School of Civil and Environmental Engineering, Faculty of Engineering and IT, University of Technology Sydney, Australia

Abstract. In the realm of natural hazard assessments within spatial domains, the advent of Artificial Intelligence (AI) represents a paradigm shift, revolutionizing the way we conceptualize, model, and interpret environmental risks. This keynote address illuminates the profound impact of AI technologies, particularly machine learning algorithms and data-driven approaches, in reshaping our understanding and prediction capabilities concerning natural disasters.

By assimilating and scrutinizing vast spatial datasets, AI-driven models offer unparalleled accuracy and efficiency, facilitating timely and precise hazard assessments. Real-time processing of geospatial information not only enables rapid predictions but also forms the cornerstone of proactive disaster management strategies. Furthermore, AI's capacity lies in its adeptness at deciphering intricate spatial patterns inherent to natural hazards, unraveling subtle cues and previously unnoticed correlations within the data fabric.

This keynote delves into how AI's nuanced interpretation, coupled with advanced algorithms, elevates hazard modeling, providing deeper insights into the spatial dynamics of environmental risks. By augmenting traditional methodologies and revealing hidden patterns, AI fosters comprehensive risk assessments, fostering informed decision-making processes. The fusion of AI and natural hazard assessments in spatial domains heralds a more resilient approach to disaster preparedness and response.

Join us in embracing this transformative era, where AI's sophisticated modeling techniques and precise spatial interpretations converge, heralding proactive and effective mitigation strategies amidst the ever-evolving landscape of environmental challenges.

Short Bio. Distinguished Professor Dr. Biswajeet Pradhan is an internationally established scientist in the field of Geospatial Information Systems (GIS), remote sensing and image processing, complex modelling/geo-computing, machine learning and soft-computing applications, natural hazards and environmental modelling. He is the Director of the Centre for Advanced Modelling and Geospatial Information Systems (CAMGIS) at the Faculty of Engineering and IT at the University of Technology, Sydney (Australia). He was listed as the World's Most Highly Cited Researcher by the Clarivate Analytics Report for five consecutive years, 2016–2020, as one of the world's most influential minds.

He ranked number one (1) in the field of "Geological & Geomatics Engineering" during the calendar year 2021–2023, according to the list published by Stanford University Researchers, USA. This list ranks the world's top 2% most highly cited researchers based on Scopus data. In 2018–2020, he was awarded as World Class Professor by the Ministry of Research, Technology and Higher Education, Indonesia. He is a recipient of the Alexander von Humboldt Research Fellowship from Germany. Between 2015–2021, he served as "Ambassador Scientist" for the Alexander Humboldt Foundation, Germany.

Professor Pradhan has received 58 awards since 2006 in recognition of his excellence in teaching, service and research. Out of his more than 850 articles (Google Scholar citation: 70,000, H-index: 129), more than 750 have been published in science citation index (SCI/SCIE) technical journals. He has authored/co-authored ten books and thirteen book chapters.

Software Engineering Research in a New Situation

Prof. Carl K. Chang

Professor Emeritus, Iowa State University, USA

Abstract. With the rise of Generative Artificial Intelligence (GAI), epitomized by Large Language Models (LLMs), a profound shift has unfolded in software engineering research. In this presentation, I will traverse my four-decade journey in software engineering research, focusing on situational awareness in the era of the Internet of Things (IoT). I have witnessed the turbulence brought forth by the AI community that demands changes in our approaches. Meanwhile, owing to the pervasiveness of services computing, services became the first-class citizen in modern-day software engineering methodologies.

I argue that situational awareness must permeate the entire lifecycle to consistently deliver software services that align with the dynamic needs of users and the ever-evolving environments. I will elucidate this argument by reviewing the Situ framework, offering a comprehensive illustration of my perspective. Furthermore, I will outline my vision regarding the formidable research challenges considering the rapidly shifting landscape dominated by an irresistible and profoundly disruptive generative AI tsunami.

Short Bio. Carl K. Chang is a former department chair and Professor Emeritus of Computer Science at Iowa State University. His research interests include requirements engineering, net-centric computing, situational software engineering and digital health. Chang was the 2004 President of the IEEE Computer Society. Previously he served as the Editor-in-Chief for IEEE Software (1991–1994), and as the Editor-in-Chief of IEEE Computer (2007–2010). He was the 2012 recipient of the Richard E. Merwin Medal from the IEEE Computer Society. Chang is a Life Fellow of IEEE, a Fellow of AAAS, and a Life Member of the European Academy of Sciences (EurASc).

Interpretability and Privacy Preservation in Large Language Models (LLMs)

Prof. My Thai

University of Florida (UF) Research Foundation Professor
Associate Director of UF Nelms Institute for the Connected World

Abstract. Large Language Models (LLMs) have transformed the AI landscape, captivating researchers and practitioners with their remarkable ability to generate human-like text and perform complex tasks. However, this transformative power comes with a set of critical challenges, particularly in the realms of interpretability and privacy preservation. In this keynote, we embark on an exploration of these pressing issues, shedding light on how LLMs operate, their limitations, and the strategies we can employ to mitigate risks. We begin by examining the interpretability in LLMs, which often function as enigmatic "black boxes." Their complex neural architectures make it challenging to understand how they arrive at specific outputs. This lack of transparency raises questions of trust and accountability. When deploying LLMs in real-world applications—whether for chatbots, content generation, or decision-making—it becomes crucial to demystify their decision paths.

We will use explainable AI (XAI) to offer faithful explanations, from the black-box to white-box models, and from feature-based [1, 2] to neuron circuits-based [3, 4] explanations. By visualizing attention mechanisms, feature importance, and saliency maps, we empower users to comprehend LLM predictions. XAI not only fosters trust but also encourages responsible utilization of LLMs.

We next turn our attention to one of the utmost concerns and challenges: data privacy. LLMs process vast amounts of data, raising risks of data leakage, model inversion, the right to be forgotten, and inadvertent exposure of sensitive information. Furthermore, the integration of LLMs into diverse applications also significantly brings these challenges to the next level [5]. This talk explores strategies to protect privacy, including differential privacy, federated learning, and data encryption.

Short Bio. My T. Thai is a University of Florida (UF) Research Foundation Professor, Associate Director of UF Nelms Institute for the Connected World, and a Fellow of IEEE and AAIA. Dr. Thai is a leading authority who has done transformative research in Trustworthy AI and Optimization, especially for complex systems with applications to healthcare, social media, critical networking infrastructure, and cybersecurity. The results of her work have led to 7 books and 350+ publications in highly ranked international journals and conferences, including several best paper awards from the IEEE, ACM, and AAAI.

In responding to a world-wide call for responsible and safe AI, Dr. Thai is a pioneer in designing deep explanations for black-box ML models, while defending against explanation-guided attacks, evident by her Distinguished Papers Award at the Association for the Advancement of Artificial Intelligence (AAAI) conference in 2023. At the same year, she was also awarded an ACM Web Science Trust Test-of-Time award, for her landmark work on combating misinformation in social media. In 2022, she received an IEEE Big Data Security Women of Achievement Award. In 2009, she was awarded the Young Investigator (YIP) from the Defense Threat Reduction Agency (DTRA), and in 2010 she won the NSF CAREER Award. She is presently the Editor-in-Chief of the Springer Journal of Combinatorial Optimization and the IET Blockchain Journal, and editor of the Springer book series Optimization and Its Applications.

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Smart, Safe, and Health Cities (SSHC 2024)

A Literature Review of the Urban Heat Island (UHI) Phenomenon Connected with Smart Cities Paradigm

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Abstract. The article aims to analyse the approach used to evaluate Urban Heat Island (UHI) to determine the most suitable parameters based on the urban features of every city. The authors want to investigate the current state of knowledge on the role of Urban Heat Island (UHI) and its associated characteristics in the field of Urban Planning and Smart Cities. This exploration will begin by discussing the concepts of UHI, Smart City, and City Dashboard. They systematise the methodology, classifications, issues, and solutions found in recent scientific studies. This literature review proposes a systematic approach, analysing the best-known databases in the field of scientific research (Google Scholar, Scopus and Science Direct) in order to catalogue and systematise the most consonant approach according to certain characteristics in the study of UHIs. This paper represents a first phase of a broader research and provides a literature base to better understand how to deal with urban heat islands, following an urban planning vision dependent on the concept of Smart Cities. This analysis led to the definition of a set of indicators useful for studying this issue from an urban planning perspective and possible new studies on the interconnection between City Dashboard, Smart Cities and UHI.

Keywords: Urban Heat Island · Smart Cities · Urban Planning · Systematic Literature Review · Sustainability · City Dashboard · Indicators

1 Introduction

Global warming is one of the most important challenges of our time, affecting the daily lives of individuals and populations around the world. The rapid increase in the planet's average temperatures, resulting from human activities, has led to a series of environmental, social, and economic consequences that manifest themselves in various ways in everyday life.

The study of global warming and its impacts therefore becomes particularly important. Understanding the reasons for climate change, monitoring its consequences, and finding ways to mitigate and adapt have become mandatory goals for a good quality of life and to ensure a sustainable future for the next generations. Through data analysis,

© The Author(s), under exclusive license to Springer Nature Switzerland AG 2024
O. Gervasi et al. (Eds.): ICCSA 2024 Workshops, LNCS 14823, pp. 3–17, 2024.
https://doi.org/10.1007/978-3-031-65329-2_1

climate modelling, impact assessment and the development of innovative solutions [1, 2], an understanding of global warming can be provided, and action can be directed towards policies and practices to address it.

One of the key elements of global warming that can be addressed through the concepts of Smart Cities is the analysis of Urban Heat Islands (UHI) effects.

UHIs are a distinctive feature of urban areas, manifesting themselves with significantly higher local temperatures than surrounding areas [3]. As a result, cities are often revealed as heat oases, where temperatures can reach significantly higher values than in the surrounding rural areas.

Increasing urbanisation and the rapid expansion of metropolitan areas are redefining the structure of our planet. The transformation of rural areas into urban settings has led to UHI being seen as one of the most relevant and debated phenomena in climate and environment.

Human activities play a significant role in accentuating the phenomenon of urban heat islands [4]. Heat emissions from vehicles, heating systems, air conditioning and industries further amplify local warming [5]. Removal of vegetation and replacement of permeable soils with impermeable surfaces contribute to exacerbating this effect [6].

Urban heat islands have significant impacts on urban life and the sustainability of cities. Rising local temperatures can lead to increased energy demand for cooling buildings, leading to rising energy costs and increased greenhouse gas emissions [7]. In addition, high temperatures put human health at risk, causing heat stress and increasing susceptibility to heat-related diseases [8].

In the context of an increasingly urbanised world, cities represent not only epicentres of economic and social activity, but also sites of complex environmental challenges. The evolving concept Smart Cities offers unprecedented opportunities to address the challenges of urbanisation in innovative and efficient ways.

To address this issue, the tools under the Smart City paradigm [9] can provide an innovative approach to urban design and management. Smart Cities combine advanced technologies with urban data and smart governance models to improve efficiency, sustainability, and quality of life for citizens. For example, to tackle this problem effectively, more and more cities can adopt innovative tools such as City Dashboards like London [10] and Florence [11].

City Dashboards [12–15] are digital platforms that collect, analyse and display data from a variety of sources, including environmental sensors, weather stations, satellite imagery, and socioeconomic data. City Dashboards are very articulate systems that provide comprehensive and up-to-date data/information on weather conditions, pollution, metro lines, the latest news. City dashboards are specifically developed to generate responsibility of public institutions towards the population [16, 17]. In addition, these tools offer an integrated, data-driven approach to monitoring and managing UHI. These platforms provide municipal administrators and stakeholders a real-time overview of environmental conditions and climate trends. This allows them to make well-informed choices and implement targeted actions to mitigate UHI.

City Dashboards are powerful tools for gathering, analysing and visualising a wide range of urban indicators [18], including those related to Urban Heat Islands (UHI). Indicators are quantitative or qualitative measures that are used to assess the condition

and progress of a city in several domains, including but not limited to the environment, economy, mobility, and health. When addressing UHIs, several indicators may be used, such as surface temperatures, relative humidity, vegetation cover, energy consumption, air quality and other factors.

The connection between indicators and City Dashboards is important for effectively understanding and managing UHIs. City Dashboards serve as centralised platforms that gather, merge, and present relevant indicators in a concise and simple-to-read way. These platforms enable citizens, urban administrators, planners, researchers, and stakeholders to monitor in real time every change related to a city and understand the level of dangerous for specific domains.

Starting from these assumptions, the main goal of this paper is to examine the scientific literature to identify approaches and methodologies for studying urban heat islands. The authors recognise the existence of previous research studies on the UHI subject [19–22]. However, this study distinguishes itself from the others by integrating previously unexplored concepts such as urban heat islands, smart cities, and city dashboards. The authors also aim to exploit concepts and indicators available in the context of Smart Cities and develop analytical strategies to address current urban planning challenges. For obtain these main goals, the paper is organised as follows: after the introduction, the second paragraph analyse concepts and methods under the main fields of smart city, UHI, and city dashboards. The third paragraph introduces the used methodology for the scientific review. Finally, the results are presented before underlining final considerations and conclusions.

2 Concepts and Methods

In today's world, cities have significant issues that are also a result of fast and unregulated urbanisation. Among these factors, UHI emerges as particularly significant, because it has direct impacts on the well-being of inhabitants and the effectiveness of urban infrastructure. However, the Smart City paradigm with its tools and its potentiality on analysing data provide opportunities to address these challenges. This paragraph analyses the concepts associated with Urban Heat Island (UHI) and Smart City, emphasising the key elements of intersections and synergies between them.

2.1 Urban Heat Island: Definitions and Impact

Urban Heat Island (UHI) is a thermal phenomenon characterised by elevated temperatures seen in cities compared to the surrounding rural or suburban regions. This phenomenon is the result of a complex interaction between various factors, such as heat absorption by urban materials, heat emission from anthropogenic activities, and significant alteration of soil characteristics [8] which leads to extra heating. UHI has many adverse consequences, such as increased energy demand for cooling buildings, degradation of air quality, and thermal stress.

The origins of urban heat islands can be traced to the configuration and land use of urban areas. Urban surfaces, such as buildings and roads, have a higher capacity to absorb and retain heat compared to rural areas [23]. This heat storage effect is particularly

pronounced during clear nights, when urban surfaces gradually release heat accumulated during the day.

2.2 Smart City and City Dashboard: Concept and Applications.

Defining a smart city can be hard due to its multifaceted nature. However, its association with a city dashboard, which will be explained later, has prompted the authors to define a smart city as a place that takes advantage of technology to improve the quality of life, the liveability, and environmental sustainability of the city [9, 24–27]. Smart cities use data from a variety of sources, such as IoT (Internet of Things) sensors, mobile devices, and monitoring systems, to optimize urban services, mobility, energy and more. Within the framework of Urban Heat Island (UHI), the principles of Smart City may be applied to identify and develop new environmentally friendly spaces, including green and white roofs, investigate the utilisation of innovative urban materials, and provide efficient and low-pollution public transportation options. These initiatives not only reduce the heat island impact but also enhance urban resilience and quality of life.

The intersection of Urban Heat Island and Smart City offers fertile ground for interdisciplinary innovation and research. The challenges related to UHI require an integrated approach that combines smart technology with sustainable urban design and whole-population engagement. Exploring these connections between the various concepts is critical to the development of resilient, sustainable, and inclusive cities. A tool that can be used to address UHI according to Smart City paradigm is the City Dashboard.

The City Dashboard is a comprehensive system that monitors and visualises data, offering a real-time summary of several metrics and indicators that impact a city. The indicators may include demographics, traffic, air quality, energy consumption, traffic accidents, crime rates, waste collection, noise levels and other metrics that reflect the functioning and quality of life in an urban community.

The main objective of a city dashboard is to provide policy makers, urban planners, local administrators, and citizens with a tool to better understand the dynamics and challenges of urban life. These systems enable them to make more informed decisions, to identify critical areas requiring action and to evaluate the effectiveness of public policies implemented.

City dashboards may have a substantial effect on urban living. Below are listed some of the most significant impacts:

1) Optimised urban planning: Improved availability of urban data empowers urban planners to make well-informed choices on urban development, transport management, green space distribution and other related aspects. For example, politicians may use this approach to determine the sites of new green zones.
2) Greater transparency and citizen involvement: City dashboards provide more openness and public engagement by providing people with access to data about their city, fostering transparency and encouraging active participation in urban life. This may result in an enhanced feeling of civic responsibility and increased engagement in the development of local policy. For instance, it might be used to apprise senior citizens of the hottest parts of the city at a certain time of the day.

3) Reducing emergency response times: City dashboards facilitate expedited and efficient emergency response by continuously monitoring data related to public safety, the environment, and urban services. This enables prompt action in circumstances such as traffic accidents, floods, or other natural disasters. For example, it might be advantageous in determining the most efficient routes inside a city by using data on accidents, temporary road closures, and several other pieces of information.
4) Optimisation of resources: Through the analysis of data gathered by city dashboards, local authorities may discover inefficiencies and bottlenecks in public services, allowing for improved allocation of resources and more effective city administration.
5) Improved quality of life: City dashboards can enhance the quality of life for urban people by using data to tackle issues like pollution, traffic congestion, and crime. This contributes to creating more liveable and sustainable cities. Politicians may use it as a tool to determine whether or not to implement traffic restrictions in certain regions based on air pollution levels.

The indicators used in the development of City Dashboard are very significant in tackling the issue of Urban Heat Island (UHI), particularly with regards to the first and final points on the list. City dashboards are a helpful tool for contemporary urban administration, offering a concise and comprehensive summary of urban life and facilitating improved planning, resource allocation, and citizen engagement.

3 Methodology

This paper examines the latest studies on urban heat islands (UHI) over the last few years, to identify the key components that are considered relevant for the functional analysis of UHI for urban planning. The research is structured into five distinct steps:

1) Investigating scientific articles that are relevant to the analysis;
2) Skimming the scientific and relevant papers by considering their abstracts;
3) Developing a clear table summarising the collected results;
4) Conducting a comparative analysis of the articles selected in step 2;
5) Identifying the most significant indicators related to urban morphology that are important for evaluating the urban heat island effect.

The selection of relevant publications was based on three criteria: the degree to which the issue aligns with an urban planning goal, publishing in open access journals, publication period. The 'Google Scholar,' 'Scopus,' and 'Science Direct' platforms were chosen due to their open access nature and their effectiveness in research findings.

Articles were retrieved from Google Scholar, Scopus, and Science Direct databases through a query containing the terms 'urban heat island,' 'urban planning' from 2020 to 2023. Due to the vast number of papers, over 56,000, it is unfeasible to examine such a substantial quantity of publications. Therefore, it was determined to further simplify the search by merely concentrating on the titles of the different publications. As a result, a total of 201 scientific publications were identified across all three search engines, and none of the duplicate papers have been eliminated from any of the search engines. The authors attempted to enhance the relevance of the text by using the phrases "Smart City" and "City Dashboard". However, their study had no results.

Therefore, the authors decided to modify the search criteria to make it more recent and targeted towards identifying interesting indicators used in city dashboards. The aim is to obtain a larger number of search results by using fewer keywords in search engines. Additionally, considering the abundance of scientific articles that discuss the use of indicators in city dashboards [13, 18, 28] it would be more effective to replace the newly added words with the single term "Indicator".

Furthermore, to align with the original objective and ensure relevance, the time frame for the search will be limited to the period from 2022 to 2023. As a result, a total of 73 articles will be included in the search.

Afterwards, by analysing the abstracts of the downloading papers, a comprehensive assessment of the articles is conducted, revealing the key components of the study.

4 Results

The results of the first step concerning the search and the various modifications in the search to arrive at a reasonable number of articles that could be analysed manually are shown in Table 1.

Table 1. Summary table of the results obtained by searching the various search engines.

	First Attempt	Second Attempt	Third Attempt	Fourth Attempt
Terms in the content	Urban Heat Island, Urban Planning		Smart City, City Dashboard	Indicator
Terms in the title		Urban Heat Island, Urban Planning	Urban Heat Island, Urban Planning	Urban Heat Island, Urban Planning
Years	2020–23	2020–23	2020–23	2022–23
Google Scholar	17,600	139	0	47
Scopus	30,439	44	0	17
Science Direct	8,273	18	0	9
Total	56,312	201	0	73
Motivation for the change of research	Research more precise	More focalised on city dashboard	Need more results and more current, looking for indicators useful for a City Dashboard	

The result of this supplementary investigation is a cumulative total of 73 publications. However, not all papers can be evaluated due to different reasons. Upon doing an initial study of the findings, the authors had to exclude any publications that were difficult

to scan or inaccessible for download. Additionally, they remove duplicates detected inside each individual search engine and duplicates of the same article across all three search engines. Furthermore, items published in languages other than English were also removed. Table 2 shows the schematisation of articles that cannot be used for search purposes. A total of 47 scientific publications were accessible for empirical analysis as a consequence of this approach.

Table 2. Table with analysis and elimination of non-downloadable, duplicate or non-English items.

		Google Scholar	Scopus	Science Direct	
Non-Downloadable		6	1	0	7
Repeated in single search engine		3	0	0	3
Repeated among all search engines	15				15
Not in English	1				1
Total to skim					26

A decision was reached to conduct a more comprehensive examination based on the abstracts of the remaining 47 publications. A total of 14 publications were selected for further investigation based on this evaluation. Table 3 provides a concise overview of the whole process used to reach the final paper skimming. Figure 1 shows the results of the skimming in more detail from the totality of the search results.

Table 3. Table summarising step-by-step cleaning of the results obtained.

Total before cleaning	Total after cleaning	Total after reading abstract
73	47	14

In order to have a thorough understanding of the most recent developments in the field of urban heat islands, the authors have opted to construct Table 4. This table includes a title, a case study, and the indicators used in the research. It helps in the identification of relevant information to do this literature review.

Land Surface Temperature (LST) is often used as the primary indicator in most papers. This is because urban temperature data has to be compared with rural data, making LST an essential factor. The most frequently used indicators, categorised accordingly, include measurements of building height [29, 41, 42], indices referring to the percentage of built-up land [29, 30, 33, 34, 38], measurements of the percentage of green and blue spaces in specific areas [30, 33–36, 38–40, 42] and wind speed [29, 32, 41].

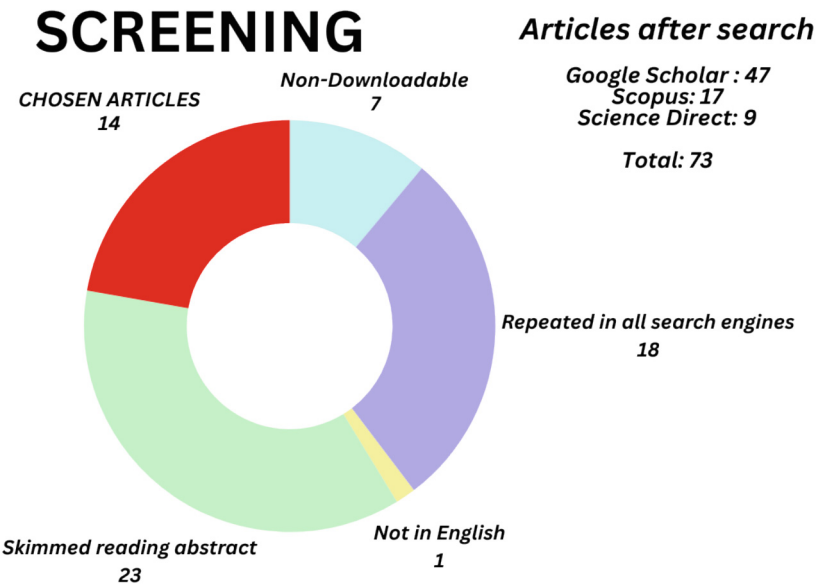

Fig. 1. Summary of the screening of articles found through searches.

Table 4. Table summarising most important information of chosen articles.

Title	Case study	Indicators
Analysing the Impact of Urban Planning and Building Typologies in Urban Heat Island Mitigation [29]	Sidney Metropolitan Area, Australia	Building Height (BH); Street Width (SW); Aspect Ratio (AR); Built Surface Ratio (BSR); Built Area Ratio (BAR); Land Surface Temperature (LST); Ambient Temperature (AT); Wind Speed (WS); Gradient of Temperature Decrease along the district axis (GTD)
Analysing the Urban Heat Island In Ho Chi Minh City In Relation To Urban Planning Processes from 2010 To 2020 [30]	Ho Chi Minh City, Vietnam	Land Surface Temperature (LST); Normalised Vegetation Index (NDVI); Normalised Difference Built-Up Index (NDBI)
Assessment of Urban Heat Islands For Land Use Based on Urban Planning: A Case Study in the Main Urban Area of Xuzhou City, China [31]	Xuzhou City, China	Land Surface Temperature (LST); Urban Development Land (UDL)

(*continued*)

Table 4. (*continued*)

Title	Case study	Indicators
Assessment of Wind Characteristics And Urban Heat Island Dynamics For Urban Planning: A Case Study Of Toulouse, France [32]	Toulose, France	Local Weather Type (LWT); Wind Intensity (WI); Local Climate Zone (LCZ)
Discerning The Success of Sustainable Planning: A Comparative Analysis of Urban Heat Island Dynamics in Korean New Towns [33]	Bundag, Ilsan, Guangyao and Songdo, South Korea	Land Surface Temperature (LST); Green Normalized Difference Vegetation Index (GNDVI); Modified Normalized Difference Water Index (MNDWI); Digital Elevation Model (DEM); Normalize Difference Built Index (NDBI); Euclidean Distance to Roads (EDR); Population Density (PD)
Effects of Urban Planning Indicators On Urban Heat Island: A Case Study of Pocket Parks In High-Rise High-Density Environment [34]	Hong Kong, China	Ratio Of A Building's Total Area To The Land Area On Which It Is Built (FAR); Building Density (BD); Park Area (PA); Tree Cover Ratio (TCR); Shrub Cover Ratio (SCR)
How Can Urban Green Spaces Be Planned To Mitigate Urban Heat Island Effect Under Different Climatic Backgrounds? A Threshold-Based Perspective [35]	Hohhot, Beijing, Shanghai and Haikou, China	Urban Green Space (UGS); Cooling Intensity (CI); Absolute Cooling Threshold (ToCabs)
How Can Urban Parks Be Planned To Mitigate Urban Heat Island Effect In "Furnace Cities"? An Accumulation Perspective [36]	Fuzhou, China	Radiative Transfer Equation (RTE); Park Cooling Intensity (PCI); Park Cooling Gradient (PCG); Park Cooling Area (PCA); Park Cooling Efficiency (PCE); Efficiency Threshold Value (TVoE)
Planning Strategies For Urban Heat Island Mitigation: An Application Of Local Climate Zone Into The High density City Of Hong Kong [37]	Hong Kong, China	Land Surface Temperature (LST); Sky View Factor (SVF)
Spatial Changes of Urban Heat Island Formation In The Colombo District, Sri Lanka: Implications For Sustainability Planning [38]	Colombo District, Sri Lanka	Land Surface Temperature (LST); Normalised Differential Vegetation Index (NDVI); Normalised Differential Accumulation Index (NDBI); Population Density (PD)

(*continued*)

Table 4. (*continued*)

Title	Case study	Indicators
Spatial Process Of Surface Urban Heat Island In Rapidly Growing Seoul Metropolitan Area For Sustainable Urban Planning Using Landsat Data (1996–2017) [39]	Seoul Metropolitan Area, South Korea	Land Surface Temperature (LST); Changes in Land Use and Land Cover (LULC); Impervious Surface (IS); Persistent IS (PIS); Newly Added IS (NAIS); Forest Area (FS)
The Urban Heat Island Of The Metropolitan City Of Turin. Strategies For A Sustainable Urban Planning [40]	Turin, Italy	Air Temperature (AT); Urban Morphology (UM); Exposure of Urban Spaces to Sunlight (EUSS); Albedo Coefficients of Outdoor Areas (ACOA); Percentage of Greenery and Water (PGW); Distance from the Built-Up Area (DBUA); Land Surface Temperature (LST)
Urban Heat Island And Thermal Comfort Conditions At Micro-Climate scale In A Tropical Planned City [41]	Putrajaya, Malaysia	Diffuse Solar Radiation (DSR); Reflected Solar Radiation (RSR); Land Surface Temperature (LST); Physiologically Equivalent Temperature (PET); Wind Speed (WS); Building Height (BH);
Urban Heat Island's Vulnerability Assessment by Integrating Urban Planning Policies: A Case Study of Montpellier Méditerranée Metropolitan Area, France [42]	Montpellier Metropolitan Area, France	Green Space (GS); Building Footprint (BF); Building Height (BH); Constraction's Location (CL); Air Conditioning (AC); Topography (T); Proximity to Natural Areas (PNA); Surface Urban Heat Island Intensity (Day and Night) (SUHII); Population Density (PD); Land Uses (Daytime) (LUD); Land Uses (Nighttime) (LUN); Sensitive Population (SP); Health and Care Facilities (HCF); Low-Income Households (LIH); Building Age (BA)

5 Discussions and Conclusions

After conducting an extensive analysis of recent scientific literature and examining the present understanding and connections between Urban Heat Islands (UHI) and Smart Cities, it is evident that there has not yet been a comprehensive method for evaluating UHI.

During extensive searches across many search engines, it became evident that there is a lack of literature that primarily focuses on urban planning and urban heat islands using

city dashboards. This field has the capacity to be a fascinating domain of investigation and development.

Some researchers attempt to categorise and provide significant details on the indicators of various Local Climate Zones (LCZ). However, their analysis is limited to just a few indicators, that always consider meteorological and urban geometry parameters. The objective of future research papers might be to identify universal indicators that can be used to categorise urban heat islands. This would include examining noteworthy aspects of the examined publications.

The key indicators analysed in the articles are Land Surface Temperature, Building Heights, Wind Speed, Vegetation and Built-up Index. An important element emphasised in this research is that in cities situated in close proximity to the sea or lakes, the distance from these bodies of water is commonly ignored.

Essentially, a comprehensive analysis of the urban heat island phenomenon reveals a complex and continuously changing scenario that mirrors the increasing understanding of the many factors that contribute to elevated temperatures in metropolitan areas. Existing literature indicates that the socialisation process of people in urban areas has a significant impact on the environment. Administrators may find it important to establish public places suitable not only for socialisation but also for those dynamics that can mitigate the negative effects of Urban Heat Island (UHI). Furthermore, the local urban warming may have a substantial impact on public health, energy efficiency, and the general quality of the urban environment.

After examining several solutions and relevant research, it is important to underline the following actions (but they are not exhaustive) to mitigate the adverse impacts of Urban Heat Island (UHI):

1) Vegetation in urban areas. Participating in tree planting and creating parks or gardens may effectively lower surface and air temperatures due to the cooling effect and humidity provided by trees.
2) Vertical gardens and green roofs. Vertical gardens and green roofs reduce heat absorption naturally. Indeed, plants absorb heat and evaporate water through the process of transpiration, cooling the surrounding air and reducing the temperature of buildings.
3) Paving with reflective materials. Using reflective materials on roads, sidewalks and roofs may decrease the heat absorbed. Light-coloured materials or specialist reflective coatings possess a greater ability to reflect solar energy in comparison to normal dark materials.
4) Urban planning initiatives and specialised Urban Master Plans that are interconnected with land use, water usage, and climate changes, in general. Urban temperatures may be controlled and reduced by designing cities to optimise natural spaces and decrease the use of asphalt surfaces. Effective planning strategies may include the establishment of green corridors that connect various parks and green spaces, as well as initiatives related to the efficient use of land and water resources. Furthermore, the promotion of sustainable mobility via the encouragement of bicycling and public transit may also result in measures that alleviate the adverse impacts of Urban Heat Island (UHI). By decreasing the number of vehicles on the road, it is possible to contribute to mitigating the impact of urban heat islands.

5) Aquatic environments. Water has a notable capacity for heat absorption due to its high specific heat, allowing it to absorb a substantial amount of heat without suffering a significant rise in temperature. Integrating fountains, ponds, or other water elements may effectively lower the temperature of the surrounding environment.
6) Monitoring and adaption measures using tools such as city dashboards. The capacity to continuously monitor all the data and indicators about urban heat island (UHI) and climate change allows for the subsequent adjustment of municipal and local policy.

It is crucial to foster collaboration among scholars, urban planners, policymakers, and local communities in the future to implement methods that mitigate and adapt to challenges. Currently, the only means of studying urban heat islands is through a multidisciplinary approach. This approach must be adopted to consider the Urban Heat Island (UHI) under the interdependence between climate change, urban planning, public health, and environmental sustainability.

City dashboards are used in the development of today's smart cities, basically to assist decision-makers in making well-informed decisions, not only in relation to the mitigation of the urban heat island phenomena [43]. These tools are valuable for collecting, assessing, and visually presenting customised indications and data.

The city dashboard provides a real-time and comprehensive overview of current conditions and trends in urban environments, whether at a local or regional level. It enables prompt reactions to urban issues and assists in determining the priorities and the key areas for action by public administrations.

Developing heat-resistant cities requires a proactive attitude and specific actions to reduce the ecological effects caused by human behaviours and activities. Similarly, effectively addressing the adverse effects of urban heat islands requires a high level of awareness and sensitivity from the entire community, aiming to establish healthy, sustainable urban environments that can withstand future climate challenges.

Acknowledgments. This study was supported by the technical-scientific collaboration agreement "PON METRO 2014–2020 AXIS 6 - Action CA6.1.1.b - Cagliari smart city: Integration of urban governance with the mitigation of urban heat islands (CA_UHI)" signed between the Municipality of Cagliari and the University of Cagliari (DICAAR - Department of Civil and Environmental Engineering and Architecture). This study was accomplished within the RETURN Extended Partnership and received funding from the European Union Next-GenerationEU (National Recovery and Resilience Plan – NRRP, Mission 4, Component 2, Investment 1.3 – D.D. 1243 2/8/2022, PE0000005).

This study was supported by the MUR through the project "SMART3R-FLITS: SMART Transport for Travellers and Freight Logistics Integration Towards Sustainability" (Project protocol: 2022J38SR9; CUP Code: F53D23005630006), financed with the PRIN 2022 (Research Projects of National Relevance) program. We authorise the MIUR to reproduce and distribute reprints for Governmental purposes, notwithstanding any copyright notations thereon. Any opinions, findings, and conclusions or recommendations expressed in this material are those of the authors and do not necessarily reflect the views of the MIUR.

Author Contributions. This paper is the result of the joint work of the authors. In particular, "Abstract" and "Results" were written by all authors. C.G. wrote "Introduction" and "Discussions

and Conclusions", M.M.M. wrote "Concepts and Methods", and "Methodology". C.G. supervised and edited the text of the manuscript.

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Exploring Urban Greenery Through Standard and Novel Monitoring Optical Tools: Preliminary Findings in the Metropolitan City of Cagliari

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Abstract. Green spaces in urban areas play a fundamental role in shaping the cityscape, gaining increasing importance in a context of growing impact of extreme weather events, global warming, and urban pollution. Innovative strategies for urban green infrastructure planning and management are essential to foster a healthier urban ecosystem. This research focuses on employing a multifaceted strategy involving novel optical technologies and the acquisition of standard vegetation parameters to examine the physiological status of specific Mediterranean plant species (*Quercus Ilex* L., *Nerium Oleander* L., and *Prunus Cerasifera* Ehrh.) from different urban habitats (central and peripheral) of Cagliari as compared to a control site in the inner part of Sardinia. Preliminarily, historical data from air quality monitoring stations for the period 2019–2022 allowed to identify two timeframes to assess the relationship between plant physiological responses and environmental parameters as well as the effects determined by pollutants: one in the post-summer period and the other one in the post-winter period. Leaf area, fresh and dry leaf weight, and trunk size, were collected. At the same time portable Normalized Difference Vegetation Index (NDVI)-, fluorescence/transmission-, and Raman-based portable sensors were used to non-invasively monitor leaf pigment-related indices, showing variations based on species and urban zones. The responses observed were characterized by imbalances in chlorophyll levels and distinct variations in polyphenols and carotenoids as well as different biometric trends. In the next measurement campaigns, an analysis of the soil will be added to assess its potential influence on plant response as well as satellite data to obtain additional information on a local base such as traffic, land temperature variations and spread of pollutants. This preliminary study lays the groundwork for developing a strategy to conscientiously monitor and manage urban greenery, contributing to the establishment of a greener and more sustainable city.

Keywords: sustainable urban development · urban green space · optical techniques

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O. Gervasi et al. (Eds.): ICCSA 2024 Workshops, LNCS 14823, pp. 18–34, 2024.
https://doi.org/10.1007/978-3-031-65329-2_2

1 Introduction

The rapid increase in urban population represents one of the major challenges of our time, with more than half of the world's population currently residing in urban areas and a projected growth of up to 70% by 2050 [1]. This phenomenon is closely related to a series of significant environmental problems, which have a direct impact on human well-being, undermining the quality of life and endangering not only the environment subject to these issues but also people's health.

Indeed, urbanization is associated with a range of processes that exacerbate existing environmental problems in the area and intensify extreme climatic events due to ongoing climate change. Urbanization involves the extensive use of impermeable materials, altering the water cycle and increasing the risk of floods [2]. This impact on soil hydrology reduces water infiltration, altering flood dynamics, and influencing water resource availability [3, 4]. Moreover, urbanization intensifies energy demand, promoting the use of fossil fuels and contributing to increased greenhouse gas emissions [5], resulting in worsened air, water, and soil pollution [6, 7]. These emissions lead to increased greenhouse effect, causing longer periods of extreme heat, reduced precipitation, and intensified storms.

Global climate change is further fueled by urbanization, including significant alteration of climatic regulation within urban areas, creating urban heat islands characterized by increased land surface and air temperatures [8]. Record temperatures, floods, destructive hailstorms, droughts, and sudden fires are some of the most devastating effects of climate change impacting Italy and the rest of the world.

This complex scenario underscores the importance of adopting holistic approaches to address the challenges associated with urbanization and mitigate its negative impacts on human health and well-being. Until now, planning has mostly focused on managing human-induced transformations on the environment and territory, within a perspective where they were essentially available to humanity. Climate planning reverses this perspective, working to reduce human impacts on the ecosystem and adapt settlements to the transformations occurring in the natural environment of which we are part.

The need for urgent, strong, and cooperative action based on trust and mutual understanding has never been higher. Similarly, it is essential for countries to strengthen their capacity to understand, plan, and manage climate risks in an ongoing process, no longer treating them as unpredictable phenomena to be managed according to the logic of urgency and emergency, but integrating them into the ordinary dimension of policies, programming, planning, and design.

Local governments are often identified as key actors in the transition towards a more sustainable society as many local decisions can directly influence environmental quality, such as regulating local transportation, constructing buildings, spatial planning, and various economic aspects.

In such a complex and articulated framework, the importance of cities is also affirmed by Goal 11 of the UN 2030 Agenda [9], aiming to make "cities and human settlements inclusive, safe, resilient, and sustainable", as well as by the New Urban Agenda and the European Urban Agenda [10], sharing the objective of improving the social, cultural, and environmental well-being of all citizens with a focus on inclusion and cohesion. This commitment is also in agreement with Goal 13 of the 2030 Agenda on climate action and

entails integrating measures for adapting to and mitigating climate change into urban and territorial planning and development processes. The latter are internationally recognized for their capacity to strengthen environmental and socioeconomic resilience, improve both mitigation and adaptation to climate change, and manage natural and environmental risks [11–13]. At the EU level, the long-term strategy for 2050 [14] acknowledges that climate change is a concerning issue among European citizens, as it is reshaping the world by amplifying instability risks in all its forms.

Addressing climate change and its effects presents a multiple challenge where two priorities can be identified for an integrated and effective approach: 'mitigation', meaning limiting future climate changes by reducing greenhouse gas emissions; 'adaptation', meaning being prepared to face the impact of inevitable climate changes in the best possible way.

Territorial and urban planning is widely recognized internationally as a powerful tool in shaping urbanization to make cities truly resilient to various risks that make them fragile, especially through nature-based solutions. Plants, as integral bioindicators, respond to pollutants and play a fundamental role in improving air quality and mitigating the effects of urban heat islands [15].

In recent years, numerous physiological studies on plants have been conducted to better understand their adaptation and response to environmental conditions [16–26]. These studies have explored a wide range of physiological aspects of plants, providing valuable information on their well-being and adaptation strategies to the environment. Aspects such as variations in levels of photosynthetic pigments (chlorophyll, carotenoids), as well as levels of secondary metabolites, are linked to adaptation and defense mechanisms, adverse environmental conditions (cold, heat, excessive light radiation, drought, etc.), biotic attacks (pathogens, molds), as well as a plant's response to interactions with pollutants. Studies on the physiological responses of primary and secondary plant metabolites have employed a wide range of tools, techniques, and types of analysis to understand their adaptation mechanisms to the urban environment. Regarding specifically non-destructive optical techniques, studies have been conducted using chlorophyll level analyzers including the most commonly used ones such as the SPAD 502PLUS (Konica Minolta) [27], the Dualex (Force A), and the CCM-200 (Opti-Sciences Inc.) that provide an estimate of leaf chlorophyll through transmittance measurements on a single leaf [28]. Other instrumentation is based on fluorescence such as the Multiplex (Force A) [29] for measuring chlorophyll content on larger areas such as a cluster of leaves. Dualex and Multiplex also allow investigating the content of epidermal flavonoids and anthocyanins [30]. The PAM [31] is also based on fluorescence techniques but is used to analyze photosynthetic efficiency. All of the aforementioned techniques are widely used in agronomy, but few studies have been carried out in urban contexts, and the literature regarding non-destructive optical analysis techniques on urban greenery is rather lacking. Furthermore, techniques such as reflectance spectroscopy use hyperspectral data for the simultaneous evaluation of pigments such as chlorophyll, carotenoids, anthocyanins, and flavonoids. In the field of vibrational spectroscopy, portable systems based on Raman spectroscopy have recently been introduced, which potentially allow deriving information on the content of the main plant components [32]. Another type of technique used is Fourier-transform infrared spectroscopy (FTIR), which has been proposed

for the classification and prediction of the contents of secondary metabolites, including flavonoids, alkaloids, phenylpropanoids, terpenes, carotenoids, amino acids, and other phenolic compounds [33]. This research project, which involves the use of portable optical detection devices for the analysis of plant physiological responses, aims to test the efficiency of such devices in urban settings. Their use in this context is accompanied by that of traditional techniques such as destructive analyses for quantifying the levels of the main leaf compounds in order to validate the outcome of the results obtained with optical instrumentation. In addition to optical analyses, the measurement strategy includes the collection of fundamental parameters related to plant vitality and age, such as leaf area, fresh and dry leaf weight, height, and trunk dimensions. Specifically, we are evaluating the use of Dualex (as mentioned above) as well as a portable Raman spectrometer for non-invasive monitoring in situ or "close to the field" of the main leaf pigments and components, whose levels can reveal the characteristic responses of plants to variations in environmental conditions and pollution.

Adopting a multidisciplinary approach that includes also a detailed assessments of urban vegetation, along with analysis of soil characteristics and atmospheric conditions, can provide a more comprehensive understanding of the complex interactions between the urban environment and vegetation. The preliminary phases of this approach are here discussed and have included the adoption of more traditional as well as of innovative analytical tools that spam from the collection of biometric plant parameters to the use of portable optical devices aimed at scrutinizing the plant physiological status as a function of its localization in the urban environment and of external factors. This innovative methodology, downstream of a correlation with relevant data on pollution and atmospheric parameters, is aimed at providing an in-depth description of the state of health of particular areas of the city and help in undertaking targeted mitigation policies.

2 Methodology

In the initial phase of our research, we selected two different areas within the urban context of the metropolitan city of Cagliari: a central neighborhood and a neighborhood situated in a more peripheral location. This selection was aimed at capturing the variety of urban landscapes and enabling an in-depth investigation of the diverse ecological facets of the Mediterranean environment of Cagliari (see Fig. 1).

The selection was also dictated by the positioning of monitoring stations under the control of the regional environmental protection agency, referred to as ARPAS, which in turn were strategically placed in various locations within the metropolitan city of Cagliari to capture the diverse urban fabric of the metropolis in question.

The station located at Via Cadello, indeed, termed as an urban traffic station in the municipality of Cagliari, offers several advantages over the others: it is centrally located relative to the urban core; it is a four-lane road (2 lanes per direction) experiencing medium to high traffic volumes; it is situated near a heavily urbanized area and is representative of pollution generated by high traffic volumes, akin to other significant thoroughfares (such as Via Dante, Via Sonnino, Viale Trieste, etc.); to the east and west, it intersects with other heavily trafficked arteries: 300 m to the east with the New Median Axis Road and 500 m to the west with Via Campania and Via Is Mirrionis; on

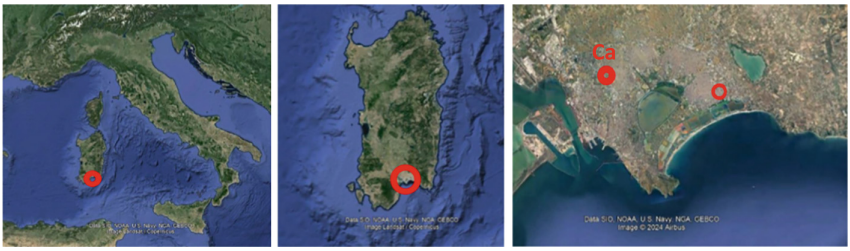

Fig. 1. Study area in southern Sardinia (left and central images) and identification of two selected sub-areas (right image) from Google Earth: a Cagliari central area (Ca) and a peripheral zone of the city situated in Quartu Sant'Elena (Qu).

the southern side, it borders a recreational green area (Monte Claro Park) that allows for the dispersion of pollutant sources (port area) and thus is not directly interfered with by sources other than traffic.

The urban background monitoring station located on Via Perdalonga in the municipality of Quartu Sant'Elena, represents a more peripheral situation. The chosen site is indeed a municipal area free from specific pollution sources such as vehicular traffic (Viale Cristoforo Colombo and Via Fiume, two roads characterized by significant traffic flows, are located at distances of 300 and 600 m from the site, respectively) or nearby industrial or artisanal emissions. Furthermore, the urban fabric of the surrounding area is very homogeneous (as required by specific APAT criteria; APAT is a national government agency for environmental protection and technical services) and densely populated. The location appears optimal for determining the levels of urban background pollution experienced by the residents of Quartu. Although this location was later replaced by another peripheral one (see below) responding better to the requirements of our research, this area has proven an exceedingly valid test field to setting up our measurement protocol.

Starting from the air quality monitoring stations, we have defined a field of action that extends up to a maximum distance of 1 km from the monitoring station. Beyond this distance, the data recorded by the station are less representative of the area (see Fig. 2).

Fig. 2. On the left is the central area of the city of Cagliari where the urban traffic monitoring station is located; on the right is the peripheral area of the city where the urban background monitoring station is located.

Firstly, we analyzed the historical data recorded by the monitoring stations from 2019 to 2022. Through the analysis of the trends of environmental parameters and pollution levels over the past four years, we were able to identify suitable time windows in which it was most feasible to observe a physiological response of the species under examination in relation to pollution and environmental stressors (see Fig. 3).

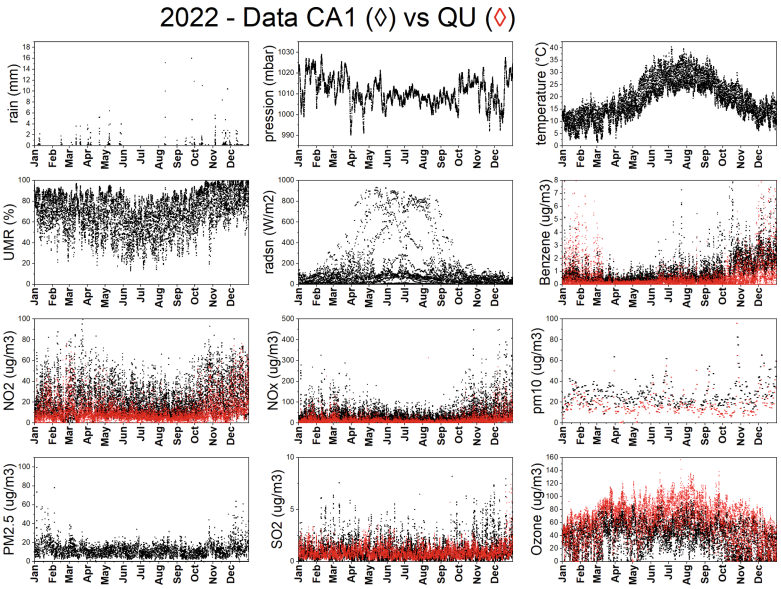

Fig. 3. An example of data analysis provided by the monitoring station of the regional environmental protection agency ARPAS for the year 2022 in the central area of the city of Cagliari and in the peripheral area of Quartu.

We identified an initial time window towards the end of February and a second time window at the end of October. These are two significant periods for conducting our measurements during a planned two-year campaign (2024–2025). The first period falls at the end of the winter season, during which typically higher levels of pollutants are observed due to domestic heating and vehicular traffic. The second period was identified at the end of the summer season, chosen following cycles of extreme meteorological events such as high temperatures, intense solar radiation, and low precipitation.

The year 2023, during which we also conducted two measurement campaigns, served to refine the protocol. Throughout this period, we made several adjustments based on the results obtained and field analyses, ultimately leading to a reliable protocol as applied in the third measurement campaign, conducted at the end of February 2024, whose results will be also briefly summarized in the followings.

Regarding the selection of species to monitor, our choice turned to plant species that were widely present in the locations considered and that were most representative of the urban context. The selected species included *Quercus Ilex* L. and *Nerium Oleander* L.,

which are evergreen arboreal and shrubby plants, respectively. Initially, the deciduous tree *Prunus Cerasifera* Ehrh. was also considered.

In the two measurement campaigns conducted in 2023, 3 plant subjects were identified for each species in each considered area, for a total of 9 subjects per study area. The use of portable detection devices, including a Normalized Difference Vegetation Index (NDVI)-based device (GreenSeeker Handheld sensor, Trimble), a leaf transmission/fluorescence analyzer [30] (Dualex, Force A) and a Raman spectrometer [32] (Mini-Raman Power Dual LightNovo with 660 and 785 nm lasers) enabled an in situ or close to field non-invasive monitoring of main leaf pigments and components whose levels can reveal characteristic plant responses to variations in environmental and pollutant conditions (see Fig. 4).

Fig. 4. Portable optical instruments used in the field to monitor plant physiological response: Greenseeker (on the left), Dualex (in the center), Raman spectrometer (on the right).

In particular, the main Dualex indices such as Chl, Flav, and Anth were collected from a total of 20 leaves per plant, focusing on the southeast orientation of the species relative to sunlight. These optical indices are proportional to the concentration of chlorophyll, epidermal flavonols (a type of flavonoids mainly involved in protection against oxidative stressors), and anthocyanins, respectively, present in the leaf [34–36]. Furthermore, selected Raman peaks were considered as representative of carotenoids and total phenols [37, 38]. For Raman spectroscopy-based analysis, 4 leaves per SE orientation subject were considered, totaling 12 leaves analyzed. A single NDVI acquisition per subject was also carried out.

It is worth specifying that in the preliminary measurement campaigns conducted in 2023, we also considered the northwest orientation of the selected subjects for the analysis. However, as no statistically significant differences between different orientations were observed on the basis of chlorophyll indexes, we finally selected the southeast orientation for future measurements. This decision was made both to ensure a more homogeneous comparison among the different sites and to better appreciate possible metabolic changes in polyphenol levels due to excessive solar radiation in the summer periods.

In addition to optical analyses, our measurement strategy included the collection of fundamental parameters related to plant vitality and age, such as leaf area, fresh and dry leaf weight, and trunk size.

The refined measurement protocol, finalized and implemented in the third measurement campaign of 2024, saw substantial changes compared to the two campaigns conducted in 2023. In this last measurement campaign, we decided to focus on a different peripheral area of the metropolitan city of Cagliari, *i.e.* that of Monserrato (Mo), where another ARPAS station for air quality monitoring is located. This station provides a more comprehensive information compared to the station located in the Quartu area because it collects a more complete selection of daily pollution data and atmospheric parameters. Furthermore, the Monserrato station is used by the regional authority as a reference station for the urban background, which also motivated us to choose this site as peripheral area to analyze. Another factor that led us to prefer the Monserrato area over the Quartu area is that, during field analyses, we noticed that the plant subjects in Quartu were not of the same age as those distributed in Cagliari and Monserrato, which represents an aspect of particular relevance for making comparable evaluations. Finally, we preferred to consider the Monserrato area instead of Quartu to exclude factors related to marine aerosols that inevitably can affect the Quartu area due to its closer proximity to the coast (see Fig. 5).

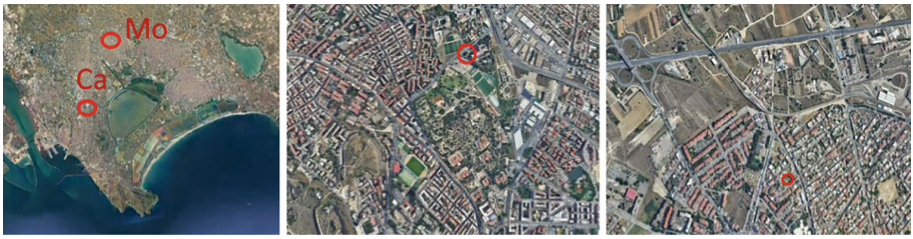

Fig. 5. In the new protocol, the central area in Cagliari (Ca) as previously considered (central image) and the new peripheral area in Monserrato (Mo, right image) are identified. Both areas (Ca and Mo) are reported in the left image.

During the third measurement campaign, we further added a background area (Se) where an ARPAS monitoring station is located, in what the regional authority calls the "Maintenance Area". This station is capable of monitoring background pollutant levels resulting mainly from natural sources and long-range transport phenomena. This area is considered a control zone. The positioning was defined by the fact that it is a relatively uncontaminated area and far from significant sources. Annual average levels of NO_2, PM10 and PM2.5 of about 1 $\mu g/m^3$, 13 $\mu g/m^3$ and 6 $\mu g/m^3$ (year 2022), respectively indicate the almost absence of pollution sources. The station is located about 3 km from the nearest inhabited center: Seulo, a village of fewer than 1000 inhabitants, 70 km north of Cagliari, at an altitude of about 700 m, located within a natural area accessible from the SS198, a road with limited traffic flow; the neighboring municipalities, well-spaced, have similar characteristics and the entire region is characterized by hilly and mountainous terrain with extensive forested areas; no significant industrial plants or dusty areas are

reported. In particular, an area cleared of trees (firebreak zone) and overlooking the valley below was identified: in this way, the station is not interfered with obstacles and also the anemometric pole can measure meteorological parameters optimally. The site had already been used previously for mobile monitoring stations, providing high-quality data, and also presents low simulated pollutant concentration values (see Fig. 6).

Fig. 6. On the left, the new and third control area added in the new measurement protocol located in Seulo, and on the right, a magnified view of the zones under analysis.

Based on the statistical analysis of the initial campaigns, it was decided to expand the number of subjects to be considered in the third campaign from 3 to 6 (of comparable size and age; *Quercus Ilex* L. subjects showing a trunk circumference within the 40–60 cm range) to reduce intraspecies variability, while simultaneously obtaining a larger representativeness of each area. Additionally, we excluded *Prunus Cerasifera* Ehrh. (not present in Monserrato and Seulo sites) to focus only on the two most widespread urban species: *Quercus Ilex* L. and *Nerium Oleander* L. (see Fig. 7).

Fig. 7. The species analyzed in the third campaign: *Quercus Ilex* L. (left image), and *Nerium Oleander* L (right image).

The number of analyses based on Raman spectroscopy was also increased (from 4 leaves to 10 leaves per subject), while the number of measurements performed with the Dualex device remained the same. It is important to emphasize that in the third campaign, Raman spectroscopy measurements were performed on collected leaves within a short (after 2 h) timespan from the in-situ measurements, while in the preparatory campaigns, the analysis was conducted in the laboratory after 1–2 days from leaves collection.

We utilized one-way ANOVA with Tukey post hoc test and a significance level of 0.05 to statistically analyze the groups corresponding to the identified zones for each chosen index. Statistical results as reported in the paper were performed under Origin Pro 2022 based on intraspecies grouping.

3 Results and Discussion

The variances noticed among the chosen plant varieties within the two designated urban areas - urban traffic site of Cagliari (Ca) and background urban site of Quartu Sant'Elena (Qu) - in the post-summer campaign provide initial perspectives into how urban vegetation reacts to its immediate surroundings (see Figs. 8 and 9). An imbalance in Dualex chlorophyll indexes (Dx Chl, see Fig. 8) between Ca and Qu sites is observed in the case of *Quercus Ilex* L. (QI), which was instead absent in *Nerium Oleander* L. (NO) and in *Prunus Cerasifera* Ehrh. (PC) This observation can suggest a peculiar response of QI as a function of the location inspected. Flavonols Dualex index (Dx Flav) kept comparable values upon different sites for NO and PC while an opposite variation with respect to Chl index was observed for QI between the two locations.

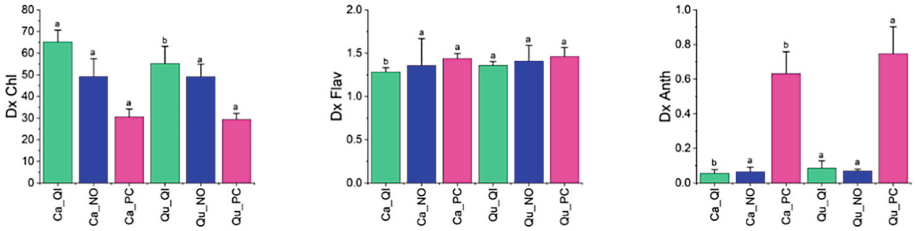

Fig. 8. Dualex analysis of the physiological responses of pigments in *Quercus Ilex* L. (QI), *Nerium Oleander* L. (NO) and Prunus Cerasifera Ehrh. (PC) in Cagliari (Ca) and in Quartu Sant'Elena (Qu). Each value represents the mean ± SD. Different letters indicate significant differences at $P < 0.05$.

Raman measurements (see Fig. 9) indicated an increase in phenols in the case of PC subjects from the Qu site, probably driven by a substantial increase in the level of anthocyanins as detected by Dualex analysis (Dx Anth, see Fig. 8). A larger Dx Anth index value was also observed for QI in the same location (Qu). The production of phenolic compounds such as flavonols and anthocyanins is generally involved in photoprotection and free radical scavenging activities, indicating a possible adaptation mechanism of the plant against environmental agents.

The results of the third measurement campaign in the post-winter window show that there is a significant increase in chlorophyll levels observed in the case of QI and to a

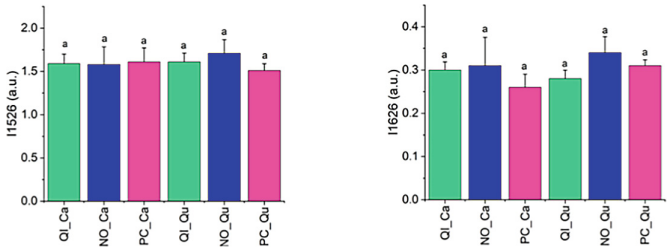

Fig. 9. Raman signal intensities at 1526 cm^{-1} (I1526) ascribed to carotenoid content (on the left) and at 1626 cm^{-1} (I1626) ascribed to total phenols content (on the right) in *Quercus Ilex* L. (QI), *Nerium Oleander* L. (NO) and *Prunus Cerasifera* Ehrh. (PC) in Cagliari (Ca) and in Quartu Sant'Elena (Qu). Each value represents the mean ± SE.

much lesser extent for NO at the Ca location compared to the peripheral (Mo) and control (Se) locations (see Fig. 10). This behavior is not uncommon for urban trees and highlights a plant response to a "mild pollution" effect, as previously noted [39]. It is hypothesized that below a certain level of air contaminants, chlorophyll content is positively affected due to compensatory mechanisms [40]. Indeed, this result is well in agreement with NOx levels for Ca (33 $\mu g/m^3$ annual average NOx in 2023) around the critical threshold for vegetation protection (i.e. 30 $\mu g/m^3$), accompanied by substantially higher levels of PM10 and PM2.5 for this location (30 $\mu g/m^3$ and 13 $\mu g/m^3$ annual average PM10 and PM2.5 in 2023, respectively) even compared to the peripheral site (7 $\mu g/m^3$, 27 $\mu g/m^3$, 7 $\mu g/m^3$ annual average NOx, PM10 and PM2.5 in 2023, respectively) and notably higher than in Se (<1 $\mu g/m^3$, 13 $\mu g/m^3$, 6 $\mu g/m^3$ annual average NOx, PM10 and PM2.5 in 2023, respectively). The result is also supported by measurements for QI from the post-summer campaign, where higher chlorophyll levels were recorded for the metropolitan site (Ca) compared to the peripheral one (Qu) as already mentioned above (see Fig. 8).

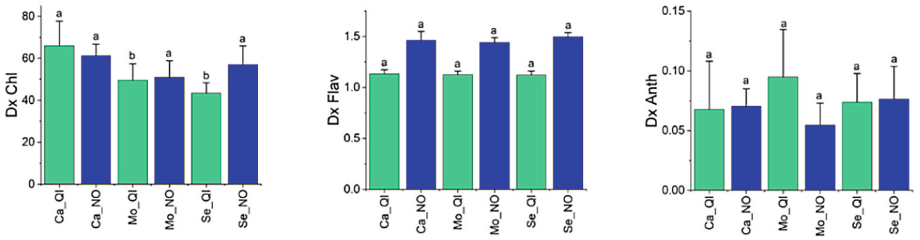

Fig. 10. Dualex analysis of the physiological responses of pigments in *Quercus Ilex* L. (QI), *Nerium Oleander* L. (NO) in Cagliari (Ca), Monserrato (Mo) and Seulo (Se). Each value represents the mean ± SD. Different letters indicate significant differences at $P < 0.05$.

The measured levels of Dx Flav exhibit a homogeneous intraspecies behavior during the post-winter campaign, which is further corroborated by Raman data I1626 (see Fig. 11). The absence of variations in both Dx Flav index and Raman I1626 suggests the absence of a defense response based on an accumulation of secondary metabolites by the

plant, eventually indicating the utilization of alternative adaptation mechanisms to urban stress situations, as observed in the case of QI for Ca, where chlorophyll levels increased. The Dx Anth index indicates very low levels of anthocyanins that remain constant across different locations, confirming the absence of a response at the secondary metabolism level of the plant.

Moreover, the levels of carotenoids highlighted by the Raman I1526 show minimal differences across locations, with an increasing trend from the metropolitan areas (Ca, Mo) to the control zone (Se) possibly indicating a partial impairment of photosynthetic centers in the former site (significative for NO of Ca), which is compensated by other plant adaptation mechanisms, as suggested above.

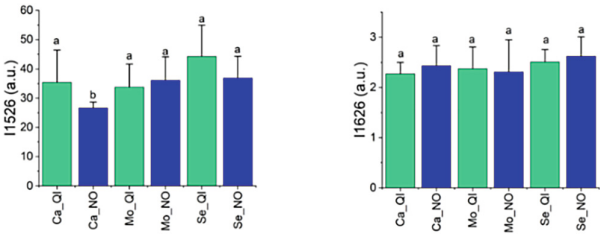

Fig. 11. Raman signal intensities at 1526 cm^{-1} (I1526) ascribed to carotenoid content (on the left) and at 1626 cm^{-1} (I1626) ascribed to total phenols content (on the right) in *Quercus Ilex* L. (QI), *Nerium Oleander* L. (NO) in Cagliari (Ca), in Monserrato (Mo), and in Seulo (Se). Each value represents the mean ± SE.

NDVI measurements (see Fig. 12) find a certain alignment with Raman observation evidencing moderately worse vegetation conditions (reduced plant vigor and/or foliage canopy density) in the case of the subjects from Ca and Mo.

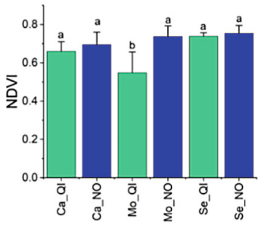

Fig. 12. NDVI measurements in Cagliari (Ca), in Monserrato (Mo), and in Seulo (Se). Each value represents the mean ± SE.

Finally, biometric data (see Fig. 13) highlight a reduced leaf expansion of both QI and NO accompanied by a lower fresh and dry weight in NO subjects from the metropolitan locations.

Overall, these results outline a fair tolerance of both plant species under examination to the higher levels of pollution observed in the metropolitan area, to which they respond through compensatory mechanisms by either an imbalance in photosynthetic pigments

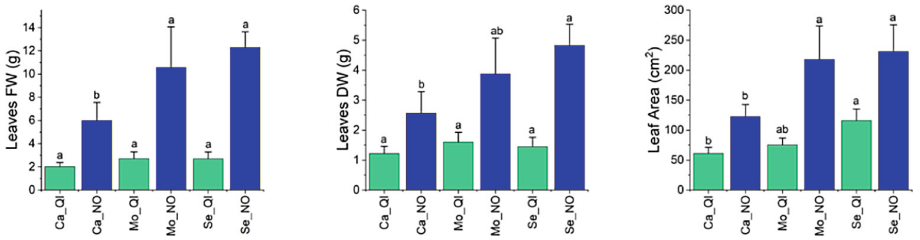

Fig. 13. Leaves fresh weight (FW), dry weight (DW) and leaf area in Cagliari (Ca), in Monserrato (Mo), and in Seulo (Se). Each value represents the mean ± SE.

(both chlorophyll and carotenoids), which is the case of QI, or reducing leaf growth levels and lushness, as observed in both QI and NO.

4 Conclusions

Cities are central to efforts aimed at addressing climate change, optimizing resources, and enhancing sustainability and resilience. The way cities are planned, built, governed, and managed directly impacts not only their own sustainability but also their broader role within interconnected systems. The main challenge lies in adopting a lifestyle that harmonizes with natural resources, recognizing their crucial role for humanity's future. When managed wisely, cities can drive human progress rather than merely being centers of problems [41, 42]. It's essential to recognize ecosystemic and ecological dynamics as integral to urban development and fully integrate them into city planning.

Within this framework, the use of simple, portable tools for rapid monitoring represents a significant step forward in assessing the conditions of urban greenery, allowing for a more detailed and precise evaluation of the physiological response of urban vegetation to environmental conditions. This data can then be promptly used to inform urban planning policies and strategies aimed at promoting more sustainable and resilient cities. The integration of innovative technologies into urban planning is essential to address the global ecological crisis and promote sustainable urban development worldwide, with a particular emphasis on the role of urban greenery in achieving this goal.

This preliminary investigation thus marks the initiation of a comprehensive exploration aimed at developing an innovative approach for monitoring urban greenery, leveraging the potential of a multifacted protocol including consolidated and novel analytical technologies. The ultimate goal is to establish a robust information framework conducive to future planning efforts, aimed at enhancing the sustainability of urban ecosystems and strengthening their adaptability. By utilizing advanced analytical tools like the optical technologies tested here, capturing detailed physiological responses of plant species to the urban environment becomes easily accessible. The real-time data generated by these cutting-edge technologies will facilitate a deeper understanding of how greenery interacts with its surroundings, suggesting how urban greenery can be managed consciously and intelligently to achieve sustainability and resilience goals, thereby attributing a positive connotation to the city in the intricate fight against climate change and urban pollution. The adoption of innovative technologies in green monitoring and management can

contribute to ensuring better air quality and mitigating the negative impacts of climate change, promoting healthier and more adaptable cities for future generations. Greater attention to green management, to which this work partly contributes, can lead cities to display functional, aware, and resilient environments, in a perspective of sustainability and inclusiveness that reflects the changing needs of contemporary society.

In future developments of this research, several avenues can be pursued to enhance its impact and applicability. Firstly, longitudinal data analysis could be implemented to track the long-term effects of urban vegetation on environmental quality and human well-being. By collecting data over extended periods, researchers can better understand the dynamics of urban ecosystems and assess the effectiveness of green infrastructure in mitigating pollution and climate change impacts. Secondly, the application of the methodology to a wide range of plant species would enrich the understanding of how different plants respond to urban conditions and pollutants. By studying various species, researchers can identify resilient species suitable for urban environments and tailor urban greening initiatives accordingly. Additionally, replicating the methodology in diverse urban contexts would strengthen the robustness of the study's conclusions and recommendations. Different cities exhibit unique environmental challenges, and applying the research methodology across various urban settings would provide insights into the universality of its findings and the adaptability of green infrastructure solutions.

Analyzing data collected through portable optical devices can provide detailed information on the health and responses of plants to local environmental conditions, enabling policymakers and urban planners to assess the effectiveness of existing policies and implement targeted interventions, allowing for the identification of best practices and solutions tailored to each urban context.

In summary, the results of this research can be used to inform and guide policy and planning decisions in various areas, including urban planning, environmental management, and climate change mitigation. Their integration into participatory and evidence-based decision-making processes can contribute to creating more sustainable, resilient cities that meet the needs of local communities.

Acknowledgments. This study was partially funded by Regione Toscana (Bando Ricerca Salute 2018, PRAMA project). We thank Dr. Giacomo Fontanelli (CNR Ifac) for granting the use of the Greenseeker. We thank the Regional Environmental Protection Agency of the Sardinia Region (ARPAS) for granting the use of the air monitoring station data.

Disclosure of Interests. The authors have no competing interests to declare that are relevant to the content of this article.

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Perceptions of Safety for Women in Urban Areas: A Spatial Regression Analysis in the City of Naples

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Abstract. One of the fundamental paradigms of contemporary urban design is "the inclusive and safe city": meaning the aim of developing spaces capable of meeting the needs of different population categories, promoting accessibility, equity, and a sense of belonging. Currently more than 4.5 billion people, or 55% of the world's population, live in urban areas, a percentage expected to rise to 68% by 2050. Such increasing urbanization generates opportunities, but also enormous challenges in achieving and maintaining environmental, economic and social sustainability. Although over half the global urban population is female, cities are often inadequately designed in terms of the needs and expectations specific to women. The current research deepens the knowledge of women's perceptions of safety as they move around the city, and evaluates which characteristics of the urban contexts, including physical, functional and socioeconomic elements, have significant impacts. In support of decision-makers, a tool is developed and proposed, based on GIS methodology, using open-source data on such contextual urban aspects. To these, the tool relates data on the safety perceived by women, derived from a mobile App (Wher) that collects women's own direct suggestions, comments and ratings on their perceptions of the safest walking routes. The GIS methodology proposed allows us to capture material and immaterial elements involved in the complex issues of perceived safety, and to focus on potentials for the relative improvements in urban landscapes. The methodology allows us to analyze the impact of the built environment on women's perceptions of walkability in different urban areas and at different times of day, identifying the relationships with various physical, functional, socioeconomic and environmental factors.

Keyword: Perception of safety · Women · Naples · Urban area

1 Introduction

One of the fundamental paradigms of contemporary urban design is "the inclusive and safe city", meaning the aim of developing spaces capable of meeting the needs of different population groups, promoting not only safety, but also accessibility, equity, and the sense

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O. Gervasi et al. (Eds.): ICCSA 2024 Workshops, LNCS 14823, pp. 35–48, 2024.
https://doi.org/10.1007/978-3-031-65329-2_3

of belonging. "Inclusion", then, means the creation of accessible urban environments for all citizens, regardless of their individual characteristics. Currently more than 4.5 billion people [1], or 55% of the world's population, live in urban areas, a percentage expected to rise to 68% by 2050 [2]. Such increasing urbanization generates cases of opportunity, but also enormous challenges in achieving and maintaining environmental, economic and social sustainability, which again relates to accessibility and inclusion. In this regard, despite the fact that more than half of the urban global population is female [3], cities are not designed to adequately address their specific needs and expectations. Urban and transport planning has long neglected the importance of the intersections between gender and mobility, and has therefore generated non-neutral urban environments, and often caused inequalities in accessibility to services and spaces for different user groups, among which women. The built environment has important effects on the quality of life experienced by women. Inadequacies can severely limit the ability of women to move within the city, to fully participate at the economic level, or to simply enjoy the spaces in which they live [4, 5]. Happily, recent experiences in urban planning and transport demonstrate a greater trend towards solutions of sustainable urban mobility, including a particular focus on walkability [6, 7]. The focus on this issue intensified significantly in 1988, with the adoption of the Charter of Pedestrian's Rights by the European Parliament, stressing the obligations of ensuring comfort and safety for pedestrians in urban areas. In 2006, the Walk21 Foundation, a British charity, introduced the International Walking Charter, outlining eight principles and thirty-two actions for improved urban walkability.

The General Theory of Walkability, proposed by Jeff Speck in 2013, offered a comprehensive framework for assessing the walkability of urban environments [8], since followed by other schemes. However, standardised methods for measuring walkability often fail to consider the needs of different populations, among which women. Approaches to measurement have traditionally focused on the spatial dimension, and it is only recently that recognition has been given to the demographics of populations and characteristics of individual users, which can concern travel purposes and mobility preferences [9, 10]. Although there are several factors that distinguish the walkability of women versus men, the safety factor is the most relevant, and is still much neglected in urban planning. Not only the objective degree of safety, but also its perception, is significant in the experience of mobility and has decisive influence on travel decisions [11, 12]. The constraints on mobility resulting from the sense of vulnerability and real and perceived risks of violence or other harms, especially at night, give rise to precautionary measures and avoidance behaviour by women, such as limiting or avoiding walking altogether. The overall effect is to significantly hinder the freedom of women in their use of public and private spaces [13–16].

Needs in mobility are not uniform among women, however. The concept of gender is complex and intersectional [17], and gender overlaps with the effects of social identities, such as race or class, making the shaping of women's experiences complex [18]. The intersectionality approach, introduced by Kimberlé Crenshaw (1989), has been used in addressing this multifactor experience.

Although urban policy-makers have devoted greater attention to gender discrimination, institutions have not invested in the collection of detailed information on women-specific safety, which would be fundamental to further action, and such indifference hinders the development of specifically dedicated tools. The understanding of the dynamics influencing urban safety remains limited, with only superficial knowledge of women's needs and expectations as pedestrians. Ultimately then, there are still few tools that could contribute to decision-making processes and facilitate interventions [19, 20].

This research aims to deepen knowledge on the issue of women's perceptions of safety during urban movement, and in particular to assess which characteristics of urban contexts, including physical, functional, socioeconomic and environmental elements, have the greatest impact [21]. The approach identifies gender as a key element influencing the experience of the urban environment, and in this regard, deals with the subjectivity of walkability criteria in relation to individual perceptions. Methodologically, the main objective is to develop a decision support tool based on GIS, capable of identifying the urban characteristics that most influence women's perceptions of walking the city. In pursuit of this objective, the work applies techniques of spatial analysis to data both on urban characteristics and on women's perceptions of safety, the latter derived from a mobile app (Wher) which suggests safer walking routes. The use of spatial statistical analysis makes it possible to study the impacts of the built environment on women's walkability in different urban areas and at different times of day, identifying relationships with different physical, functional, socio-economic and environmental factors. This identification of tangible and intangible elements, contributing to the complex matter of perceived safety, can facilitate decision-making for improvements in the urban environment and thereby promote greater accessibility and inclusion for women and others.

This research includes some theoretical outcomes of the know-how developed in the project "STEP-UP—Walkability for Women in Milan" (Grant No. 2022-1643), financed by Fondazione Cariplo under the call for proposals "Inequalities Research - Generating new knowledge to reduce inequalities."

2 Methodology

In the governance of urban transformations, policy-makers and administrators are called to take into account the issues of women's perceptions of safety. To do this, they would benefit from quantitative methodologies in support of their decision-making processes.

To define the list of proxy indicators, the study used the research outcomes of project "STEP UP—Walkability for Women in Milan". In particular, project proposes a subdivision in three main factors that influence the perception of safety for women in urban areas: (i) Spatial Features (space characteristics/morphological features); (ii) City Use (traces of behaviour and presence of other city users); and (iii) Hotspots (safe havens and no-go areas). The main factors are divided in nineteen different sub-factors as show in the Fig. 1.

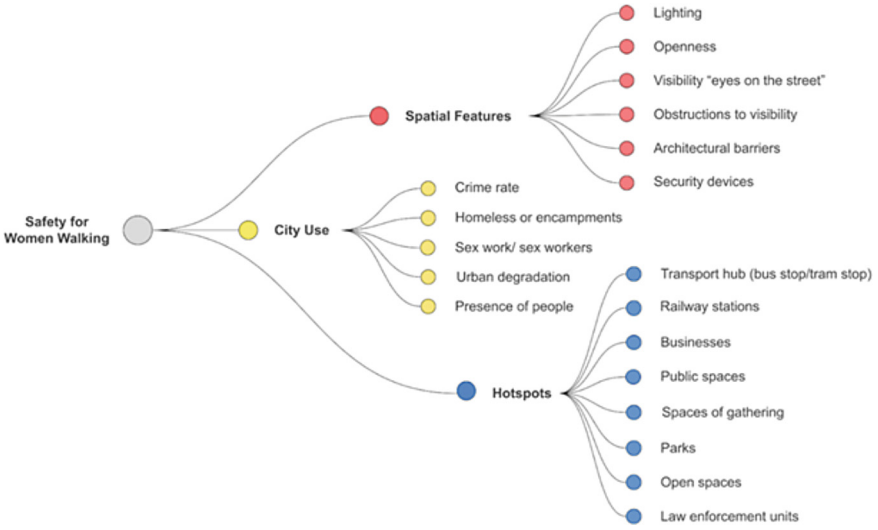

Fig. 1. Safety factors and sub-factors for women walking (STEP UP project elaboration)

On the base of STEP UP outcomes, this study proposes a selection of proxy indicators to cover the different Safety Factor categories. Table 1 shows the potential proxy indicators explanatory of women's perceptions of safety while walking at night, as proposed for the current methodology. The 18 indicators were advanced based on, in order of importance: i) their potential revelation of underlying safety factors, ii) availability of data in open format, iii) data in sufficient spatial detail (i.e., relatable to Italian census sections). Since the current study focuses specifically on women's perceptions of safety at night, the selection of indicators is balanced with this in mind.

On the other hand, the summary indicator of women's actually experienced perceptions of safety while walking at night is derived using a mobile app for grading of urban places, managed by the Walk21 Foundation. This App, called "Wher", allows women in cities such as Naples to rank georeferenced locations according to their perceived levels of safety while walking, as a cooperative device to assist other women in their mobility choices.

On further experimentation of the methodology, a decision was made to reduce the proxy indicators explanatory of women's perceptions from the proposed 18 to 11. This was done to ensure two criteria of effectiveness:

- Spatial consistency: the indicators are uniformly measurable in different parts of the city, limiting discrepancies caused by geographical variability and ensuring comparability;
- Temporality: the indicators are limited to those relevant to the night time period, i.e. from 8:00 PM to 6:00 AM (the most unsafe time interval of the day).

Table 1. Selected proxy indicators of safety for women walking at night

ID	Safety Factor		Indicator	Provider	Description
V1	Spatial Features	Openness	Ability to see and move in all directions	OSM	Layers describing vehicular, pedestrian and other public spaces
V2		Visibility "eyes on the street"	Night-time commercial activities	ISTAT	Number of pubs, restaurants, discos, coffee-shops, etc
V3			Residential buildings	ISTAT	City blocks of buildings with residences within first 2 floors
V4		Architectural barriers	Length of tunnels	DBSN	Locations of tunnels, by types
V5			Length of underpasses	DBSN	Locations of underpasses, by types
V6	City Use	Presence of people	Count of working population in selected roles	ISTAT ATECO	Density of working population in census tracts in 2021
V7			Count of resident female population	ISTAT	Density of resident population in census tracts in 2021
V8	Hot Spots	Transport hub	Count of public transport stops	OSM	Locations of bus and tram stops and train stations
V9		Public spaces	Surface of pedestrian spaces	OSM	Extension of pedestrian areas
V10			Surface of limited traffic zones	OSM	Extension of limited vehicular traffic areas
V11			Surface of urban green flowerbeds	DBSN	Extension s of urban green flowerbeds
V12		Spaces of gathering	Count of night-entertainment establishments	Google Earth	Locations of discos, night clubs, etc

(*continued*)

Table 1. (*continued*)

ID	Safety Factor		Indicator	Provider	Description
V13		Parks	Extension of urban parks	DBSN	Extension of wooded areas and parks
V14		Open spaces	Count of abandoned places	DBSN	Location of abandoned and degraded buildings
V15			Count of parking areas	OSM	Include parking areas greater than 250 square meters
V16			Count of industrial areas	OSM	Locations of Industrial agglomerations
V17			Count of industrial buildings	DBSN	Locations of industrial buildings
V18		Law enforcement units	Count of Enforcement presence	OSM	Locations of municipal and national police headquarters

OSM: OpenStreetMap
ISTAT: National Institute for Statistics
DBSN: National Synthesis Database
ATECO: National Classification of Economic Activities

After removal of the proposed indicators not meeting the above criteria, the ones remaining were: V1, V2, V3, V6, V7, V8 V9, V10, V12, V13 and V17. Subsequently, the data were collected for calculation of the 11 indicators over the minimum territorial reference unit, which in this case is the Italian census section.

The application of spatial statistical analysis typically offers important advantages in addressing large datasets, deriving explanatory and even predictive models of the relevant phenomena. The analytical procedures, however, can sometimes fail in providing sufficient precision concerning the spatial distribution of the analysed phenomena. The complexity of these techniques also requires a calibration phase in which the number of neighbouring elements or the distance with respect to which the values constituting the interpretative models to be defined are selected, on the basis of the phenomenon analysed. The different statistical techniques of spatial analysis useful for defining interpretative models of spatial phenomena are based on regression techniques. Although sharing commonalities, such techniques also have considerable differences. The classical Ordinary Least Squares (OLS) is a simple linear regression, but it does not consider the differences in spatial variables due to the non-stationarity of spatial locations. The Geographically Weighted Regression (GWR) provides a solution to non-smoothness in spatial coordinates, as its coefficients change with the variation of spatial coordinates [23]. The Multiscale Geographic Weighted Regression (MGWR) finds the optimal

bandwidth for each dependent variable, also showing the scale of action of the explanatory variables and further improving the model performance [24]. The objective of the current study, as stated, is to derive an explanatory model capable of individuating the critical factors influencing women's perceptions of safety while walking in urban areas. To achieve this objective, we propose a method using spatial statistic models, specifically GWR and MGWR, to determine the fit between the dependent variables (X_1, X_2, …, X_n) and the independent variable (Y). The application of GWR and MGWR requires a series of preliminary investigations, during which collinearity is eliminated using exploratory regressions. More specifically, the exploratory regressions individuate the set of statistical model variables with: adjusted R^2 greater than 0.3, p coefficient greater than 0.05, variance inflation factor (VIF) less than 5, and for which Jarque–Bera and spatial autocorrelation tests demonstrate the minimum acceptable value of 0.1. Naples is a considerable city with some of the highest population densities in Europe and a wide range of socio-economic and morphological complexities. These characteristics amplify the criticalities of urban planning and make the management of spatial phenomena particularly complex.

3 Case Study: The City of Naples

Naples is the third largest Italian city by population, within the second most populous metropolitan area. With 913,462 inhabitants, of which 474,264 female (ISTAT data, 2022), distributed over an area of 119.02 km^2, the average density is just over 7,600 persons per km^2. The city is divided into thirty districts for functional and physical characteristics and ten administrative municipalities. The historic centre of Naples, inscribed on the UNESCO World Heritage list in 1995, comprises the districts of Avvocata, Montecalvario, San Giuseppe, Porto, Pendino, Mercato, Chiaia, San Ferdinando, Stella, San Carlo all'Arena, San Lorenzo and Vicaria, as well as parts of the Vomero and Posillipo hills. Several of these districts are characterised by some of the highest population densities of Europe.

On the basis of their differing attributes, the thirty districts can be categorised as belonging to three fundamental types: Central, Semi-central and Peripheral (Fig. 2). The historic centre of Naples, rich in cultural attractions and economic services, is the most densely populated area. The districts of Chiaia and Posillipo, with some of the highest property values, are noted for premium residences, services and shops. Suburban districts such as Poggioreale and Ponticelli have lower population densities and lower property values, with intermixtures of residential, industrial, commercial and undeveloped areas.

The first phase of collecting data on the representative indicators was carried out using open access sources: the Urban Atlas of the European Environment Agency, the National Geoportal, OpenStreetMap, and ISTAT and City of Naples databases. The independent variable (perception of safety for women walking) was assessed using the data obtained via the Wher app. This indicator was calculated as the mean of the safety values reported on the app for evening (8:00–12:00 PM) and night (12:00 PM–6:00 AM), resulting in the definition of a single summary indicator of the level of perceived safety, from 8:00 PM to 6:00 AM.

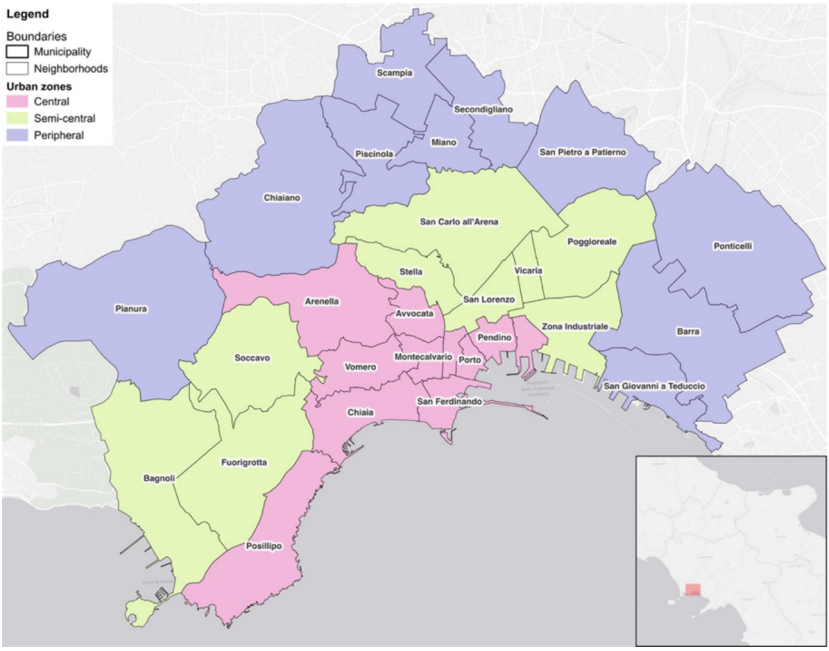

Fig. 2. The territory of city of Naples divided in the thirty districts (Municipality of Naples).

The mapping of perceived safety by district (Fig. 3) immediately reveals the low level of perceived safety for women walking at night in suburban districts, such as Barra, Chiaiano, Miano, Piscinola, Scampia and Secondigliano. The central districts and some semi-central residential areas, such as Arenella, Bagnoli and Fuorigrotta, show the highest values of perceived safety.

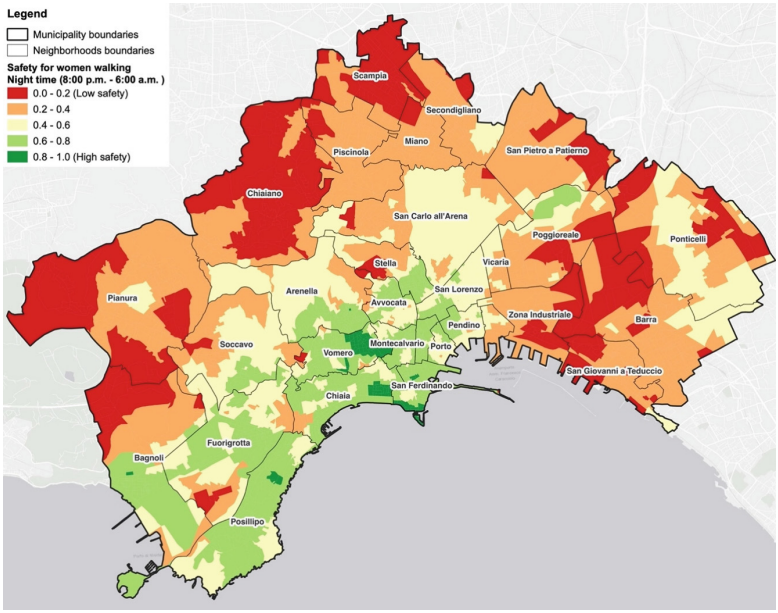

Fig. 3. Map of perception of safety for women walking at night (8:00 PM–6:00 AM).

Our next step is to evaluate all possible combinations of the candidate dependent variables, looking for OLS models that best explain the dependent variable within the context of user-specified criteria. The analysis was conducted considering all possible combinations of between three and eighteen dependent variables, applying the indispensable conditions: adjusted R^2 value of the variable greater than 0.3; p coefficient of significance greater than 0.05; variance inflation factor (VIF) less than 5; Jarque–Bera and spatial autocorrelation test values not less than 0.1. On this basis, the model developed included seven indicators of the original eighteen for which data were collected (V2, V3, V6, V7, V11, V13, V17) (Table 2).

Table 2. Comparing the fit of GWR and MGWR models

Model	Adj-R^2	AICc
GWR	0.360	10,300.94
MGWR	0.426	9,597.17

The results obtained show that the goodness of fit for the MGWR model is 0.426, significantly better than for the GWR model. The corrected Akaike Information Criteria (AICc) value for MGWR is also far lower than for GWR. We conclude that, for the city of Naples, MGWR is the better model of the relations between urban characteristics and women's perceptions of safety (Fig. 4).

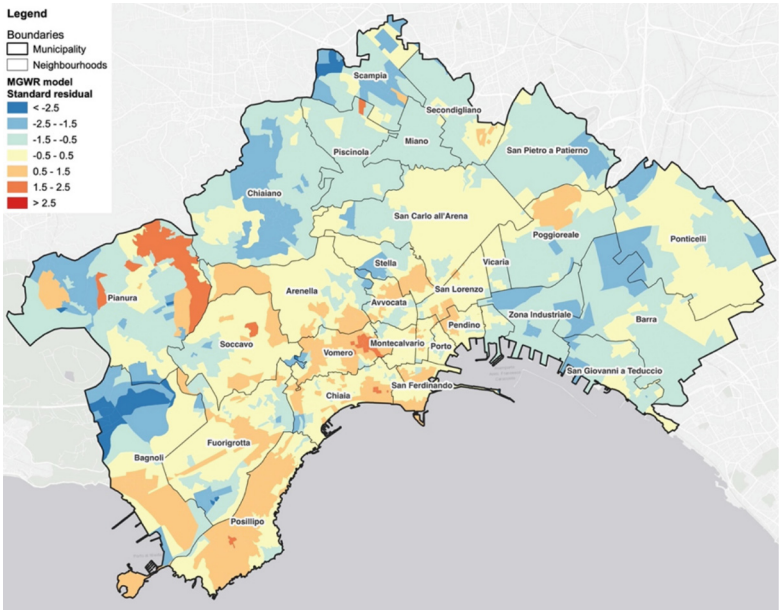

Fig. 4. Distribution of standardized residuals of MGWR model.

The representation of the standardized residuals detected nuclei that presented anomalies, with some exceeding the mean by more than 2.5 and less than −2.5 times the standard deviation. The neighborhoods with residuals greatly exceeding the mean were: Bagnoli, Chiaia, Chiaiano, Pianura, Posillipo, Vomero, Scampia and Soccavo.

The local R^2 indicates the level of performance for the applied local regression model. Results closer to 1 indicate a perfect fit to the local equation, while values below 0.3 indicate a lower fit. The results evidence 2,135 census tracts with a local R^2 value greater than 0.3, representing more than 60% of the total Neapolitan territory. The neighborhoods with highest local R^2 values are San Giovanni a Teduccio, Zona Industriale, San Carlo all'Arena, and Barra, all of which fall within Semi-central and Peripheral urban zones. The neighborhoods of the central urban zone evidence low values of local R^2, with reduced fit between the model local equation and variability of indicators (Fig. 5).

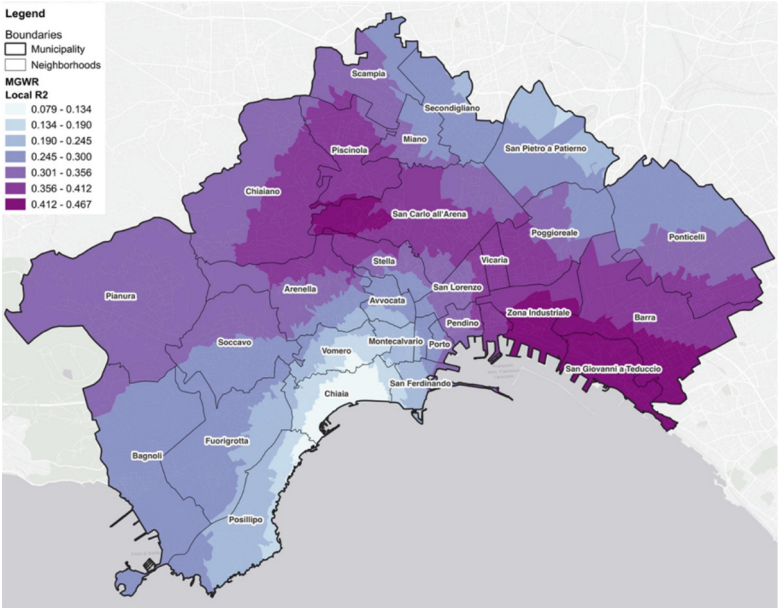

Fig. 5. Distribution of local R^2 of MGWR model.

From the observed variation of local R^2 values (Fig. 6), it appears that the obtained MGWR model fits with the variability of indicators in areas with a low level of safety. On the contrary, where women's perceptions of safety are higher at night, the model does not adapt to the variability of indicators.

These observations of results evidence that the use of spatial statistic techniques can be useful in understanding the relations between a spatial phenomenon, i.e. women's perception of safety, and certain urban characteristics. In interpreting the results, however, care must be taken to understand where and how the model is reliable in individuating the relations between the phenomenon of interest and the selected urban characteristics.

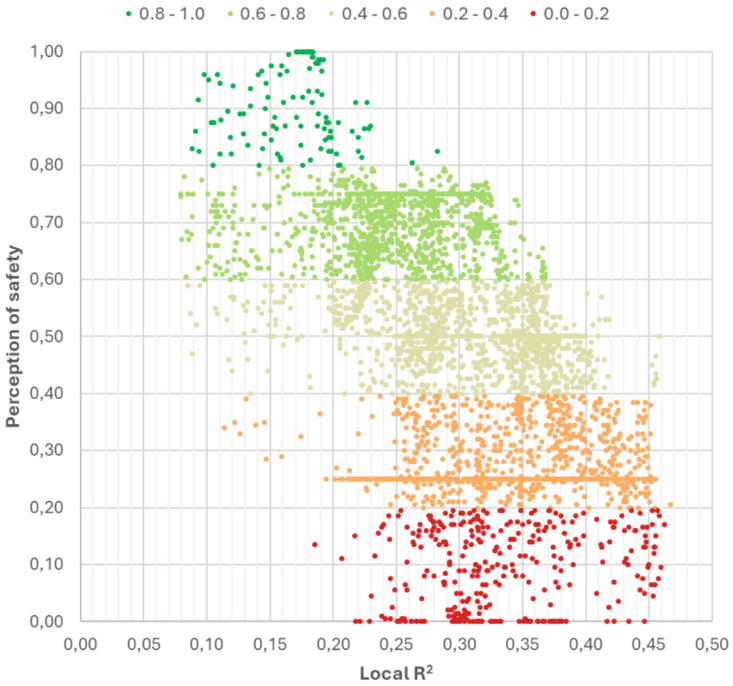

Fig. 6. Graph with the perception of safety for women walking during the night time (8:00 p.m.–6:00 a.m.) and the variation of local R^2.

4 Discussion and Conclusions

The UN Department of Economic and Social Affairs predicts that by 2050, 68% of the world's population will live in cities. Although more than half of the population is female, urban planning has generally failed to account for the particular needs of women. The generally low levels of urban liveability, in particular for females, result from concomitant causes. The complex phenomena are difficult to read and interpret, and the tasks are made still more difficult by the inadequacy of urban planning tools, which have long ignored the intersections between gender and the urban environment. In support of contemporary urban decision-makers, however, we do have the tools for identification and analysis of gender-related issues: by developing methodologies based on the collection of socio-economic, physical and functional data, and their processing through spatial statistical analysis.

Women's perceptions of safety are a particular concern, since these affect their mobility decisions in all aspects of urban life. The perception of safety does not adhere to objectively fixed rules, and is instead a complex function of physical, economic, cultural and traditional aspects of the different spatial contexts. The perception of urban space, and of safety, is therefore largely subjective in character, meaning that it can be particularly useful to develop methodologies of spatial statistical analysis on such perceptions in relation to socio-economic, physical and functional data collected on specific urban

environments. To this end, the current work has taken an integrated approach to understanding the relationships between the different urban aspects and women's perceptions of safety.

The contribution provides an initial research step in developing a tool to support decision-making processes aimed at improving women's perceptions of safety in the urban areas. The broader aim is to promote inclusive urban planning methodologies which account for gender-related needs, applicable to urban planning in general and transport planning in particular. The study, and its results, promote analytical methodologies that consider both tangible and intangible elements in perceptions of safety, improve understanding based on empirically collected data, and account for the specific needs and behaviours of women and gender minorities. Integrating information from women and under-represented groups into decision-making processes is in fact crucial, not only for increasing perceptions of safety, but for general improvements in the urban environment, appreciable and useful to all.

The main limitation of this study is the lack of useful data to calculate further proxy indicators representative of each safety factor category.

The proposed methodology provides the planning and administrative authorities of Naples with a tool for greater understanding of the urban context, based on quantitative and measurable data. The methodology could be further improved by incorporating additional data sources, such as on levels of crime or provision of street lighting. Our intention is to share the current research with local actors, hoping to verify the validity of the various results and associate them with practical recommendations.

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A Digital Humanities Approach to Study Women's Perceptions of Safety in the City of Milan: The STEP uP Project

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Abstract. This paper outlines the data collection phase of the "STEP UP - Walkability for Women in Milan" project, funded by Fondazione Cariplo (Grant No. 2022-1643), which aimed to assess walkability for women in Milan using geospatial data analysis methods. The project, which ended in February 2024, involved three phases: use case definition, data collection, and data analysis through advanced GIS mapping techniques. This paper focuses on the data collection phase, employing a digital humanities approach to gather location-based open data, Wher app data, survey questionnaires, and focus group discussions. Location-based open data and Wher app georeferenced data about women's safety perceptions in the city of Milan were subsequently used to develop a statistical GIS analysis through a Geographically Weighted Regression model aimed at understanding the relationship between ratings of women's safety perceptions and the built environment. Over 70,000 ratings and 4000 comments submitted by female users through the Wher app provided insights into their perceived security while walking. Additionally, a survey questionnaire and focus groups were conducted to evaluate participants' needs and perceptions of safety. These data aimed to facilitate a detailed spatial analysis of nighttime safety perceptions for women and gender minorities in Milan, emphasizing a human-centered approach to gender-inclusive mobility research and addressing gaps in data collection for complex socio-spatial issues.

Keywords: Data Collection · Digital Humanities · GIS Analysis · Gender Inclusion · Walkability

1 Introduction

Increasing urbanization has led to a heightened focus on issues related to spatial inequality and urban safety, including the safety perceptions of women in cities. "STEPUP: Walkability for Women in Milan" addresses one of the critical challenges in tackling

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O. Gervasi et al. (Eds.): ICCSA 2024 Workshops, LNCS 14823, pp. 49–65, 2024.
https://doi.org/10.1007/978-3-031-65329-2_4

this sensitive topic: the collection and selection of data. Women's safety on city streets is a complex and multifaceted issue that requires a deep understanding of the most significant indicators influencing such perceptions.

One of the main challenges addressed in this research is the difficulty in collecting specific data on this subject. Institutions often show a lack of interest in gathering detailed information on safety issues specific to women, creating a gap in overall understanding. This indifferent attitude results in a lack of dedicated tools and resources, limiting the ability to fully comprehend the dynamics that generate urban safety factors. Another significant challenge pertains to the absence of sector-specific data focusing exclusively on women's experiences. Generic data often does not allow for a detailed analysis of gender differences concerning specific aspects of the urban environment. This lack of sector-specific data limits the ability to formulate targeted policies and specific interventions that can effectively address safety issues affecting women.

In this context, the project aims to critically examine the challenges related to the collection and selection of data on urban safety for women, emphasizing the importance of addressing these gaps to develop more effective strategies for targeted user groups. Through in-depth analysis of multisource data, the goal is to explore women's perceptions of safety in the city, contributing to a more complete and accurate understanding of urban safety dynamics and walkability in relation to gender.

1.1 Inclusive and Safe Cities

The vision of inclusive and safe cities represents a fundamental paradigm in contemporary urban design, aiming to create spaces that meet the needs of the entire population, promoting accessibility, equity, and a sense of belonging. Inclusivity, in this context, refers to the design of urban environments that are welcoming to all citizens, regardless of their individual characteristics (Whitzman et al., 2013). The design of inclusive cities involves a significant commitment to removing physical and economic barriers. This means ensuring that urban spaces are accessible to people with physical disabilities but goes beyond, considering economic, cultural, and social accessibility. This includes creating accessible pedestrian environments and establishing public services that cater to everyone, irrespective of age, gender, or socio-economic background.

Walkability, namely referring to how friendly the urban environment is for walking, is gendered. Women generally experience the city differently than men, partly because they are more concerned with safety issues related to aggression and harassment (Koskela, 1999). Safety perception disparities tend to be especially exacerbated at night, when women's experiences tend to be significantly limited by fears of violence. This often leads to travel behavioral modifications, as evidence shows that women often suppress or modify their routes as a result (Loukaitou-Sideris, 2014). Transport planning tools and methods have often been slow in recognizing fundamental differences between the genders in their mobility patterns, largely overlooking women's needs in transport environments (Levy, 2013).

2 Methodology

2.1 A Digital Humanities Approach

Data collection in the framework of the STEP UP scientific research project follows a digital humanities approach, combining traditional and digital data collection and interpretative techniques to develop a transdisciplinary research at the intersection of computing, digital technologies and the disciplines of the humanities (Berry, 2011). This approach was deemed essential in the study of complex socio-spatial phenomena, such as the perception of safety of a specific demographic group, namely women.

The advent of digital technology has given rise to new research environments, offering new mediums for exploration using hybrid tools of data analysis that effectively mediate between new and conventional research mediums, and provides integrated and transdisciplinary methods for studying complex urban phenomena. Emerging digital technologies and data collection methods have significantly impacted the means of data production and interpretation, opening up numerous avenues for reading and understanding the urban experience through a user-centric approach (Zhang et al., 2024).

2.2 Objectives of the Research

The aim of this paper is to detail the collection and validation process for a series of relevant datasets useful to carry out the analysis in the framework of the goals of the STEP UP project. The paper is divided into four main sections discussing the collection methodology and outputs for four different data types and tools utilized in the research: Location-based Open Data (Sect. 3), Wher App Data (Sect. 4), Survey Questionnaires (Sect. 5) and Focus Groups (Sect. 6). It is important to note that these four branches of the data collection process are not mutually exclusive but are often interlinked and combined to refine one another.

Gender-disaggregated data sets collected through the four data groups are consequently analyzed through an extended Geographic Information Systems (GIS) analysis and advanced statistical techniques, as well as a series of quantitative and qualitative analyses for non-locational data, aimed to support and enrich the mapping results with further evidence from women users of the city. Techniques used to collect and analyze each data type are detailed in the following sections.

3 Location-Based Data

A series of relevant geolocated datasets were retrieved, sorted, validated, and filtered from open and proprietary data repositories and geoportals with the aim to populate a spatial regression model. The process outlined below shows the selection process of indicators leading to a final selection of eight indicators that were used to calibrate the Geographically Weighted Regression (GWR) Model to further analyze the relationship between said indicators and safety perception votes as observed through the Wher app. Data collected ranges from open to proprietary data from a wide range of sources.

3.1 Data Selection Methodology

In this study, proxy indicators were used to represent factors that are not directly observable among the list of safety factors identified as relevant in the literature in earlier phases of the STEP UP project. Within the framework of the STEP UP project, a total of 19 safety factors (SF_L2) were defined, classified into three types of safety factors (SF_L1): spatial features, city use and hotspots (Scarponi et al., 2023). A full list of these safety factors can be reviewed in Table 1 in the Annex. The set of proxy indicators identified in this research was cataloged and gathered by considering the following identified criteria: availability in the study area, alignment with the safety factors, reliability of the sources, sub-urban scale and spatial data. The complete dataset of proxy indicators was further reduced through a verifiable selection process as shown in Fig. 1.

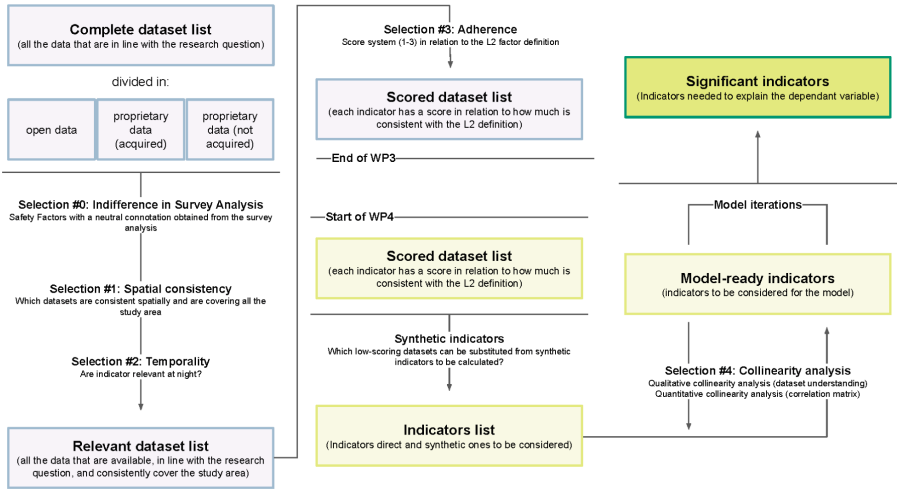

Fig. 1. Data gathering and selection methodology.

Identifying selection criteria can be a crucial step in reducing a set of indicators that describe urban characteristics more effectively and meaningfully. This process helps focus attention on more relevant indicators, thereby improving the quality and clarity of information. The selection criteria defined in the research were (i) Survey Analysis, focusing on indicators that emerged as significant in the survey results; (ii) Spatial Consistency, selecting indicators that are represented consistently in different parts of the city; (iii) Temporality, only selecting indicators that are relevant to nighttime (8pm–6am), thereby excluding activities that are only active during the day; (iv) Representativeness, which refers to the relevance of certain indicators as supported by the literature on the topic; (v) Adherence to safety factors definition, as defined in earlier phases of the research (see Table 1 in Annex). The final selection of 16 indicators to be imported in the GWR model is shown below:

1. Public Lighting
2. Space Syntax - 300m connectivity
3. Count of Food & Beverage destinations
4. Perpendicular Residential Building Curtains
5. Space Syntax - 300m choice
6. SOS Devices
7. Resident Population
8. Worker Population
9. Yearly Night Strava Users Flow
10. Overground PT Frequency
11. Railway Station Buildings
12. Discos and Night Clubs
13. Green Areas
14. Abandoned places
15. Industrial Buildings
16. Police Headquarters

4 Wher App Data

Data regarding the perceived level of security of women while walking was collected through 'Wher', a route planner application operated by Walk21 Foundation. Wher is an effective tool for collecting geo-localized data about women's perceived level of security while walking in urban areas (Carpentieri et al., 2023a, 2023b). It is a crowd-sourced mapping tool allowing women in a particular city to rank geo-referenced locations according to their perceived level of safety. As of the 1st of April 2019, in the city of Milan, the app had 5667 ratings, including 3850 textual ratings, collected from a total of 7844 users and 1296 reporters. Over 50% of the city extension (in kilometers) was rated through the application.

4.1 Methodology

Two types of data from the Wher App were analysed: (*i*) point data to be integrated in a GIS model, and (*ii*) corpus of textual comments. For the point data analysis, a road graph made using OpenStreetMap was joined to the point Wher App data to visualize ratings distribution and identify areas with the highest number of ratings, to provide insights into the spatial distribution of user perceptions. In the comments analysis, textual data was anlaysed through textometric analysis using IRAMUTEQ software to uncover common themes, and a sentiment analysis using Kimola software to derive sentiment classifications and identify frequently occurring terms.

Data distribution Analysis
The Wher App dataset is structured as single ratings, with the information regarding the creator of the comment and the timeslot of the day. Each score is positioned by the user on the geometric barycentre of the arc forming the road graph from OSM (OpenStreetMap), so that the geometric consistency of the dataset is a set of points. The same rating can be attributed to more than one point on the map, giving the user the chance to select a larger area with the same security perception characteristics, by including similar street segments considered similar to the main one. This divides the ratings in two typologies, the ratings associated with a single point on the map and the ratings associated with more than one point on the map (indicating an area that can vary). Most street segments are characterized by more than one comment or rating and a representation of the rating distribution across the city (see Fig. 2b).

App Rating Procedure and User Profiles
Users are asked to review a selected stretch of road on the application's map through a user rating and optional comment. They are asked to: (i) select a time slot between day, evening and night; (ii) rate the lighting from "Not at all" to "A lot"; (iii) specify the level of crowding from "Deserted" to "Very crowded"; and (iv) select advisability, with respect to perceived safety (Avoid, be careful and go easy). The ratings are provided with geolocation and time reference (date and time of transcription) and the points are distributed across three time segments (day, evening, and night, 06:00–20:00, 20:00–24:00, and 24:00–06:00, respectively).

Basic biographical information is also collected through the application, allowing to have some segmented information about city users. Each data point includes the following information: User ID; Creation time; Birthday; City; Occupation; Transport; Mapped meters; Ratings; Vote on perception; Vote on light; Vote on crowd; Timeslots; Rating data; Longitude; Latitude. In particular, the analysis summaries on user data, occupation, age and distribution of ratings over time, shows some data bias towards younger age groups (81.7% of users are in the 15–30 age group), and a concentration of comments in the year 2019 (2822 comments in 2019 representing over 71% of total comments collected on the App between 2017 and 2023).

4.2 Wher Data Analysis

Wher Data Analysis for GWR Model
The dataset available in the city of Milan consists of data from 2018 to 2023 with a coverage of the road graph of over 50% of rated roads. Considering the availability of data and the direction of interest of the project, the Wher App dataset submitted to further analysis is the data relative to the timeslots of evening and night (8:00pm–6:00am) from the year 2019, where two thirds of the data are concentrated. Only ratings within the boundaries Municipality of Milan are considered.

The Wher Road Graph Map
The Wher App point dataset was joined with the OpenStreetMap graph, only selecting data relevant to pedestrian flow. Arcs of sidewalks were split to a maximum length of 100 m, to be able to represent the Wher Data accurately. The resulting graph contained univocal information of each rating composed of the ID of the user, the time and date of the rating and the univocal information of each arc of the graph, such that overlapping arcs are equal to the number of ratings that were produced for each arc.

Two different maps were obtained, the first based on the ID of each rating (ID of the user and time and date of said rating), the second based on the ID of each arc of the graph. Figure 2a shows the distribution of the ratings on the city of Milan, with the overlapping of different votes and ratings of different dimensions. Ratings go from a vote of 1 to 3 and don't necessarily refer to one point. Within this image it is possible to see the overlapping of votes: some areas are characterized by similar votes, resulting in a strong red or a strong green, whereas some areas are characterized by diverging results (see Fig. 2a). Figure 2b shows the total sum of ratings for each arc, ranging from a minimum of one rating to a maximum of over 160 ratings.

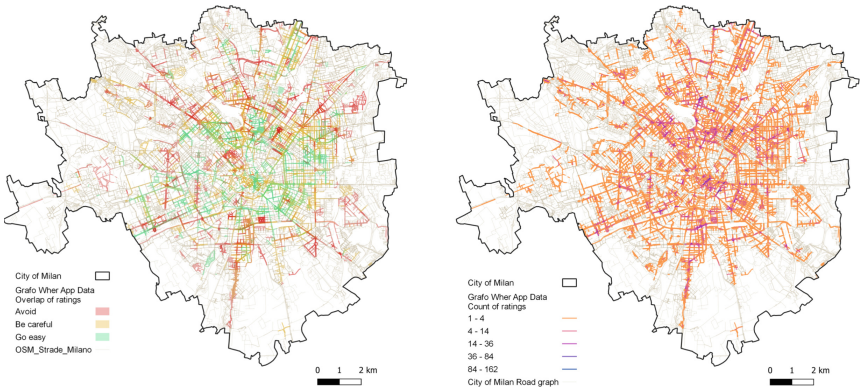

Fig. 2. (a) Wher App Data - Overlap of ratings; (b) Wher App Data - Count of ratings

Textual Comments Analysis

Textometric Analysis

Textometric analysis, also known as textual analysis or text mining, is a methodology used in the field of computational linguistics and natural language processing (NLP) to analyze and extract meaningful information from large bodies of text. The goal of textometric analysis is to uncover patterns, trends, and insights within textual data (Carpentieri et al. 2023a, 2023b). In this research, the open-source software tool IRAMUTEQ was used, which stands for Interface de R pour les Analyses Multidimensionnelles de Textes et de Questionnaires (Interface of R for Multidimensional Text and Questionnaire Analysis). IRAMUTEQ can be a powerful tool for qualitative text analysis, helping to uncover valuable insights from user ratings on Wher App.

The textual data from Wher ratings was preprocessed through data cleaning, tokenization, stopword removal, and stemming and lemmatization. Once imported into the software, the data was explored to give an overview of the word frequency and identify any immediate patterns, classifications, or themes.

IRAMUTEQ uses various statistical techniques for text analysis, including Principal Component Analysis (PCA), Multiple Correspondence Analysis (MCA), and Hierarchical Cluster Analysis (HCA). The findings were represented graphically using IRAMUTEQ's visualization tools. By clustering and grouping similar ratings or themes within the dataset, the tool helped identify commonalities and differences in women's experiences while walking. Figure 3a shows a factor analysis corresponding to the increasing frequency of forms and lemmas, where Factor 1 and Factor 2 represent the values and percentages of each class. Figure 3b visualizes the textometric analysis word graph based on word clustering.

Sentiment Analysis

Sentiment analysis describes the field of study concerned with analyzing the opinions, attitudes and emotions of individuals towards entities such as products, services, organizations, locations and events (Liu, 2012). Over the last two decades, the field has become increasingly active given the vast real-world applications to a plethora of disciplines. For the first time in history, researchers have access to huge volumes of freely accessible data

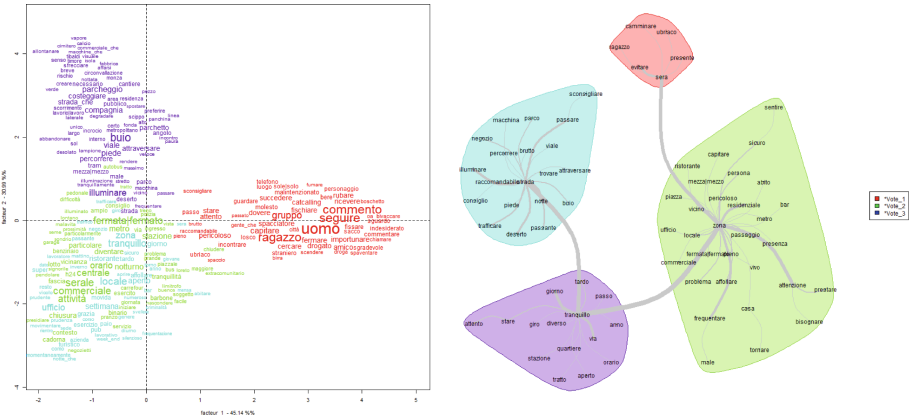

Fig. 3. (a) Textometric Analysis Classes Graph; (b) Textometric Analysis Word graph.

published by individuals online, can be analyzed through sentiment analysis (Roberts et al., 2018).

This analysis is performed using Kimola, a platform dedicated to social research and machine learning, primarily designed for obtaining consumer insights and enhancing marketing strategies. Automatic classifiers are generated, grounded in prevalent comment themes, with associated Sentiment Classifications. The analysis resulted in the following classifiers: (i) Crowded and busy Streets; (ii) Homeless people; (iii) Drug activity; (iv) Poor lighting; (v) Sex workers or the activity of sex work; (vi) Quiet residential areas; and (vii) Safety concerns at night. Figure 4 shows the sentiment polarity linked to each classifier as well as the geographic variation for the classifier "Crowded and busy Streets" by neighborhood NIL (Nuclei d'Identita Locale), the neighborhood unit in the city of Milan.

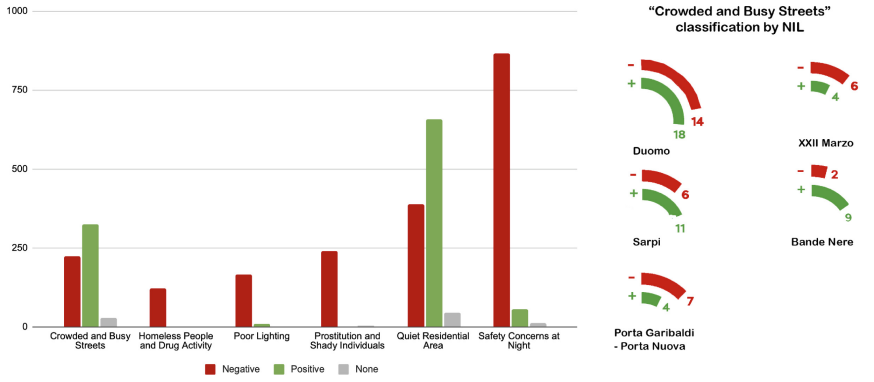

Fig. 4. Sentiment polarity total classification count and distribution by NIL for the classifier "Crowded and Busy Streets" (Kimola analysis)

5 Survey Questionnaires

A survey questionnaire was designed to intercept the participants' priorities in relation to perception of safety while walking, as well as to enrich the data collected through the Wher App filling in gaps about women's perceptions of safety, in relation to intersectional differences between respondents. The use of surveys as a data collection method for intersectional analysis has been highlighted in previous research (Fernandez et al., 2016; Hughes et al., 2022; Safer Parks Consortium, 2023).

5.1 Survey Methodology

The survey combines quantitative and qualitative questions with the aim to understand the relationship between user profiles, mobility patterns and their perceptions of safety in the city. It was disseminated in Italian and English, to target diverse populations in the city of Milan. The online survey was active for a duration of 4 months, between July 2023 and October 2023, with the aim to gather at least 500 responses from users of the city of Milan. It was disseminated primarily through social media platforms as well as by email to the researchers' extended networks, targeting active NGOs and community groups in the city of Milan as well as academic networks and Universities. The actual number of responses collected reached 1,808 responses (Italian version: 1762, English version: 46) by the end of the dissemination period.

5.2 Survey Structure

The questionnaire was designed around three main sections: (i) "Walkability in Milan profile" of each respondent collecting mobility data and general perception of safety in the city of Milan; (ii) view on perception of safety in relation to the predefined list of safety factors, elaborated on through a Likert scale, and (iii) extensive demographic data section including information on participants' age, sex, gender, sexual orientation, citizenship, physical and cultural ethnicity, and disability, among others. Some of these aspects were further investigated, and the response to each of these categories was always kept optional. Open-ended questions were also included to gather further insight into unstructured input from the participants.

5.3 Survey Results

Survey responses were cleaned to remove inconsistencies, and English responses were translated to Italian to unify the dataset for analysis. Some analyses cover the full 1,808 responses, while others focused only on responses from people who identified as women or gender minorities (1,667 responses).

Quantitative Analysis
Demographic Analysis
Detailed demographic data was gathered through the survey, and consequently regrouped into combined categories where sample sizes were too small, considering a benchmark

of a minimum of 15 people for each group to ensure representativeness (see Fig. 5). Demographic diversity of the respondent base is limited in several areas, especially with respect to nationality (96% Italian), ethnicity (95% white) and gender identity (92% women and gender minorities). On the other hand, the respondent sample base showed a fairly representative distribution in terms of age, sexual orientation, education level and economic status, as shown in Fig. 5.

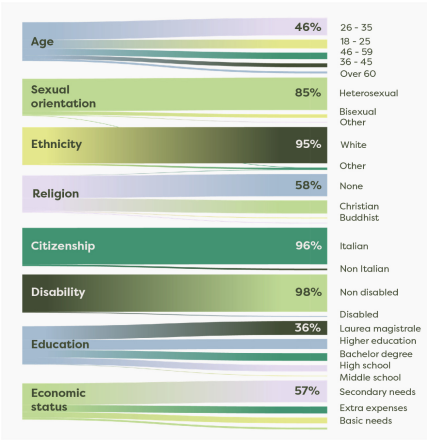

Fig. 5. Demographic distribution of survey participants (Graphics: Amina Salama).

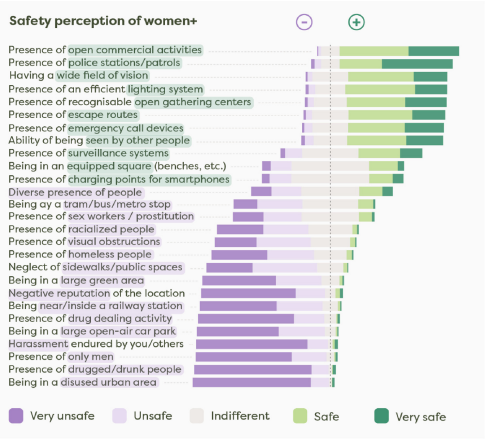

Fig. 6. Safety perception of women and gender minorities by factor (Graphics: Amina Salama)

Mobility Analysis

Within the women and gender minorities participant group, walking and metro were the most popular transport modes used. Around 90% of women and gender minorities reported walking in the city at least 30 min per day, most commonly during the evening

(7–11pm). These results are significant in showing the importance of walking in women and gender minorities' daily routines and thereby, the importance of enhancing their sense of safety around the clock.

Safety Perception Analysis
Results highlight significant difference between perception of safety of women and gender minorities compared to men during both night and day. This difference is especially accentuated during nighttime hours where 57.05% of women and gender minorities report feeling unsafe while walking compared to 8.27% of men. Men are also more likely to go out in the evening and nighttime, and to feel safe doing so. Significant findings regarding women and gender minorities' safety perceptions include:

- A significant portion of women and gender minorities experienced sexual harassment (63%) and violence (17%) while walking, leading to heightened feelings of unsafety when walking alone at night (8 in 10, compared to 6 in 10 for those who rarely or never experienced harassment or violence). This is a personal factor that has an a priori influence on perception of safety irrespective of the physical environment for walking.
- Older women are significantly more likely to have a higher perception of safety both by day and night than younger groups (25.7% of the Over 60 group reported high perceptions of safety, compared to 2.4% of those between 18 and 25 years old). Older age groups are also nearly twice as likely to feel safe or mostly feel safe in their own neighborhoods (Over 60: 54.2%; 18–25: 27.1%).

Safety Factors Analysis
Questions about safety factors were structured according to the Likert rating scale, providing information on the relevance of each factor as well as the connotation (whether positive or negative). Inherent limitations of the Likert scale include the interpretation of the numbers as continuous variables (Jamieson, 2004) (Cohen et al., 2002) and ambiguity in the meaning of the neutral value (Nadler et al., 2015). Figure 6 shows aggregated results for nighttime safety perception by safety factor for all respondents identifying as women or gender minorities. To enable a comparison among different groups, the quantitative analysis was performed by analyzing the average values of the ratings, as visualized in Fig. 7 below.

- Safety factors are generally perceived more neutrally for men compared to women and gender minorities, with a variation of up to ± 1 scale points.

Intersectional differences among women and gender minorities include the presence of police stations/patrols which vary by sexual orientation, "presence of men", "railway station" and "tram/bus/metro station", which vary by age, the possibility to be seen by other people which various by ability/disability.

Qualitative Content Analysis
A qualitative analysis was carried out on questions with open-ended answers, providing insight into (i) factors contributing to a sense of safety in specific areas, (ii) factors contributing to a sense of unsafety in specific areas, and (iii) strategies adopted by

Fig. 7. Intersectional analysis of nighttime safety perception (Graphics: Amina Salama)

respondents to feel safer when walking alone at night. Only responses from women and gender minorities were considered here. The methodology for analysis is divided into two parts: (a) frequency counts relying on automated classification techniques; and (b) a qualitative interpretation of the content through a manual review of the responses.

The frequency count was carried out using the GPT-3.5 Open AI language generation model, recognized as a strong interpretative tool to classify thousands of responses through deep learning techniques. The model was trained on a representative sample selection of 50 responses, and consequently run on the entire list of responses, automatically classifying and labeling the unstructured text data. The GPT model could identify additional factors, expanding on the list of factors from the initial manual selection.

In sum, the results from open-answer questions in the survey largely complimented and reinforced the safety factors identified at the start of the research. Additional themes emerged from these user and respondent inputs that had not been included in the safety factor list derived from the literature. These include specific land uses, such as residential areas; pedestrian areas and high-end retail (all viewed as positive), city use features, such as neighborhood affluence or appearance of affluence (viewed as positive), and road traffic conditions, associated with a negative perception of safety.

Respondents also reported various strategies adopted to feel safer while walking at night. These can be split into three main categories: a) manipulating the urban environment, b) manipulating one's person or changing behavior, and c) social strategies, i.e. reaching out to others for help. It is also noteworthy that several of the strategies mentioned involve the use of some functionality of a personal mobile device (Apps, phone call, location sharing, etc.). This highlights the importance of handheld devices in enhancing women and gender minorities' perceptions of safety while walking in the city, emphasizing the potential role of digital communication and navigation services.

6 Focus Groups

6.1 Methodology

Area Selection Process
Areas selected for focus groups were based on inputs from the Wher App data and the survey responses. Whereas Wher App data gives us more accurate georeferenced data, the input from the survey is based on a wider diversity of respondents. Thus, it is important to consider input from both sources when selecting areas for focus group discussions. Given the lack of congruence between rated areas and NIL divisions, the areas defined for the purpose of this study are based on a wider neighborhood approach.

Three neighborhoods were selected in total, out of which two are among the most negatively perceived (Centrale and Loreto-Padova), and one is among the areas most positively perceived by users (Sarpi). This is done to allow for a cross-examination between both groups. The area selection process was based on the following criteria: (i) data coverage (95th percentile), (ii) score or safety rating, (iii) overlap of Wher and survey results, (iv) population diversity. Areas rated outside the city of Milan and data positioned in non-walkable environments (e.g. highways) were excluded.

Participant Selection Criteria
Participants were selected to encompass a wide diversity of women with respect to age, ethnicity and nationality, with the precondition of residing in or frequenting the neighborhoods under study on a regular basis. Non-heterosexual males were also considered to potentially offer insights aligned with the LGBTQI+ community. Furthermore, participants were required to have previously expressed their perceptions of safety through the survey discussed in Sect. 5. This ensured inclusion of individuals who had already articulated their viewpoints on the subject and have a good grasp of the framework of the project.

Structure of the Focus Group Discussions (FGDs)
The focus group sessions were designed as semi-structured discussions using participatory mapping tools. The sessions lasted about two hours each and involved 4–6 participants in each of three focus areas. The moderators facilitated the discussions to delve into factors that evoke feelings of discomfort or feelings of safety while walking in these neighborhoods as well as brainstorming solutions or potential intervention strategies where needed. Recurring patterns and noteworthy observations are highlighted in the results.

6.2 Focus Group Results

The three focus groups highlighted various positive and negative factors. Negative elements focused on problematizing other person groups, highlighting concerns about male only presence, homelessness, inebriated individuals, and (male) immigrant groups. These perceptions are often exacerbated by biased media portrayals and/or direct personal experiences. Car-centric environments were also highlighted hostile environments that impinge on personal safety. On the other hand, positive factors include vibrant, and

well-maintained spaces, well-lit areas at night, presence of security, pedestrian areas and community activities that foster community engagement. Solutions proposed by participants include revitalizing specific areas, improving lighting, and promoting active citizenship. Design solutions to enhance visibility, and infrastructure improvements such as dedicated cycle paths and parking facilities were also highlighted as measures to enhance safety perception.

7 Conclusions

The approach adopted in this research contributes significantly to enhancing the understanding of safety factors in urban environments, particularly in the context of space perception, city use, and hotspots. The process of defining and gathering potential proxy indicators for location-based data, through a multiple criteria selection, has resulted in a refined dataset of 16 indicators for statistical spatial analysis. The process of defining proxy indicators to represent safety factors posed challenges and limitations. The scarcity of and restricted access to certain proprietary data, and the limitations of spatial localization for others, presented limitations. Despite these challenges, a substantial, relevant list of datasets emerged, providing a foundation for a multivariate spatial analysis for consequent phases of the project.

The integration of technology through the Wher App brings a valuable dimension to the assessment of safety perception. The inclusion of various parameters, along with the option for users to provide free-form comments, enriches the data with geolocalized user-generated insights. Applied textometric and sentiment analysis techniques offer a deeper layer of understanding, unveiling common patterns and relationships within user comments. Sentiment analysis allowed for a nuanced exploration of spatialized sentiment variation of specific themes. The findings suggest that certain factors elicit a higher negative sentiment, providing valuable insights for urban planning and safety enhancement measures. This multi-faceted approach offers a robust framework for identifying common indicators across diverse urban zones.

The online user survey reveals some key findings about women and gender minorities' experiences while walking in the city, especially at night. The findings both confirm assumptions based on previously reviewed literature on the topic as well as highlight new themes, opening new avenues for exploration on the theme of women's safety in the night city. Beyond differences in perceptions of safety between genders, the survey also revealed differences by age, sexual orientation, and disability, emphasizing the importance of intersectionality for gender-responsive urban planning. Qualitative results shed light on additional safety factors that were not considered in the study. These range from urban characteristics to personal, subjective factors, such as proximity to one's home. Despite these findings, the survey's limitations in participant diversity restrict the broad applicability of its results. A more targeted dissemination approach could help to reduce or eliminate these biases.

The focus groups enabled a qualitative investigation providing deeper insight through dialogue and discussion. The restriction of focus group participants to individuals who (i) had completed the survey, and (ii) had a strong connection to the focus areas enhanced and focused the outputs of the FGDs. What emerges is an expertise of the participants

regarding their perceived safety based on their everyday life experience while walking in specific areas of the city. The discussion around potential solutions was successful in directing these findings and local knowledge into actionable outputs. One of the striking results of the FGDs is the alignment that emerged between sustainable mobility goals and perceptions of safety, highlighted through discourses around car-centric environments as hostile elements reducing women and gender minorities' urban sense of safety. Alternatively, pedestrianized areas and enhanced cycling infrastructure were noted as positive contributors to sense of safety. This result is also in line with results emerging from open-ended questions in the survey, which highlighted the role of transport environments in enhancing or inhibiting women's sense of safety.

7.1 Final Discussion

Overall, the data collection approach demonstrated in this paper follows a digital humanities approach that mixes between conventional and digital modes of data production and analysis, providing a solid foundation for the development of a detailed spatial analysis of the perception of safety of women and gender minorities in Milan. This mixed data collection methodology allowed the researchers to integrate between quantitative and qualitative insights from large sets of open and proprietary data, as well as compensate for limitations of data in terms of depth and bias. This also allowed for cross-analysis of data, whereby insights from one data type were leveraged to inform and refine the methodology of data collection from another data source. Finally, the data collected through the site-specific focus group discussions, as well as other qualitative data collection tools allowed for deeper qualitative insights, further used in consequent phases of the project to inform policy guidelines for the city of Milan and recommendations for gender-sensitive urban planning principles.

Acknowledgements. This research was part of a one-year funded scientific research project, titled 'STEP UP - Walkability for Women in Milan", funded by Fondazione Cariplo (Grant No. 2022-1643) under the call for proposals "INEQUALITIES RESEARCH - Generating new knowledge to reduce inequalities". The research was coordinated by Transform Transport in collaboration with TeMA Lab - Università degli Studi di Napoli Federico II, Sex and the City, and Walk21 Foundation. The analyzed data were treated according to the GDPR-General Data Protection Regulation (EU, 2016/679).

Disclosure of Interests. The authors have no competing interests to declare that are relevant to the content of this article.

Appendix – Scored Dataset List

Table 1. Scored Dataset List

Safety Factor				Selection #0	Selection #1	Selection #2		Selection #3	
Level 1	Level 2	Indicator	Dataset Name	Survey Analysis Indifference	Spatial Consistency	Temporality	Score	Representativeness	Adherence to SF definitions
Spatial Features	Lighting	Count of Public Lighting	Public Lighting	No	x	x	2	x	3
	Openness	Ability to see and move in all directions	Roads Surface	No	x	x	2	No	1
	Visibility "eyes on the street"	Count of F&B	Food and Beverage Services	No	x	x	2	x	3
			Integrated Food and Beverage Services	No	x	x	2	x	2
	Obstructions to visibility	Count of residential buildings	Residential Buildings	No	x	x	2	No	2
		Count of partition elements	Partition Elements	No	x	x	2	No	1
		Count of isolated trees	Trees	No	x	x	2	No	1
	Architectural Barriers	Length of tunnels	Tunnels	No	x	x	2	No	1
		Length of bridges	Bridges	No	x	x	2	No	1
		Average Distance from Crossings	Highways	No	x	x	2	No	2
	Security devices	Count of Security Devices	SOS Devices	No	x	x	2	No	3
City Use	Presence of people	Count of Resident Population	Resident Population	No	x	x	2	x	2
		Count of Working Population (on selected Ateco codes)	Worker Population	No	x	x	2	x	2
		Count of F&B	Food and Beverage Services	No	x	x	2	x	3
			Integrated Food and Beverage Services	No	x	x	2	x	2
		Strava Metro Flows	Yearly Night Strava Users Flow	No	x	x	2	No	2
	Transport hub (bus/tram stop)	Count of Bus and tram stations	Surface Public Transport Stops	No	x	x	2	No	2
	Railway stations	Count of Railway Stations with external buildings	Railway Station Buildings	No	x	x	2	No	3
Hotspots	Businesses	Count of F&B	Food and Beverage Services	No	x	x	2	x	3
			Integrated Food and Beverage Services	No	x	x	2	x	2
	Spaces of gathering	Count of discos and night clubs	Discos and Night Clubs	No	x	x	2	No	3
	Parks	Count of Green Areas	Green Areas	No	x	x	2	x	3
	Open spaces	Count of abandoned and not activated places	Abandoned Buildings	No	x	x	2	No	2
			Areas of degradation	No	x	x	2	No	3
			Parking Lots With Area > 250sqm	No	x	x	2	x	2
		Count of industrial buildings	Industrial Buildings	No	x	x	2	No	2
	Law enforcement units	Count of Enforcement presence	Police Headquarters	No	x	x	2	No	2

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Warsaw's Smart City Mirage: Unmasking Ranking Variations and Methodological Mysteries of IMD Smart City Index Report

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Abstract. Although the smart city concept is widely adopted globally, there is a growing need to assess the advancement of spatial entities. International Institute for Management Development (IMD) Smart City Index has been providing an annual rating of the smartest cities worldwide since 2019. However, because of the changed methodology for 2023, the comparison is not as straightforward as one would expect. The purpose is to illustrate how ranking position comparison can't be the unique method as a suitable way for judging a city's downgrade or promotion, giving a more friendly form of study for decision makers' assessments. This paper conducts a comparative analysis of the 2019 and 2023 IMD Smart City Index reports, using Warsaw as a case study. The significance and originality of this study is in emphasising the challenge of assessing cities only based on their ranking. Instead, the objective is to assign more value to the individual factors studied in the ranking, consequently proposing a more direct comparison among them. The authors demonstrate how the alteration in methodology impacted Warsaw's ranking position. Subsequently, a contrary trend was identified, rather than increasing as first suggested, Warsaw declined in the ranking, which corresponds to the worsening of most of the parameters examined in the research. Hence, the updated calculation methodology used in the IMD Smart City Index is more precise and may be regarded as a metric for assessing advancements in the search for smartness.

Keywords: smart city · sustainability · IMD · Smart City Index · Warsaw

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O. Gervasi et al. (Eds.): ICCSA 2024 Workshops, LNCS 14823, pp. 66–78, 2024.
https://doi.org/10.1007/978-3-031-65329-2_5

1 Introduction

In recent decades, urban areas have seen rapid and continuous growth. According to the 2022 World City Report published by UN-Habitat, the urban population accounted for 57% of the global population in 2021. The forecast indicates that there would be a projected growth to 68% by the year 2050, resulting in a total of 2.2 billion people living in urban areas [1]. The ongoing process of urbanisation and its resulting consequences in all aspects of urban life have led to a growing focus on sustainable development [2].

The concept of a "smart city" has become more popular worldwide as a way to tackle urbanisation, economic and technological growth and environmental issues [3, 4]. Furthermore, the relevance of this topic is increasing as technology assumes a more significant role part in everyday lives [5].

Despite being recognised since the early 1990s, there is no universally accepted definition for what constitutes a "smart city" or a "smart and sustainable city" [6–9]. Some researchers focus on the aspect of safety [10], other on healthcare innovations [11, 12], and still another on people' engagement and empowerment [13–15]. Most studies focus on three main groups of aspects such as socio-cultural, techno-informational, and organizational aspects of smart city notion [16]. Hui et al. [17] define a smart city as a city that is both sustainable and efficient from several perspectives. It achieves this by improving mobility, optimising the use of resources, enhancing health and safety, promoting economic and social growth, and enabling participatory governance through not only face to face communication, but also the use of information and communication technologies, cooperation, and investment in social capital. Ahmed et al. [18] concentrate on the use of cutting-edge technologies in the management of urban environments. Sarker [19] defines a smart city as "an urban environment" or an advanced contemporary context, able to guarantee the accessibilities of the city amenities, to enhance the citizens wellbeing.

Pandiyan et al. [20] discuss addressing urban challenges by optimising resources and maximising productivity in the mobility, waste management and the energy sectors. The authors emphasise the significant impact of socio-cultural aspects on improving urban quality of life through suitable environmental and mobility planning.

The rise of the smart city idea has led to several research papers predicting the assessment and ranking of cities globally based on their initiatives. The IESE Cities in Motion Index ("Instituto de Estudios Superiores de la Empresa"), the Smart Cities Index, the ISUI Smart City Index ("International Society for Urban Informatics"), the Digital City Index, the Innovation Cities Index, and the IMD Smart City Index are a few examples [21]. The Swiss International Institute for Management and Development's report (the IMD Smart City Index) focuses on the technical, economic, and social elements of cities, by analysing all aspects with indicators [22].

Indicators and rankings are important tools for evaluating the progress in smart development because they provide easily interpretable quantitative data. In order to effectively quantify the impact of using such ranking to monitor the development, it was important to concentrate the attention on a single aspect (analysing all 141 cities in the ranking would be inefficient). Warsaw was chosen as a case study because of its representative significance. Warsaw is the capital and largest city of Poland, and it is also one of two Polish cities included in the ranking. Furthermore, the city has been

honoured with several smart city awards and certificates. Upon examining the data, an anomaly was observed: despite the indicators worsening, the city's rating improved, which seemed to be a significant phenomenon.

For these reasons, the authors will examine Warsaw's scenario in the IMD Smart City Index research, with a particular emphasis on methodology. The index was selected due to its utilisation of citizen interviews and data collection across several cities, making it a highly regarded tool for policy makers and for attracting worldwide media attention. Furthermore, the researchers created case studies on several kinds of smart cities to demonstrate the varying phases of growth and diverse experiences in each city. The objective was to highlight the applicability of the index in multiple circumstances. To direct the research, the following research question was formulated: "What impact did changes in methodology and priorities have on Warsaw's Smart City Index rankings between 2019 and 2023, and what were the contributing factors to these shifts?" The authors further explore this topic by examining the changes made to the methodology of the IMD Smart City Index between 2019 and 2023 and how these changes impact the comparability of Warsaw's rankings in those two years. To accomplish this, the paper starts with an introduction (this section, the Sect. 1), that emphasises the growing notion of smart cities. The discussion then turns to analysing Warsaw as a smart city (Sect. 2) and the IMD Smart City Index, by discussing how the index assesses cities (Sect. 3). The Sects. 4 analyses the methodology employed and the results for this comparative analysis. Finally, the discussion and conclusions are focuses on Sect. 5. This section not only explores the implications of methodological alterations on Warsaw's ranking fluctuations, but also provides suggestions for policymakers.

2 Warsaw as Case Study

Warsaw, the capital of Poland is located in the centre of the country (Fig. 1). According to the Central Statistical Office, Warsaw covers 517.2 km^2 and has a population of 1,861,975 inhabitants, according to the Central Statistical Office [23]. This makes Warsaw the biggest and most populated city in Poland. The capital is also the 9^{th} most populous in the EU [24]. Warsaw is situated in the Mazovian Region, which is the biggest and most populated in the country. It's located 300 km from the Carpathian Mountains and 260 km from the Baltic Sea. It operates as a central intellectual, political, cultural, and economic centre.

Warsaw is a city that is recognised as the smartest in Poland. In 2019, it won the Smart City Award in the category for cities with 500,000 inhabitants and more [25]. The Smart City Award aims to recognise people and initiatives that have significantly contributed to the progress of policies for developing smart cities in Poland. The award is designed for members of the business community and local government officials who improve the competitiveness of Polish cities, the country's economy, and businesses by using innovative ideas and management practices in their initiatives [26].

Warsaw was appreciated for its technological development with a view to the well-being of the citizens and tourists [25]. That year, the capital of Poland received the platinum certificate of ISO 37120 norm from the World Council on City Data (WCCD). It is an international standard to quantify indicators of quality of life and urban services

and therefore assess sustainable social development of cities. Certificates are awarded at five different levels: aspirational, bronze, silver, gold, and platinum, based on the number of indicators are submitted and verified.

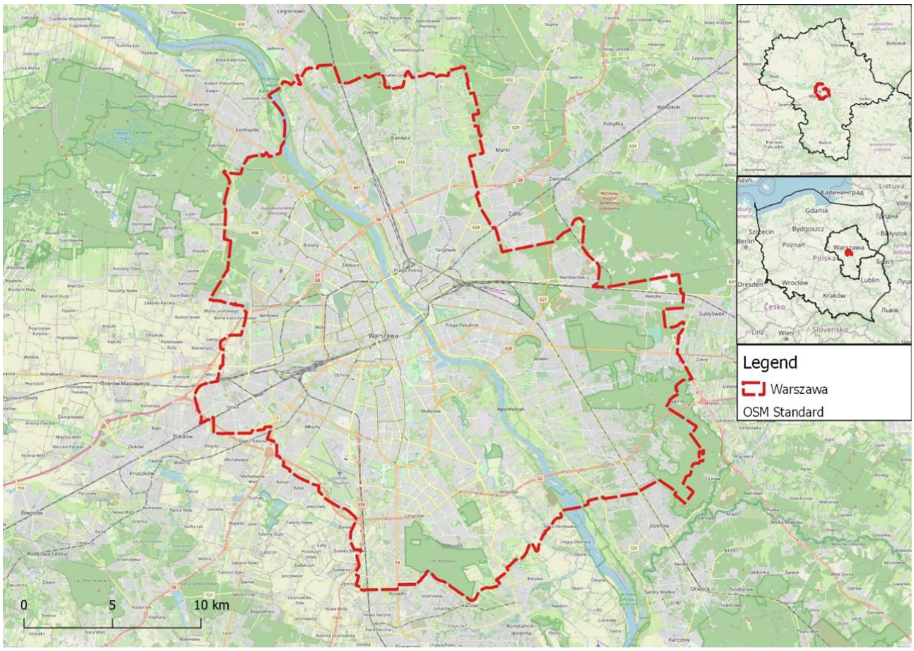

Fig. 1. Map of Warsaw (Source: Authors elaboration)

The certification procedure involves verifying 100 indicators, including 46 core indicators necessary for certification and 54 additional indicators. Those indicators are divided into seventeen categories. The auditors from the WCCD assessed several aspects of urban life in Warsaw, including urban planning, transportation, sanitation, recreation, education, and safety [27]. Knight Frank, a well-known real estate, and consultancy business produced two reports in 2018 on the aspirations of two Polish cities to become 'smart', one of them was Warsaw. The research examined the city across six areas of smartness: smart mobility, smart environment, smart economy, smart society, smart living, and smart government [28]. The selection of these parameters is not arbitrary but rather based on the recognition that they are internationally recognised as the key factors used to create the IMD Smart City Index, the most significant measure for evaluating the smartness of cities.

The selection of Warsaw as a case study for this research is ideal because it effectively demonstrates the significant discrepancies in rankings resulting from the use of two different assessment procedures to compute the IMD Index. It strongly emphasises the need of considering factors beyond just geographical comparison in order to accurately assess the city's development. By re-evaluating the calculating technique, it becomes evident that there has really been a decline in the city's growth.

3 IMD Smart City Index

The Smart City Index introduced by IMD evaluates both social, economic, and technological elements of the city. The former refers to inclusiveness, quality of life and environment. The index measures citizens' perceptions in five key areas (Table 1): health & safety, mobility, activities, opportunities (work & school) and governance, captured in two categories: structures and technologies.

Table 1. Key areas of IMD Smart City Index report. (Source: Authors elaboration)

Structures	Technologies
Health & safety	
Mobility	
Activities	
Opportunities	
Governance	

A total of 120 people from each city were polled for assessment. There are 15 indications offered under major categories. Survey participants are also asked to choose the 5 most important aspects for them, which constitute priority categories [29, 30]. The Human Development Index (HDI) is finally used to compute the final score. This index is computed based on predicted years of life, schooling, mean schooling period and Gross National Income per capita. Subsequently, the HDI is used to categorise cities into four groups. Cities within these are rated from AAA to D based on citizens' feedback [30]. Hence the score is relative. Moreover, the scores from past years are used into the calculation of the current year's results. What are the methodological changes between 2019 and 2023?

Initially, the number of cities featured has increased from 102 in 2019 to 141 in 2023. In addition, a new knowledge partner, The World Smart Sustainable Cities Organisation, provided guidelines for smart cities. Finally, the approach was revised. The 2023 IMD Smart City Index highlights that the alteration in calculation methodology is a response to the evolving global environment of smart cities. This transformation at the city level serves as a valuable signal of what the future could bring.

The SCI's methodology (Smart City Index) was enhanced by including more data at the municipal level. The SCI was developed as an analysis tool for the improvement of cities by using surveys to evaluate people' perceptions. Therefore, it is of utmost importance that the data collected is perfectly placed in the context of the cities examined.

The 2021 Index, as well as all previous years, depended on country-level Human Development Index (HDI) data provided by the United Nations Development Programme (UNDP). In 2022, the International Institute for Management Development intends to use HDI data at the city level, in order to provide a more realistic depiction of the socio-economic environment of specific cities [29].

4 Analytical Approaches in Analysing the Two Smart City Index Reports (2019–2023)

As previously mentioned, the research is based on comparing two Smart City Index reports created by International Institute for Management Development in Switzerland. The research focused just on these two years due to a recent change in methodology. Including two years in between (with no data for 2022) would not provide any new insights to the analysis. The modifications made to the calculation procedure between the 2019 and 2023 reports were carefully analysed to identify the changes affecting the ranking outcomes. Moreover, changes in the indicators were examined, especially in the priority areas. Analysis of trends revealed a substantial reversal in Warsaw's expected economic trajectory. Warsaw's rating decreased as expected due to lower scores on many parameters outlined in the revised approach.

Warsaw made its debut in the smart city rankings in 2019. Various changes have occurred in the indicators and overall rating for four years. Warsaw was ranked 61st out of 102 cities in 2019 and 44th out of 141 cities in 2023. The overall rating increased by 17 positions in the individual Smart City Index rankings. Comparing the metrics from 2019 and 2023 in the smart city index is remarkable. It is important to note that the methodology for generating the index in the 2023 Smart City Index has been changed.

The 2023 IMD Smart City Index enhanced the technique for calculating the index and comparing it to the previous version by introducing a new approach for calculating indicator methodology. So, according to new rankings published in the SCI 2023, in 2019 Warsaw should have been placed in 14th position instead of 61st. This paper examines and contrasts the first signs to comprehend the decline in Warsaw's ranks from 14th to 44th position.

Priority Areas

Figure 2 shows the IMD Smart City Index priority areas, which were selected from a list of 15 indicators. Survey participants were asked to choose 5 indications they considered most critical for their city. The top three top problems identified by survey respondents in 2019 were traffic congestion, air pollution, and affordable housing. Compared to 2023, only affordable housing is still in the top three. Affordable housing, security and health services have been the most highlighted indicators [29].

In 2023, there have been different changes in several priority areas compared to 2019. Participants in the survey said that some key topics had shifted since 2019. Figure 1 shows that among the 14 overall priority categories, only six, including affordable housing, recycling, basic utilities, school education, social mobility, and unemployment, were considered more concerning to the city in 2023 compared to the 2019 data.

Priority areas in Fig. 2 linked to traffic, such as road congestion and air pollution, have decreased in rank from the top positions to 5th and 6th place. Meanwhile, concerns about affordable housing and security are moving to the top. Conversely, the concern over unemployment has marginally risen, but citizen engagement has decreased. Additional factors such as employment, recycling, green spaces, and transport have been consistently identified as areas of concern with no notable improvements in Smart City Reports [29].

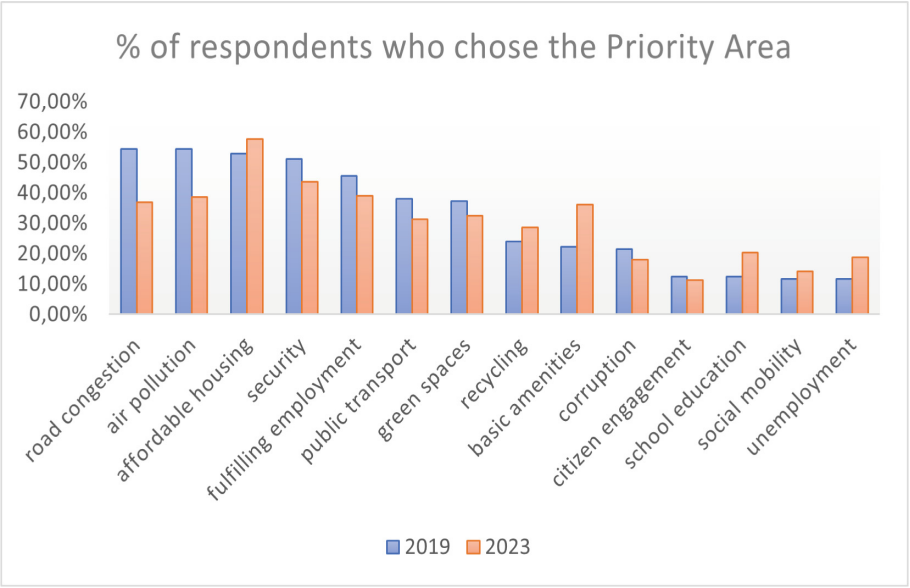

Fig. 2. Priority Areas, from 2019 to 2023, according to IMD Smart City Index (Source: Authors elaboration)

On comparing the indicator changes on Table 2, it is evident that several indicators have declined in the Smart City Index 2019 comparison to the 2023 SCI. Merely examining the ranking position without reviewing the whole record, it would have given the impression that Warsaw had improved (moving from 61st place to 44th). Warsaw fell from 14th rank in 2019 to 44th in SCI 2023 due to a general reduction in most metrics, with just three showing improvement. That proves that individual comparison of old ranking positions in the IMD Smart City Index with the new one is not relevant due to the changes in methodology.

Table 2. Structures Index, from 2019 to 2023, according to IMD Smart City Index [29, 31]

Index	2019	2023
Basic sanitation meets the needs of the poorest areas	74.66	64.1
Recycling services are satisfactory	61.98	61.3
Public safety is not a problem	66.39	61.1
Air pollution is not a problem	27.55	31.6
Medical services provision is satisfactory	47.93	46.3
Finding housing with rent equal to 30% or less of a monthly salary is not a problem	–	28.6

(*continued*)

Table 2. (*continued*)

Index	2019	2023
Traffic congestion is not a problem	32.51	31.4
Public transport is satisfactory	64.33	63.0
Green spaces are satisfactory	71.9	63.0
Cultural activities (shows, bars, and museums) are satisfactory	80.17	77.6
Employment finding services are readily available	77.96	65.4
Most children have access to a good school	78.4	68.4
Lifelong learning opportunities are provided by local institutions	75.48	70.4
Businesses are creating new jobs	78.93	69.3
Minorities feel welcome	61.43	58.3
Information on local government decisions are easily accessible	71.49	62.1
Corruption of city officials is not an issue of concern	40.5	40.7
Residents contribute to decision making of local government	59.37	54.7
Residents provide feedback on local government projects	65.43	63.3

It is necessary to study each increase or decrease of the individual parameter in order to be able to analyse the change in the city in detail (Table 3).

Table 3. Technologies index, from 2019 to 2023, according to IMD Smart City Index

Index	2019	2023
Online reporting of city maintenance problems provides a speedy solution	57.3	51.3
A website or App allows residents to easily give away unwanted items	66.67	62.2
Free public Wi-Fi has improved access to city services	71.49	62.6
CCTV cameras (Closed-circuit television camera) has made residents feel safer	71.21	55.2
A website or App allows residents to effectively monitor air pollution	73.42	64.4
Arranging medical appointments online has improved access	69.28	66.4
Car-sharing Apps have reduced congestion	55.1	49.1
Apps that direct you to an available parking space have reduced journey time	59.64	50.7
Bicycle hiring has reduced congestion	64.74	59.6

(*continued*)

Table 3. (*continued*)

Index	2019	2023
Online scheduling and ticket sales has made public transport easier to use	77.41	71.8
The city provides information on traffic congestion through mobile phones	-	50.1
Online purchasing of tickets to shows and museums has made it easier to attend	84.99	78.7
Online access to job listings has made it easier to find work	83.2	78.7
IT skills are taught well in schools	66.39	58.7
Online services provided by the city has made it easier to start a new business	68.32	63.7
The current internet speed and reliability meet connectivity needs	-	71.3
Online public access to city finances has reduced corruption	46.97	45.2
Online voting has increased participation	54.55	57.6
An online platform where residents can propose ideas has improved city life	68.04	63.7
Processing Identification Documents online has reduced waiting times	75.07	67.3
Ranking position	**61/102**	**44/141**
New ranking position	**14/102**	**44/141**

A significant aspect to consider is the methodology changes in the 2023 Smart City Index, impacting the comparison between 2019 and 2023. The index calculation method was improved, and a new way of calculating indicators was implemented. Therefore Warsaw, in updated rankings from previous years, published in SCI 2023, secured 14th place, a substantial improvement from its 61st position in the original SCI 2019.

The methodology changes involved transitioning from using country-level Human Development Index (HDI) as a proxy for evaluating health, knowledge, and standard of living dimensions to city-level HDI, provided by the Global Data Lab. This modification enhances the accuracy of city rankings and allows for better comparisons between cities.

The drop in ranking from 14th to 44th in IMD 2023 reflects the impact of these methodology changes, highlighting the necessity to consider the altered calculation approach when interpreting Smart City Index results. In addition, the analysis of the individual old parameters shows that almost all of them (33 out of 36) had a decrease compared to 2019.

5 Discussions and Conclusions

This paper presented research based on the case study of Warsaw as a smart city, based on the comparative analysis of the IMD Smart City Index Reports from 2019 and 2023. The main focus was on the methodology alternation that affected the relevance of the previous reports; therefore, it is important to discuss the significance of this change.

Here, the rationale behind the change as well as the impact on relevance and accuracy will be presented.

First of all, the changes made to the IMD Smart City Index methodology in 2019 and 2023 indicate a concerted attempt to improve the precision and relevance of city rankings. The Human Development Index (HDI) at the city level was adopted in place of the country-level HDI due to the realisation that city-specific data might provide a more detailed and accurate evaluation of urban regions. The knowledge that cities can differ greatly from their national averages in terms of development, infrastructure, and quality of life probably led to the decision to include city-level HDI. Rather than making generalisations based on national measures, the index sought to provide a more customised assessment by utilising city-level data to capture the distinctive qualities and accomplishments of particular cities. Secondly, the transition to the city-level HDI brought in an assessment approach that was more context-and locally-specific. The purpose of this modification was to improve the IMD Smart City Index's city rankings' relevance and accuracy.

The index aimed to provide a more accurate depiction of a city's development by considering characteristics unique to its urban environment by utilising data relevant to individual cities. This modification was made in order to reflect the different specifics of cities more accurately across the globe, considering their unique efforts, strengths, and problems as they work to become smarter. However, it was difficult to compare rankings directly between the two years due to the change in calculation techniques, particularly the addition of city-level HDI. Warsaw's move up the rankings—from 61st in 2019 to 44th in 2023—might at first seem to indicate improvement. But rather than being a direct outcome of the city's smart city efforts getting better, this change in rank was the consequence of methodological changes.

Caution should be used when interpreting ranking discrepancies due to the necessary methodological corrections. Comparing rankings from different methodologies without considering methodological adjustments may lead to erroneous findings. It is important to highlight that the altered approach may lead to variations in a city's ranking, which may not accurately represent the advancements made in its smart city projects. This highlights the importance of understanding the context and paying careful attention to methodological subtleties when evaluating changes in rankings. The subtleties produced by the methodological changes emphasise the need of recognising these variations to avoid misinterpretations and provide a more precise assessment of a city's progress throughout time.

There are a few limits to this research. Firstly, in order to accurately compare the ratings of each city and comprehend the underlying causes, the analysis of individual items is rather extensive. Additionally, because the analysis is based on surveys, it is highly dependent on the selection of the sample, making it especially sensitive to this decision.

The paper also addressed the changes in priority areas in Warsaw from 2019 to 2023. Therefore, it is crucial to examine its importance and implications. The surveys conducted by the IMD Smart City Index have identified significant shifts in crucial domains that are crucial for understanding the evolving needs and preferences of residents in the context of smart cities. These changes reflect the changing perspectives and

concerns of residents regarding the most significant issues impacting their quality of life and urban experiences.

These alternations have a multitude of impacts on smart city initiatives and projects. Primarily, they provide precious information that assists politicians and urban planners in adapting their plans and initiatives to more effectively meet the evolving needs of the population. Initiatives focused on enhancing safety measures, increasing healthcare accessibility, and strengthening emergency services may get more money and attention if security and health services have been identified as priority areas. Additionally, they indicate the need for a more comprehensive strategy for the development of smart cities. Initiatives should prioritise several areas of urban life, including social inclusion, affordable housing, security, healthcare, and environmental sustainability. Policymakers should use the Index's findings as a guide when developing integrated solutions to address these varied and changing objectives.

Local governments may use adaptive governance techniques in response to these evolving challenges. This requires the implementation of adaptable policy-making methods that can accommodate the dynamic demands of the people and the constantly evolving urban environment. For instance, if authorities see that restoring community participation in decision-making processes has diminished in significance, they may seek innovative methods to achieve this goal by using technology and community engagement platforms [32, 33].

In addition, the results of the Index can force an assessment of current programmes and policies to make sure they are in line with the priorities of the present. Budgets may need to be reorganised in order to allocate funds to sectors that the public believes have become more important, as indicated by the Index's highlighted citizen perceptions.

In summary, methodological changes make it difficult to compare Smart City Index ranks between years. Changes in methodology, like going from a country-level HDI to a city-level HDI, have an immediate effect on the assessment's criteria and statistics. This results in a fundamental change in the assessment of cities, complicating direct year-over-year comparisons. However, changes in priority areas and direct comparison of individual parameters may serve as a suggestion for policymakers to adjust or alternate existing strategies.

Acknowledgments. This study was supported by the technical-scientific collaboration agreement "PON METRO 2014–2020 AXIS 6 - Action CA6.1.1.b - Cagliari smart city: Integration of urban governance with the mitigation of urban heat islands (CA_UHI)" signed between the Municipality of Cagliari and the University of Cagliari (DICAAR - Department of Civil and Environmental Engineering and Architecture). This study was accomplished within the RETURN Extended Partnership and received funding from the European Union Next-GenerationEU (National Recovery and Resilience Plan – NRRP, Mission 4, Component 2, Investment 1.3 – D.D. 1243 2/8/2022, PE0000005).

This study was supported by the MUR through the project SMART3R-FLITS: SMART Transport for Travellers and Freight Logistics Integration Towards Sustainability" (Project protocol: 2022J38SR9; CUP Code: F53D23005630006), financed with the PRIN 2022 (Research Projects of National Relevance) program. We authorise the MIUR to reproduce and distribute reprints for Governmental purposes, notwithstanding any copyright notations thereon. Any opinions, findings, and conclusions or recommendations expressed in this material are those of the authors and do not necessarily reflect the views of the MIUR.

Author Contributions. This paper is the result of the joint work of the authors. In particular, the "Abstract" and "IMD Smart City Index" were written by all authors. M.M.M. wrote "Introduction", K.G. wrote "Warsaw as Case study", K.G., J.A.V. and V.M. wrote "Analytical approaches in Analysing the two Smart City Index Reports (2019–2023)" and C.G. wrote "Discussions and Conclusions". C.G. supervised and edited the text of the manuscript.

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The Downgrade of Bilbao, Spain's Leading Smart City

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Abstract. This article aims to analyse the main variables responsible for the downgrade in the ranking of Bilbao in Spain as the top smart city, according to the International Institute for Management Development (IMD) index. The factors that will undergo rigorous study are those that contribute to either improvement or exacerbation between 2019 and 2023. The objective is to identify the primary causes for the decline in Bilbao's ranking places. This research may be of interest to cities seeking to enhance the quality of life for its residents by gaining insights from this report. This study examines the primary enhancements and failures that the city has implemented in certain areas. Gaining knowledge on how to prevent these failures and implementing enhancements in future urban areas is significant and remarkable.

Keywords: Smart city · Urban · Sustainability · Health and safety · Mobility · Technology · Governance · Liveable

1 Introduction

A smart city is a place where human and social capitals as well as a robust communication infrastructure (ICT) contribute to both economic progress and an improved quality of life and happiness of people [1–7]. A city is also smart where individuals can conveniently access all necessary destinations by either walking or using environmentally friendly public transportation. A smart city is also characterised by its devotion not only to competitiveness [8], but also to sustainability, prioritising environmental care and demonstrating knowledge of its own pollution emission [9]. Various research across several disciplines attempted to provide a clear definition of a smart city by identifying and categorising its associated factors and features. Nevertheless, the literature concurs in delineating the key aspects that a smart city must encompass, namely an effective health and safety infrastructure, a well-functioning public transport system, engaging recreational options and environmentally friendly areas for the residents, provisions for job seeking and educational grants, and a responsible and open governance.

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O. Gervasi et al. (Eds.): ICCSA 2024 Workshops, LNCS 14823, pp. 79–95, 2024.
https://doi.org/10.1007/978-3-031-65329-2_6

In their study, Harrison et al. [10] provided a definition of a smart city, as the need to increase the urban smartness, by integrating its physical, social, commercial, and information communication technology (ICT) infrastructure. Kondepudi [11] defines a smart city as a modern city that needs ICT to enhance the quality of life and public services for its citizens. These two definitions illustrate that a smart city is a technologically advanced urban environment that incorporates information and communication technology (ICT) to enhance everyday activities and the well-being of its residents. However, the current idea of "smart cities" has become associated with city rankings, which serve as the most influential and efficient tool for driving economic, social, and spatial developments in cities. Giffinger et al. [12] provided an initial definition of a smart city as the integration of i) ICT, ii) data, iii) actions taken by decision makers, iv) economy and v) the well-being of the residents themselves. This integration leads to a sustainable development over time and encompasses six key pillars: Smart Economy (competitiveness), Smart People (social and human capital), Smart Governance (participation), Smart Mobility (transport and ICT), Smart Environment (natural resources) and Smart Living (quality of life).

The "smart cities" concept proposed by Dashkevych et al. [13] encompasses various identification criteria that include the key aspects of sustainable development (environment, society, economy, and technology). These criteria are directly linked to enhancing the overall quality of life for citizens. The suggested classification [14] differs from traditional Smart Cities categorizations, in which some categories contain more metrics than others, and many metrics are general technological measures not directly related to human well-being. Correia et al. [15] propose composite indicators to define and classify a smart city, firstly based on the respective smart city category of the projects (ultimately related to the smart city conception phase) and secondly considering the population density of each area (organised by classes). This prevents smaller cities from often being overlooked and disregarded when discussing smart cities. The ranking incorporates both smaller and medium cities, emphasising the notion that significant choices made in smaller cities may have a greater influence than those made in medium cities. This approach introduces new insights to the ongoing debate on the essential characteristics of a smart city. City rankings are important because they serve as a tool that depends on urban expertise and the capacity to use the findings efficiently. City rankings are a valuable and efficient tool for guiding economic, social, and spatial processes in cities. They provide recommendations for researchers and analysts involved in the design and methodology of city rankings, as well as for local governments and stakeholders regarding the reasonable management of the results [16].

Starting from assumptions, this study aims to evaluate the reasons for Bilbao's decline in the International Institute for Management Development (IMD) smart city index, specifically examining the causes for its shift from being the leading smart city in Spain to the 27th best in the world. To achieve these goals, the paper is organised as follows: section two describes the case study, the third section explains the methodology, the fourth part analyses the results and finally, a general conclusion will be described.

2 Case Study

Bilbao, situated in the northern part of Spain (Fig. 1), is the most densely populated city in the province of Bizkaia and in the Basque region. Additionally, it is the biggest city in northern Spain and the tenth-largest city in the country, with a population of 347,000 residents (2023), resulting in a density of 8,339 inhabitants per square kilometre.

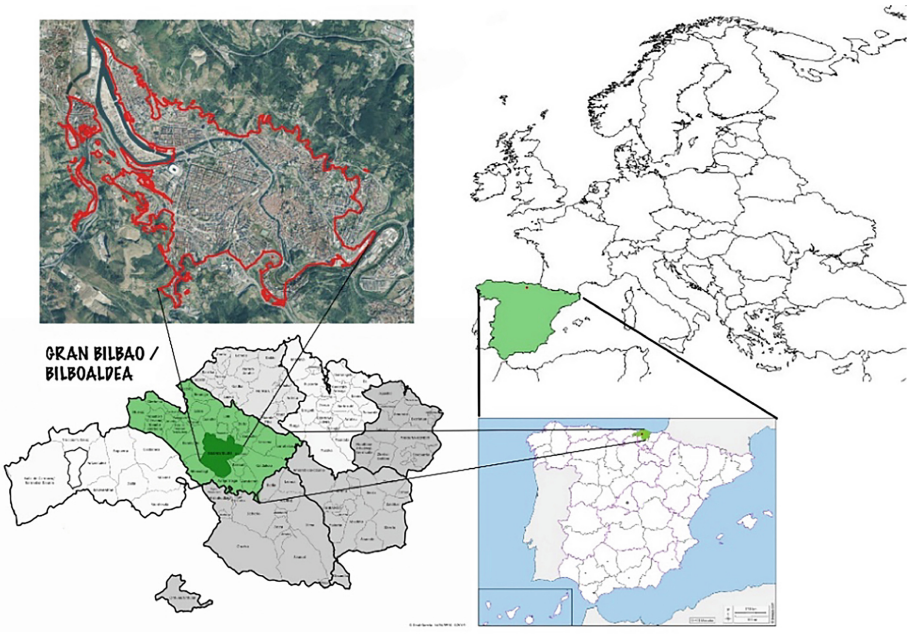

Fig. 1. Map of Europe, Spain, Province of Bizkaia and finally the city of Bilbao.

Furthermore, considering the metropolitan region, the population significantly grows, surpassing one million residents. Recent data from the Spanish National Statistics Institute reveals that Bilbao covers an area of approximately 41 km^2. Although Bilbao is relatively small in size, it serves as a crucial focal point for cultural, economic, and political endeavours in the Basque Country. The city is geographically positioned about 14 km to the south of the Bay of Biscay, providing direct access to the Atlantic Ocean. This geographical advantage greatly strengthens its importance as a marine gateway. The urban environment of Bilbao is characterised by its cutting-edge infrastructure, prominently including the world-famous Guggenheim Museum. This architectural masterpiece serves as a symbol of the city's dedication to contemporary design and cultural revitalisation.

This paper examines a Spanish city due to the European Union's designation of the Iberian Peninsula as an energy island with the ability to meet its own energy needs. Consequently, the towns in this region are prime candidates to become highly advanced smart cities.

Bilbao is an ideal city in Spain for promoting and implementing green infrastructures and technology due to its optimal size, which may serve as a model for other cities. It has also the potential to serve as an ideal urban environment for testing and evaluating innovative technologies on a smaller scale. The tables below (Table 1 and Table 2) show the IMD smart city index rankings for 2019 and 2023, highlighting the decline of Bilbao in the rankings and identifying the new cities that have surpassed Bilbao. A more comprehensive study of the ranking will be conducted later in the methodological approach section.

Table 1. IMD Smart City Index 2019 [17]

IMD Smart City Index 2019			
1. Singapore	4. Geneva	6. Auckland	8. Helsinki
2. Zurich	5. Copenhagen	7. Taipei City	9. **BILBAO**
3. Oslo			10. Dusseldorf

Table 2. IMD Smart City Index 2023 [18]

IMD Smart City Index 2023			
1. Zurich	8. Helsinki	15. Amsterdam	22. Auckland
2. Oslo	9. Geneva	16. Seoul	23. Wellington
3. Camberra	10. Stockholm	17.Dubai	24. Brisbane
4. Copenhagen	11. Hamburg	18. Sydney	25. Shanghai
5. Lausanne	12. Beijing	19. Hong Kong	26. Reykjavik
6. London	13. Abu Dhabi	20. Munich	27. **BILBAO**
7. Singapore	14. Prague	21. New York	28. Vienna

In order to properly understand the ranking, it is important to be aware of the specific parameters used by the IMD index to categorise the cities included in the ranking. After analysing the particular variables surrounding each indicator associated with the cities, a comparison will be conducted to identify any changes that have impacted the city of Bilbao over the past few years. This analysis aims to provide justification for the city's decline in the ranking. The analysis will provide a logical explanation for the fluctuations in indicators that have occurred due to changes in government and extraordinary circumstances over the past four years. The most prominent instance is the COVID-19 pandemic, which had a significant impact on the economies and politics of all governments and cities worldwide.

3 Methodological Approach

Rankings are an effective method for assessing smart cities because they provide an evaluation of the fundamental concept and its first development. Additional rankings, such as the IESE Cities in Motion Index conducted by the University of Navarra, as well as others conducted by various institutions, exist. This study uses the IMD rank due to its comprehensive analysis of a larger number of metrics and cities compared to other rankings. The research focused on particular ranking indicators that have the greatest impact on Bilbao's decline in position. These indicators are closely aligned with the goal of prioritising the evaluation of citizen well-being.

Bilbao ranked 9th in the IMD Smart City Index 2019, conducted by the prestigious IMD World Competitiveness Centre, a leading business school in Switzerland that is globally recognised. Bilbao is among the top cities on this ranking, surpassing places such as Singapore (1), Zurich (2), Oslo (3), Geneva (4), Copenhagen (5), Auckland (6), Taipei (7), Helsinki (8), and Dusseldorf (10).

The latest research of 2023 studied 141 cities (compared to 118 cities in 2019) and examined the perceptions of 120 inhabitants to assess the cities. Bilbao has dropped to the 27th place in this position.

The World Talent Ranking assesses the degree to which economies experience growth, attract, and retain highly skilled employees. In an ever-changing world where artificial intelligence, robots, and other emerging technologies are reshaping current and future challenges for business, policy makers, and educational institutions, fostering a skilled and knowledgeable workforce enhances competitiveness and fosters sustainable prosperity in the long run. The determination of the criteria for defining a smart city is crucial due to the expected ongoing advancements in technology, which will provide new solutions to urgent global issues such as climate change, inequality, health, and education. However, due to their intricate nature and reliance on insufficient or inconsistent information, these choices can pose difficulties for officials from municipalities, investors, and residents.

IMD Smart City Index Main Parameters:

Health and Safety: The healthcare system in the Basque Country ranks as the second highest-performing in Spain. Nevertheless, after the COVID-19 pandemic, assessments within the healthcare system have declined. Regarding the waiting lists, those in the Basque Country are among the most compact in Spain. The ratio of health professionals to residents is 4.85 staff members per 1,000 persons. The overall feeling of security experienced by inhabitants in this city, as in other parts of the globe, is dependent on the specific neighbourhood they find themselves in. On average, the people of Bilbao rate their city with a score over 6. The poll revealed that over 90% of respondents reported no instances of criminal activity inside the city in the last 4 months. Regarding police efficacy, a majority of over 45% of residents expressed their intention to contact the municipal police, while about 40% said their preference for contacting the Ertzaintza.

Mobility: Bilbao has the most efficient public transport system in Spain, outperforming bigger cities such as Madrid or Barcelona, despite their larger size and population. Private transport is rarely utilised in this city and its predominant mode of transportation

is the underground. The transport system consists of three primary routes that link the outside districts with the city core. It is also capable of facilitating transportation to other communities within the province. In terms of bus transportation, this city has a network of 43 routes and over 500 strategically located stations.

Activities: Bilbao has lately acquired a significant number of green areas for its residents. In the last year, the city has added almost 20,000 m^2 of natural areas, together with 1500 newly planted trees that create a green belt around the city. The municipal government declared that they had opened up 10,873 m^2 of grounds. The government plans also to include 12,566 m of additional green areas with the implementation of the Master Urban Plan in March. The areas are now in various stages of development. The construction of 3,392 m^2 of gardens in the Pinar de Zorroza group is nearing completion, and an additional 3,464 m^2 will be obtained from various plots in San Ignacio. Regarding cultural activities, residents seem satisfied with the IMD ratings during the years.

Opportunities (Work and School): The Bilbao City Council has implemented new procedures for the recruitment of additional staff. The youth employment strategy aims to enhance their prospects in this area. Bilbao Ekintza, a municipal company that aims to promote the generation of economic and social wealth for Bilbao, develops pragmatic training initiatives as part of the Employment Plan and Youth Employment Plan, aiming to enhance the competencies of unemployed persons engaged in these programmes. The objective is to stimulate job creation and economic growth in Bilbao by adhering to the principles of sustainability, innovation, and collaboration. This will involve prioritising the city's strategic sectors while also focusing on talent retention and development. Additionally, efforts will be made to bridge the gap between young people and the labour market by aligning their personal and professional skills with the needs of businesses.

Governance: The government's official website offers people opportunities to access information and have a comprehensive understanding of how their taxes are being used. Additionally, they consider whether the government values the opinions of its people. Table 3 illustrates the fluctuations in Bilbao's rates from 2019 to 2023, excluding the rank for 2022, according to several elements of the IMD smart city index.

4 Results

This section of the paper examines the reasons for the IMD index's drop from 2019 to 2023. Because these are some of the variables that have either improved or become worse in Bilbao over the past five years, the study analyses them. In addition, as they are the most crucial markers to guarantee inhabitants a decent standard of living.

A. Decline in the Quality of Healthcare Services.

The medical care in Bilbao has declined, as reported by the interviewed people, as a result of reductions in government funding. Research conducted by the Euskadi medical union (EMU) reveal that the COVID-19 crisis has significantly exacerbated the previously existing condition in the community, as shown in 2019 [21].

The main difficulties faced by people include the scarcity of new family physicians in the healthcare system, resulting in a higher number of retiring doctors compared to those entering the profession after graduation [22].

Table 3. IMD Smart City Index 2019 (p. 36) [17], IMD Smart City Index 2020 (p. 26) [19], IMD Smart City Index 2021 (p. 26) [20], IMD Smart City Index 2023 (p. 52) [18].

INDICATOR	Meanings	BILBAO				
STRUCTURES		2019	2020	2021	2022	2023
Health & Safety						
Basic sanitation meets the needs of the poorest areas	If the communities where residents who are in weaker financial circumstances move are equally clean	74.59	77.3	77.4		76.4
Recycling services are satisfactory	If the city has facilities to handle the trash and a good system to assist residents in recycling	77.05	77.7	74.3		76.0
Public safety is not a problem	Is it safe to walk at night in every street and neighbourhood and if there is enough police	59.70	64.3	64.3		62.2
Air pollution is not a problem	The quality of the air of the city is good for the health of the citizens and for the environment	51.37	53.1	52.6		50.2
Medical services provision is satisfactory	The city has enough hospitals or ambulatories to take care of all the population	75.14	78.0	75.1		69.0
Finding housing with rent equal to 30% or less of a monthly salary is not a problem	Is it possible to pay rent inside the city without using the biggest part of your monthly salary	x	27.6	27.8		25.4
Mobility						
Traffic congestion is not a problem	If the most used roads and streets have a normal traffic quantity to be able to reach your destination without congestion	43.17	44.0	47.8		47.0
Public transport is satisfactory	The public transport of the city is enough to go to all the parts of the city and it is fast. Also the frequency is good and they have a good app to help citizens to reach their destination	81.97	82.4	81.4		82.8
Activities						
Green spaces are satisfactory	The city has enough parks and trees to walk around and have a break	77.87	76.6	77.1		78.9
Cultural activities (shows, bars, and museums) are satisfactory	The city has bars, cinemas, museums, theatres to supply to the citizens cultural entertainment	81.28	80.3	80.8		84.0

(*continued*)

Table 3. (*continued*)

INDICATOR	Meanings	BILBAO				
STRUCTURES		2019	2020	2021	2022	2023
Opportunities (Work & School)						
Employment finding services are available	The city has a good system to help citizens to find jobs	74.45	73.8	75.5		75.4
Most children have access to a good school	The public schools are good enough to ensure a good education to all the children of the city. No matter how much money they have their families	78.83	78.7	76.3		76.2
Lifelong learning opportunities are provided by local institutions	If the universities or study centres are able to offer learning opportunities to the citizens during the time they live	80.60	81.0	77.4		76.2
Businesses are creating new jobs	If the businesses are creating new kinds of jobs according to the new studies and careers	54.37	50.2	49.3		50.9
Minorities feel welcome	In the city the minorities feel comfortable and don't have problems with the rest of the citizens	65.57	62.9	63.1		63.8
Governance						
Information on local government decisions is easily accessible	It is easy to know about what the government is doing or going to do with the city to improve the citizens lives	60.93	62.1	61.8		61.9
Corruption of city officials is not an issue of concern	If around the people who manage the city there is no corruption	50.14	53.1	52.6		51.6
Residents contribute to the decision making of local government	If the citizens are able to take part in the decisions for improving the city	51.37	49.3	50.1		48.4
Residents provide feedback on local government projects	If citizens are used to giving their impressions about the decisions taken by the government	61.48	58.3	56.1		54.9
TECHNOLOGIES		2019	2020	2021	2022	2023
Health and safety						
Online reporting of city maintenance problems provides a speedy solution	If the government could help the citizens using online ways, it could be faster and easier for all	59.97	60.0	54.3		55.4
A website or app allows to give away unwanted items to other city residents	If the citizens could shop or sell the things, they do not want the easier way possible	53.83	53.4	54.6		55.8

(*continued*)

Table 3. (*continued*)

TECHNOLOGIES		2019	2020	2021	2022	2023
Free public Wi-Fi has improved access to services	If the city could offer free WiFi for the citizens in public areas, for all the people to have access to it	62.16	60.4	58.4		58.7
CCTV cameras make residents feel safer	If the city has vigilance, the citizens won't be afraid of walking in the night alone or in more conflicted areas	51.09	51.2	50.1		50.3
A website or App allows effective monitoring of air pollution	If the govern could offer an App for monitoring the air pollution the citizens could choose to go to the place they prefer the most	50.00	50.5	47.3		43.2
Arranging medical appointments online has improved access	This could help the people on their medical issues and the medical system stop to be collapsed	76.50	75.2	71.0		68.0
Mobility						
Car-sharing Apps have reduced congestion	If this type of App is improved it could help with all the problems that are caused by cars, such as traffic jams, pollution…	45.22	45.3	42.5		47.2
Apps that direct you to an available parking space have reduced journey time	You can go directly to a parking lot with available places and not waste time or fuel looking for one free. It will help with the pollution and the traffic congestion too	52.05	51.3	47.8		48.6
Bicycle hiring has reduced congestion	The improve of the bicycle in the city help the environment and the traffic jams to be reduced	58.47	60.1	61.8		60.7
Online scheduling and ticket sales make public transport easier to use	The new Apps for the public transport help the people to know what bus or train they had to catch and pay it in a easier way	74.73	73.6	71.4		72.7
Activities						
Online purchasing of tickets to shows and museums has made it easier to attend	The websites of the touristic places help them to make themselves known for more people	83.33	83.5	82.7		82.5
Opportunities (Work & School)						
Online access to job listings has made it easier to find work	This kind of websites and list could help the people to find a work faster than in the traditional way	69.77	67.5	62.5		65.1

(*continued*)

Table 3. (*continued*)

TECHNOLOGIES		2019	2020	2021	2022	2023
IT skills are taught well in schools	Informatic technologies are a very important skill for the students, so if they are well teaching in the school in the future those children will had more capacity in the using of a computer	65.16	64.4	63.4		62.7
Online services provided by the city has made it easier to start a new business	The advantages of the IT (Information technologies) in the online services help the citizens in their issues when they need information about starting a new business	59.02	58.8	54.3		52.3
Governance						
Online public access to city finances has reduced corruption	The local government publishes the financial data managed by the city council, with the aim of being more transparent to citizens	46.17	44.4	41.6		41.7
Online voting has increased participation	With online voting, the number of people who want to vote has increased	43.85	46.0	42.9		42.7
An online platform where residents can propose ideas has improved city life	This online resource in which citizens can propose new ways to improve the city	58.33	59.7	58.7		56.1
Processing Identification Documents online has reduced waiting times	With the new online identification methods, people in the city avoid having to go in person and can carry out their transactions online	63.66	64.9	65.3		65.4

Healthcare professionals are reluctant to work inside the oppressive Osakidetza system (institution created in 1984 in charge of the public healthcare system in the autonomous community of the Basque Country), prompting many to transition to fields with less round-the-clock shifts, private healthcare sectors, or even seek opportunities abroad where they may get better treatment [23]. Prior to the COVID-19 epidemic, over 4,000 certificates were granted to community members for employment in foreign countries, all of whom were negatively impacted by the aforementioned issue of poor working conditions.

In addition, after the 2010 crisis that impacted the whole of Spain, the funding given to healthcare has seen a significant reduction. As of the start of 2021, a significant 58% of employees within the Basque health system were employed on temporary contracts, despite possessing over 8 years of professional experience.

In comparison to the 2019 data, the healthcare taxes allocated in the Basque Country are 2% points lower than the allocation made by the European Union. Therefore, in order to meet the European average, the healthcare budget in the Basque Country would need to be increased by 40%.

The hospital employment rate is lower compared to other European countries, with just 3.6 health professionals per 1,000 residents, whereas the European average is 8.8 per 1,000.

B. The Excessive Rental Costs for Houses.

During the previous four years the conditions and rates to rent a property in the city of Bilbao have grown unequal. The primary factor is the city's high level of tourism and the preference of citizens who own secondary homes to rent them out as tourist apartments. This allows them to generate higher income compared to renting to students or professionals who need to reside in Bilbao for educational or work-related purposes.

Additionally, the city's restricted urban space in the centre region is due to its mountainous surroundings, leaving the only viable option for expanding the metropolitan area on the opposite sides of the mountains. The demand for homes in the city centre has increased due to people's preference for living there, as it offers proximity to both their workplaces and social amenities. Consequently, this leads to an escalation in housing prices.

According to the Department of Territorial Planning, Housing and Transport of Spain, Bizkaia in Basque language has the highest number of uninhabited houses, with a total of 6707. Most of these houses are located in the metropolitan area of Bilbao. It is worth noting that these houses are primarily rented out as tourist apartments. This condition is exacerbating the rising costs of rental rates in the city. The current public administrators decided to impose taxes on homeowners whose properties are potentially rentable, beginning in 2024. In light of the tourist issue, it is more usual to see various indicators such as AT ("apartamento para uso turístico", apartment for tourist use), VT ("vivienda para uso turístico", housing for tourist use) or HT ("habitación de vivienda particular para uso turístico", room in a house for tourist use) displayed in the corridors of many downtown residences, denoting their status as tourist accommodations.

These flats are considered legal because they are controlled by the government and fulfil their tax obligations. However, the issue arises with those units that are being leased in violation of the law. The inspectors saw a discrepancy between the number of units listed on booking platforms such as AirBnb or Booking and the number of flats recorded in their system. it is expected that in the future, the flats offered for rent on the internet were 40% larger than their legally registered size and complied with the present requirements [24]. This scenario is a dual issue, both for the government and for those who lawfully rent out their tourist apartments. The absence of regulation creates a sense of insecurity, leading to a significant loss of consumers. This is mostly due to the fact that potential renters tend to choose for the cheapest options, which often happen to be the illegal ones. While the issue poses a challenge for rental property owners, it has significantly worsened over the past four years for citizens seeking to rent a house for residential purposes. Presently, it is virtually impossible to secure a house in the city centre without incurring a monthly cost of approximately 1,000 €.

The examined indicator, due to its downgrading, suggests that it is possible to rent a property while allocating less than 30% of the monthly income. Evidently, this indicator has deteriorated in 2022, because the mean rental housing price was at 1,103 € per month. Consequently, an individual earning the interprofessional minimum salary would need to dedicate 110% of their income to cover this expense.

C. Traffic Congestion Is Not Something to Worry About.

Bilbao has been actively engaged in the European Mobility Week from the year 2000. Throughout this period, the city has collaborated with the European Commission to achieve the shared goal of implementing optimal strategies to minimise automobile use and thus mitigate atmospheric and noise pollution. The capital city has successfully implemented a measure to reduce the speed limit of all its streets to 30 km per hour. This initiative has earned the city the European Union Urban Road Safety Award, which acknowledges the exceptional and innovative efforts made by local authorities in promoting road safety.

In addition to decreasing the speed limit inside the city, Bilbao has implemented a comprehensive and sustainable mobility strategy aimed at promoting longer and healthier lives for its residents. One notable project, such as "Red de caminantes" [25] or the walkers' network, has developed 15 distinct walking routes to explore Bilbao in a healthy manner. Furthermore, there are supervised walks for students to ensure their safety while commuting to and from school. Another significant initiative involves the closure of major roads in the city centre every Sunday, which were previously congested with cars, in order to promote pedestrianisation. The primary purpose of this is to provide those who have the opportunity to engage in leisurely biking, skating, or walking in the city centre, free from noise pollution and the need to be mindful of traffic. According to research conducted by OCU (Organisation of consumers and users of Spain), the public transportation system in Bilbao is ranked among the top in Spain. The study analysed timeliness and overcrowding in transportation across 21 Spanish towns [26].

Following this organisation (OCU), the tram in Spain is considered the best due to its exceptional performance in terms of punctuality, with only 6% of delays, none of which exceed two minutes. Furthermore, the tram is appreciated for its informative screens and ample available space. In addition, the municipal buses in Spain are also highly regarded, particularly in the cities of Logroño and Pamplona, as they experience a mere 21% of delays. The subterranean system has the second most favourable position in the nation, being topped only by the underground system of Malaga. Despite being somewhat delayed 17% of the time, it achieved the highest ranking in terms of agglomerations.

Another important aspect associated with the lowering of the usage of vehicles within the city is the excellent system of electric bikes, "BilbaoBizi". Bilbao has the European system with the largest bicycle utilisation. The system has had around 5 million utilisations since its establishment, surpassing any other European cities with similar services, with an average of over 20 uses per bicycle on peak hours. Prior to 2018, the service saw an average daily utilisation of 500 on traditional bicycles. By 2022, there will be many occasions when the number of uses will exceed 8,000 or 9,000.

With the addition of a cycling network spanning over 60 km in a city measuring only 41 km^2, the implementation of secure parking in municipal lots, and financial support for the acquisition of electric bicycles, the bicycle has gained significant popularity. It now stands alongside walking and public transportation as the main means of transportation in this city, where 64% of journeys are made on foot, 24% by public transportation, and 11% by car.

This system is very advantageous for intra-city transport. However, this year, the administration of Bizkaia has introduced a new system named "BizkaiBizi" with the aim of linking the neighbouring towns of the metropolitan region to the city core. The Provincial Council of Bizkaia, in collaboration with the municipalities of Barakaldo, Berango, Bilbao, Erandio, Getxo, Leioa, Portugalete, Santurtzi, and Sestao, implemented the BizkaiBizi public bicycle service. The service comprises a fleet of 650 electric bicycles, accompanied by 62 dedicated parking and charging facilities. In the future, this number will increase to 78 anchoring sites, representing the whole of the service. The issue of traffic congestion in Bilbao has significantly diminished with the government's adoption of a new legislation aimed at preserving air quality by reducing harmful emissions inside the city core. Furthermore, the bicycle rental system is implemented both inside the city and its surrounding metropolitan region. This is further enhanced by an exceptional transit and underground system.

D. The Prevalence of Unemployment Increases.

Before 2019, Bilbao's economy had considerable stability, with an unemployment rate that consistently remained below the national average of Spain. The city has evolved into a prominent centre for services, tourism, and culture, generating employment opportunities in several sectors. The employment in Bilbao was significantly influenced by the construction, industrial, and tourism industries.

A critical turning point was achieved in 2020 when the COVID-19 pandemic hit. Bilbao's position became precarious due to mobility constraints, the shutdown of non-essential businesses, and a significant downturn in tourism. Many firms were forced to cancel employment contracts or initiate staff layoffs. The sectors that saw the greatest effect were hospitality, tourism, and culture.

The implementation of pandemic containment measures had a detrimental impact on the local economy, resulting in a significant increase in the region's unemployment rate. People who had previously had secure and dependable employment unexpectedly found themselves unemployed and unable to provide financial assistance for their families. The increase in unemployment has had a significant effect on the residents of Bilbao. People who become unemployed often face financial difficulties and undergo feelings of stress and anxiety.

The uncertainty over the future and the ability to fulfil basic needs may have a significant emotional and psychological impact on individuals and their families. Furthermore, unemployment may lead to a decrease in an individual's self-assurance and confidence, which can adversely affect their mental well-being.

Rising unemployment may also engender feelings of unease and distrust towards the stability of the economy, thereby influencing individuals' choices about investment and expenditure. The local economy may see enduring repercussions from the relentless cycle of unemployment. The whole can therefore be graphically summarised in Fig. 2 in which the data for the previously mentioned items are displayed.

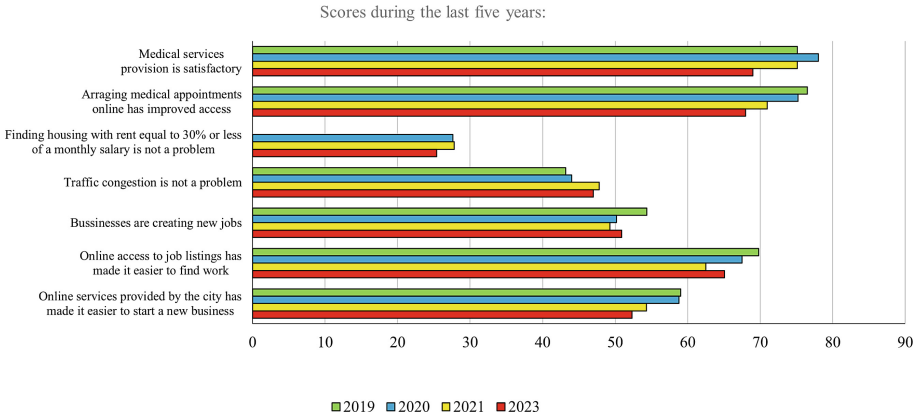

Fig. 2. Visual illustration of the indicators which are analysed from 2019 to 2023.

5 Discussions and Conclusions

This article demonstrates that between 2019 and 2023, the city of Bilbao experiences a decline in the ratings given by its residents. The first aspect is the decline in health services, mostly attributed to the COVID-19 epidemic. Additionally, the reduction in healthcare funding allocated by the state in preceding years has contributed to this situation. Another factor is the adverse working circumstances experienced by physicians, as well as the growing number of newly graduated doctors who choose to pursue their specialisation in a foreign country.

Another issue faced by the residents is the exorbitant rental prices for houses. One of the primary causes of this problem is the limited construction area in Bilbao due to its mountainous location. Additionally, individuals who own second homes in the city often choose to rent them out as vacation houses in order to maximise their profitability. The annual rental cost of the flat exceeds 30% of an individual's monthly income. The last factor that negatively impacted the ranking was the job environment, which was adversely affected by the movement restrictions imposed during the COVID-19 epidemic. Consequently, the local economy suffered significant harm.

The Vasque Government has identified many projects that might assist individuals in addressing these issues. Some of these efforts include:

Harmonise the public expenditure (GDP) of Euskadi with that of Europe by allocating a maximum of 7% of public expenditures on healthcare. Prioritise the use of public health above private health. Enhancing the scope of public health insurance and promoting its use among the population. Ensure universal access to a cost-free, high-quality healthcare system for all individuals. The objective is to provide more employment opportunities and enhance the quality of life for healthcare workers.

As to the findings of the Vasque Government observatory, if tourist residences were subject to appropriate taxation, it would alleviate the strain on the regular rental market. This would result in an increase in the number of available rental properties and a decrease in average rental costs.

The recovery has been systematic despite the allocation of resources towards economic transformation and steps to mitigate the impact. To ensure a robust and enduring recovery, it is imperative for the government, companies, and society as a whole to implement cohesive and synchronised measures to tackle the economic crisis and unemployment in Bilbao. Bilbao's economic outlook is characterised by its potential for adaptability and future resilience. The city of Bilbao has successfully alleviated traffic congestion with the construction of an exceptional public transport system, and the introduction of a new public bicycle service.

In conclusion, the decline in the ranking of Bilbao may be attributed to the issues outlined in this research, which have resulted in a decrease in their scores over the last five years. These are the primary factors contributing to the decline in rankings. Additionally, it is important to consider that in recent years, additional cities have been included in the index, resulting in a little decrease in Bilbao's place on the list.

The difficulties, potential remedies, enhancements, and conclusions outlined in this paper may serve as a valuable source of information and inspiration for other communities facing comparable circumstances. This study can contribute to conducting additional analyses to identify new indicators or modify existing ones for assessing and tracking the effects of technological innovations on the advancement of smart cities and the promotion of sustainable visions [27]. These analyses aim to address concerns related to contemporary society.

Essentially, Bilbao is an ideal city for analysis due to its compact size, which allows for a comprehensive examination of problem-solving and the implementation of innovative urban systems. After conducting an analysis of the impact of the policies implemented in Bilbao, it is possible to extrapolate their applicability to bigger European cities or specific districts within those cities.

Acknowledgments. This study was supported by the technical-scientific collaboration agreement "PON METRO 2014–2020 AXIS 6 - Action CA6.1.1.b - Cagliari smart city: Integration of urban governance with the mitigation of urban heat islands (CA_UHI)" signed between the Municipality of Cagliari and the University of Cagliari (DICAAR - Department of Civil and Environmental Engineering and Architecture).

This study was supported by the MUR through the project "SMART3R-FLITS: SMART Transport for Travellers and Freight Logistics Integration Towards Sustainability" (Project protocol: 2022J38SR9; CUP Code: F53D23005630006), financed with the PRIN 2022 (Research Projects of National Relevance) program. We authorise the MUR to reproduce and distribute reprints for Governmental purposes, notwithstanding any copyright notations thereon. Any opinions, findings, and conclusions or recommendations expressed in this material are those of the authors and do not necessarily reflect the views of the MUR.

Author Contributions. This paper is the result of the joint work of the authors. In particular, the "Abstract" "Results" were written by all authors, M.M.M. wrote "Introduction", A.A. wrote "Case Study", C.M. wrote "Methodological approach" and C.G. wrote "Discussions and Conclusions". C.G. supervised and coordinated all paper.

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Mitigating Risks in Pedestrian Pathways of Railway Station Districts: A Parma Case Analysis.

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Abstract. Enhancing walkability can involve optimizing pedestrian movements, ensuring both convenience and safety. This proves to be particularly relevant in the context of railway stations as they can be identified as collectors of urban mobility flows and at the same time as central and interconnected urban spaces, able to give integrated responses to new social needs linked both to daily life and tourism. Thus, enhancing active mobility in these areas includes facilitating seamless access to the station, platforms, and surrounding areas, thereby promoting sustainability in transportation, encouraging an active lifestyle, and enhancing the overall experience for railway station users. To address walkability risks within railway station districts, the study seeks to contribute to minimising security risks and optimizing safety perceptions on pedestrian paths and crossings. Leveraging the Parma case study, the research introduces a methodology for evaluating walkability within a specified buffer zone around the station, using two Key Performance Indicators (KPIs) defined as Safety and Security, applied to the pedestrian network graph. The research proposes a methodology considering specific factors relevant to the Safety and Security KPIs. The results highlight critical issues within the study area, pinpointing high-risk zones through graphical representation. Results might help prioritising interventions, providing essential support for sustainable mobility planning. Future research endeavours will encompass an expansion of the analysis with additional datasets, aiming to identify further essential KPIs for assessing walkability comprehensively.

Keywords: GIS · Walkability · Safety and Security · Railway Station District

1 Introduction

In recent years, there has been an increasing emphasis on the principles of sustainable urban development and mobility, as outlined in Sustainable Development Goal No. 11, and exemplified by major metropolitan cities such as Barcelona, Paris, and Milan [1–4]. This shift in paradigm, underlining the significance of prioritizing sustainable and active mobility as a primary mode of transportation, is widely recognized in the scientific

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O. Gervasi et al. (Eds.): ICCSA 2024 Workshops, LNCS 14823, pp. 96–113, 2024.
https://doi.org/10.1007/978-3-031-65329-2_7

community [i.a. 5, 6]. Walking, specifically, emerges as a central element not only for its environmental benefits but also for its substantial positive influence on individual health, encompassing both mental and physical well-being, as well as overall quality of life [i.a., 7–10].

Integration of spatial planning and urban planning, as advocated by several scholars [i.a. 11], is key to achieving sustainable urban mobility. Thus, concurrent with this transition is the imperative to regenerate public open spaces and pedestrian paths to foster safer, more appealing, and comfortable active mobility travel [12–14].

Acquisition and assessment of comprehensive data pertaining to the urban context and attributes of pedestrian infrastructure becomes a key element for identifying critical scenarios and planning effective strategies and interventions. Despite the abundance of literature presenting methodologies for studying and assessing walkability [i.a. 15–18], a universally adopted approach remains elusive [19]. While many existing methodologies share similarities, none have achieved widespread adoption. Moreover, comprehensive methodologies offering a holistic perspective on walkability are relatively underexplored and underutilised. The challenge inherent in this more holistic approach lies in the intricate nature of data collection and the complexities in its practical application by public administrations and stakeholders.

Within this framework, the authors have developed a methodology to evaluate the pedestrian infrastructure, providing insights into the urban environment's efficacy in promoting and facilitating pedestrian mobility. The research focuses on delineating criteria and Key Performance Indicators (KPIs) rooted in the principles of accessibility, safety and security, inclusive design, and enjoyment.

This contribution presents the methodology for calculating the defined KPIs of Safety and Security and its application to the case study of the station district of a medium-sized city in the Emilia-Romagna region, Parma. The KPIs of Safety and Security assess the safeguarding level for pedestrians within the urban environment, identifying potential risks and ensuring a secure experience for users. This aspect of walkability proves to be of particular relevance in the surrounding area of train stations and transit environments [20–23] as they can be identified as collectors of urban mobility flows and at the same time as central and interconnected urban spaces, able to give integrated responses to new social needs linked to daily life and tourism.

The paper is structured as follows: Sect. 2 describes a literature review focusing on relevant features for evaluating safety and security, and the station district delimitation. Section 3 outlines the proposed methodology for calculation of the Safety and Security KPIs. Section 4 introduces the case study district and presents the methodology's application results. Finally, Sect. 5 provides conclusions on the methodology's application to the proposed case study, highlighting its strengths and limitations, and suggests potential avenues for further research.

2 Literature Review

2.1 Factors Affecting Safety and Security

As highlighted in the introduction, various methodologies have been employed to assess walkability in urban areas [24]. Within this context, road safety and protection from crimes (i.e. social security) emerge as distinct yet essential factors shaping individuals' inclination towards active modes of transportation. Indeed, the susceptibility of pedestrians and non-motorized users to road accidents [25], as well as the documented correlation between personal security perceptions and transportation choices, [26, 27] are well-documented in the literature.

The table provided below (Table 1) outlines the principal characteristics of both the urban environment and pedestrian infrastructure deemed significant in enhancing safety and security aspects of walkability, as discussed in the literature.

Regarding the improvement of road safety, central elements include reducing speed limits alongside safeguarding the pedestrian infrastructure from vehicular traffic. As emphasized by the Mid-American Regional Council (MARC) [28], heightened vehicle speeds amplify the risk of accidents, as faster speeds diminish drivers' capacity to identify and evade potential conflicts [31]. Furthermore, high-speed collisions between pedestrians and vehicles increase the probability of fatal outcomes [30, 31]. Consequently, when speed reduction efforts [32] are not possible, it is important to incorporate protective features for areas dedicated to vulnerable users (e.g., kerbs, bollards, trees, etc.) [28, 33–35].

Alongside the aforementioned factors, another relevant element for ensuring road safety is the presence of dedicated signage and markings [28, 36–38] as these elements enable pedestrians and other road users to clearly identify the dedicated area for pedestrian movement and crossing.

Regarding pedestrian crossings, safety can be further enhanced by increasing visibility through measures such as curbs extensions to restrict vehicle transit areas and removing obstructive elements like parked cars or urban furniture [28, 32, 37–40]. Additionally, improving lighting systems is crucial to ensure that pedestrians are visible to approaching vehicles [28, 32]. The installation of traffic lights also plays a significant role in promoting safer crossing experiences [33, 38, 40].

An important aspect to consider regarding crossings is their typology, which impacts both safety and security. Raised crossings enhance pedestrians' visibility for vehicle users while also compelling vehicles to reduce speed near them [28, 33, 37, 39, 41, 42]. Conversely, pedestrian overpasses and subways completely separate pedestrians from vehicles, allowing safety during crossings of high traffic roads but potentially impacting social security [32, 43, 44].

Lastly, other elements related to social security on pedestrian paths include adequate lighting [24, 45–47] and the vibrancy of the street environment [47–49].

Table 1. Literature review on factors affecting road safety and social security.

Factor	References
Vehicular speed limit	[28–33]
Protection from vehicular traffic	[28, 33–35]
Signage and Markings	[28, 36–38]
Crossing visibility	[28, 29, 32, 37, 38, 40]
Traffic light	[33, 38, 40]
Crossing typology (road level or raised)	[28, 33, 37, 39, 42]
Crossing typology (overpass or subway)	[32, 43, 44]
Lighting	[24, 45–47]
Road vitality and economic activities	[47–49]

2.2 Station District Definition

The concepts of safety and security assume a peculiar meaning when applied to the area surrounding metro or railway stations [50]. The station and its surroundings are places where different needs take places and where the conflict between the mobility infrastructure and the city is more intense [51]. This complexity is reflected in the duality infrastructure node/urban place which constitute one of the main conceptual frameworks used in literature to explore the issue [52, 53]. In fact, the station neighborhood is the urban area where the integration of mobility and urban development agendas is more needed, not to mention other social, economic, and cultural aspects [54]. Transportation nodes attract and concentrate different flows of diverse users and travelers, according to its relevance [55].

To delineate the boundaries of the station environment, Bertolini [52] and Pucci [56] suggest several approaches. These include defining a walking radius of influence based on time or distance, investigating historical form or topographical landmarks, identifying an urban transect centred around the station, or considering a defined perimeter for transformation or redevelopment projects. However, despite these proposals, the definition remains ambiguous and does not clearly establish the limits of this context. Yang also identifies a possible way to assess a station area of influence by determining a suitable walking distance to access the station, with additional other approaches emphasising criteria such as urban compactness or focus on specific urban design features [57].

In conclusion, for the purposes of this study, the station district area is delineated using a 1-km isoline originating from the station and distributed along the road graph. This isochrone corresponds approximately to 15-min walk at a 4 km/h speed. This choice does not take into account impedance factors, such as lower speeds of vulnerable users (elderly people, children) and is purposedly made to consider the broadest possible area of analysis.

3 Materials and Methods

This section describes the methodology used for calculating the KPIs of Road Safety and Social Security respectively.

As previously stated, the KPIs of Safety and Security assess the protection level for pedestrians within the urban environment by identifying potential risks and ensuring a secure experience for pedestrians. The Road Safety KPI focuses on assessing conflicts with motor vehicles and the risk of road accidents, while the Social Security KPI concentrates on factors related to the sense of social security, such as exposure to potential crimes (e.g. theft or vandalism).

The aim of this methodology is to create a systematic data collection protocol that can ensure adaptability, reproducibility, and transferability to other urban contexts. Thus, some of the attributes listed below could prove to be less relevant in specific urban contexts and be excluded from the calculation of the KPI to make it more adaptive in relation to the characteristics of the area.

To assess the degree of safety and security of the pedestrian infrastructure, a comprehensive approach is adopted, based on a review of the scientific literature (Sect. 2.1). This guides the development of a systematic data collection protocol, which includes searching for data from official sources and carrying on remote and in-field inspections. Furthermore, the observation phase is useful to grasp features, vulnerabilities, and peculiarities of paths at different scales. Surveys' results are then represented through a graph structure.

Subsequently, the assessment process assigns a numerical value to each of the domains of factors analysed by the data collection protocol. The highest value within each domain identifies the optimal condition for promoting road safety or social security (e.g. presence of lighting along the path). However, in certain instances, the maximum value identified within the domain corresponds to 0, for example with signage and markings, whereas present. This occurs when the characteristics being studied are tightly regulated by existing standards, indicating that they should already be met in the construction phase. These numerical values are then used to calculate the KPIs.

The attributes of pedestrian infrastructure and its urban context considered for these calculations are listed in Table 2, and further classified for each individual KPI.

While most factors are determined by assigning specific levels to the analysed characteristics, the Facilities density factor involves a spatial analysis using buffer areas. A 15-m buffer is applied from the path segment, and the count of services within each buffer is calculated. This enables the identification of services along each segment of the pedestrian infrastructure. Subsequently, the number of services is divided by the length of the segment. The resulting value is then normalized between 0 and 1 relative to the maximum density identified across all segments in the city under study. Services considered for this Security KPI include services where people gather and remain open in the evening hours, such as catering activities and commercial activities fostering social presence along the path (i.e. shops).

As evidenced by the attributes list under consideration, it is useful to provide a differentiation criterion based on the segment type, to distinguish between segments representing pedestrian paths and those representing pedestrian crossings. This subdivision is justified by two main considerations: firstly, the distinct attributes characterizing

Table 2. Safety and Security KPIs - Evaluation criteria adopted, and values assigned.

KPI	Attributes	Evaluation	Values
Road safety	Protection from vehicular traffic	High or no interaction	1
		Medium	0
		Low	−1
		Absent	−2
	Speed limit	None	2
		30 km/h	1
		50 km/h	−1
	Crossing location	Road level	−1
		Artificial bump	1
	Crossing visibility	High	1
		Medium	0
		Low	−1
	Traffic light	Yes	1
		No	0
	Signage	Yes	0
		No	−1
	Markings	Yes	0
		No	−1
Social security	Crossing location	Overpass	−1
		Subway	−1
	Lighting	Yes	1
		No	−1
	Facilities density (Food services + Shops)	Number of facilities/segment length	

crossings require a separate analysis from other segments, respecting the presence of certain specific characteristics that relate exclusively to pedestrian crossings. Secondly, crossings emerge as critical points associated with a higher risk in interactions among vehicles and vulnerable users, whereas interaction with vehicles should be restricted or absent in pedestrian paths. Thus, for the assessment of the Safety and Security KPI, pedestrian paths and pedestrian crossings are considered separately.

The table below (Table 3) delineates the attributes considered for each segment type (i.e. paths and crossings).

Each KPI is respectively derived by calculating the average of the appropriate factors.

The values obtained, for both KPIs, are then normalized between 0 and 1 based on the maximum and minimum values obtained through the calculation. The normalization

Table 3. Selection of distinct attributes for pedestrian paths and crossings.

KPI		ATTRIBUTES	CRITERIA	
			PATH	CROSSING
SAFETY AND SECURITY KPIs	Road Safety	Protection From Vehicular Traffic	•	
		Speed Limit	•	•
		Crossing location		•
		Crossing visibility		•
		Traffic Light		•
		Signage	•	•
		Markings	•	•
	Social Security	Crossing location		•
		Lighting	•	•
		Facilities Density (Food Services + Shops)	•	

process standardizes data, facilitating equitable comparisons across diverse KPIs (i.e. for paths and crossings) and enabling a more precise assessment of overall performance. This systematic approach ensures a comprehensive evaluation by accounting for variations in scale and magnitude, thereby enhancing robustness and reliability.

For the analysis of the designated case study and the graphical representation of associated maps, pertinent data are systematically gathered from various official sources. These sources include the Geographical Information System managed by the Municipality of Parma and the Geoportal administered by the Emilia-Romagna Region. They provide cartographic data on buildings, road networks, railway lines, road accidents, urban lots, green areas, and water bodies. Public data sources, such as OpenStreetMap, are accessed to identify existing public facilities, secondary schools, and commercial establishments. Specifically, for commercial services, information is extracted from the Points of Interest (POIs) layer in OpenStreetMap. The focus is on services with attribute codes 23xx and 25xx to ensure a targeted and relevant dataset for the Social Security KPI. Furthermore, data on pedestrian paths and crossings, along with their attributes, are collected through on-site surveys conducted by the authors.

4 Results and Discussion

4.1 Case Study: Parma's Railway Station District

The case study selected for testing the methodology involves the surrounding area of Parma's railway station, situated in the Emilia-Romagna region of Italy, within a 1-kilometre isoline from the station (Fig.1).

Parma serves as the capital of the province and is categorized as a medium-sized city (approximately 198,000 inhabitants in 2023 [58]), easily accessible on foot due to its size and layout.

Renowned for its historic landmarks, including monumental buildings, museums, and theatres, as well as its food and wine productions, the city notably held the title of European Capital of Culture for the two-year period spanning 2020 and 2021 [35]. Parma attracts a significant influx of tourists, with nearly 400,000 visitors annually, a figure steadily increasing according to statistics from the Emilia-Romagna Region [59].

Moreover, Parma is recognized as a university hub, boasting a student population of 30,600 as of 2021 [60], including a considerable number of non-local students. Additionally, as the provincial capital, Parma also draws secondary school students from surrounding areas.

The railway station in Parma is a medium to large-sized facility, accommodating a daily average of passengers ranging between 10,000 and 25,000 [61]. Strategically positioned on the periphery of the city's historic walls, the station can potentially make the city centre easily accessible on foot.

Fig. 1. Parma's railway station. Source: authors' elaboration.

The area surrounding the railway station (Fig. 2) includes four districts of the municipality of Parma: Centro Storico (south-east), Oltretorrente (south-west), San Leonardo (north), and Pablo (north-west). The urban fabric is characterized by predominantly residential buildings, while economic activities are primarily concentrated within the historic centre and along via Trento, extending northwards from the station.

Relevant public facilities within the study area include a secondary school and one of the University of Parma's premises. Furthermore, extending the walking time from the station by two minutes grants access to the University of Parma's headquarters, and seat of the Faculty of Law.

In terms of mobility, the case study area experiences various restrictions on motorised private vehicles. Specifically, the entire Centro Storico district, along with a portion of the Oltretorrente district and the immediate vicinity of the train station, are subject to limited traffic (Limited Traffic Zone - LTZ). Moreover, vehicular mobility faces an added constraint due to the presence of a 30 km/h speed restriction zone (Zone 30) in the northeastern part of the San Leonardo district. Regarding the infrastructure network related to active mobility, a preliminary assessment confirms its extensive coverage throughout the study area, potentially providing a high level of pedestrian accessibility.

In terms of traffic accidents, an analysis of pedestrian-related road accidents from the year 2022 [62] shows numerous crashes within the study area, with a notable concentration near the station and along the via Trieste Road axis.

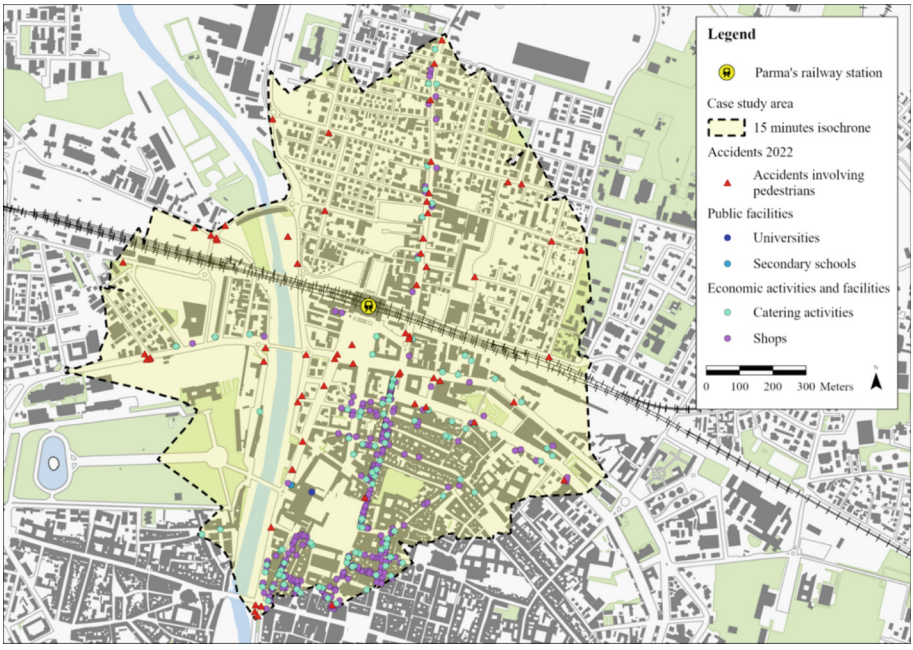

Fig. 2. Case study area with relevant data considered. Source: authors' elaboration.

4.2 Safety and Security KPIs Assessment Results

As previously defined, the Safety and Security KPIs encompass complementary aspects. Firstly, the results obtained for each KPI are presented, followed by an analysis of the

overall values assigned to each segment of the pedestrian infrastructure for the Safety and Security KPIs.

The results are visually represented using a natural interval scale (Jenkins) and a graduated colour scale ranging from red (highlighting critical segments) to green (indicating segments with favourable characteristics). To enhance clarity in distinguishing between pedestrian paths and crossings, it is decided to represent the latter using point geometry.

The analysis of the Road Safety KPI (Fig. 3) reveals that segments linked to pedestrian paths, situated south of the railway line and east of the Parma River and encompassing the Centro Storico district, are characterised by an overall good level of road safety. Furthermore, as previously mentioned, the area is also included within the LTZ, resulting in reduced vehicular traffic flows. Additionally, further improvement is anticipated with the implementation of a Zone 30 in this area, as indicated by Parma's Traffic Management Plan [63], which will further positively impact the assessment of road safety in the area. Critical segments, on the other hand, are primarily located in the northern part of the analysis area, corresponding to the San Leonardo district and northwest of the study area (i.e. Pablo district). However, a notable exception exists within these areas of concern, represented by a small portion of the San Leonardo district located to the northeast, where the level of road safety is notably less critical. This exception is justified by the presence in that area of a Zone 30. It is important to highlight that, despite the critical nature of these segments, except for via Trento, via Venezia, viale Europa, and viale Piacenza,

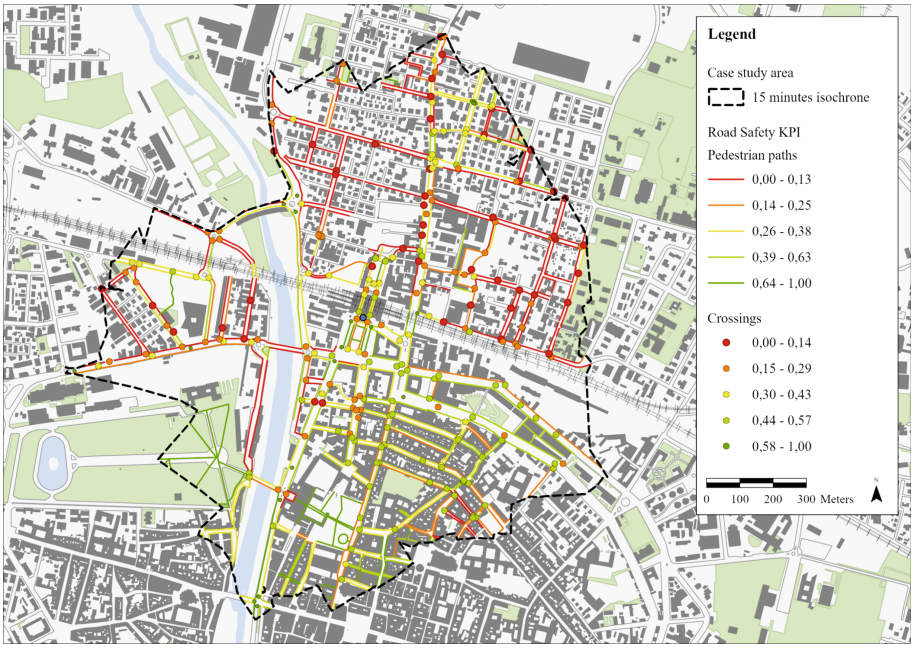

Fig. 3. Road Safety KPI. Source: authors' elaboration.

they are predominantly located within residential areas. Consequently, the vehicular and pedestrian flow along these roads is low, as their local street function suggests.

Turning to pedestrian crossings, the situation closely reflects that highlighted by pedestrian paths. However, it is necessary to emphasize that numerous crossing infrastructures are absent, particularly in the predominantly residential areas within the San Leonardo district. The most critical area is represented by the via Trieste axis where, in addition to a high criticality of pedestrian crossings, numerous accidents involving pedestrians are also recorded. This could be due not only to the limited safety of the crossings but also to a reduced number of crossings or suboptimal location.

Moving on to the Social Security KPI (Fig. 4), it is necessary to begin with a premise regarding the evaluation assigned to pedestrian crossings. Indeed, one of the protocol factors considered (i.e. the presence of pedestrian overpasses or subways) appears to have minimal relevance for this specific study area.

Fig. 4. Social Security KPI. Source: authors' elaboration.

Notably, the area lacks such infrastructure typologies, thereby making the social security assessment of crossings solely reliant on the presence of lighting. Consequently, for this KPI, pedestrian crossings are categorized with values equal to either 0 or 1. As for the evaluation of social security for pedestrian paths, it is possible to highlight how the most critical areas are represented by residential areas where the presence of commercial activities considered by the protocol is absent or extremely reduced. Additionally, a concentration of critical segments and crossings can be noted in the immediate vicinity of the station. This can strongly affect people's propensity to walk, as even a single

portion of the path, albeit limited, if present within the user's route, can compromise their modal choice or lead to route variations that can still discourage walkability. Overall, the outcomes highlight significant disparities between the northern and southern areas of the railway station, outlining distinctive urban peculiarities. These zones are primarily distinguished by their morphological and functional characteristics, revealing notable differences in terms of walkability. The southern portion stands out for its densely compact urban configuration, primarily represented by the historic center, whereas the northern zone is characterized by being a predominantly residential periphery with an industrial history. This diversity in urban contexts is directly reflected in walkability metrics, which are affected by the various morphologies and differing infrastructural provisions, influencing commuting habits and the accessibility of public spaces in both areas. Considering the KPIs, it is possible to observe how the evaluation of segments and crossings in the southern portion of the historic center is less critical than the conditions identified in the northern portion. Nevertheless, a further distinction should be made for the two northern portions of railway station, represented by the San Leonardo district and in a minor part of the northwest portion represented by the Pablo district, as they have the most critical conditions. Additionally, a concentration of pedestrian crossings in critical conditions is also found in the central portion of the study area near the station. Lastly, it can also be noted how the Road Safety KPI shows more critical issues than the Social Safety KPI, as expected given the greater number of factors considered.

The following figures (Fig. 5 and Fig. 6) show some examples of relevant paths and crossing evaluations collected across the station district area.

Fig. 5. Road safety. Frome left to right, examples of pedestrian path values, from excellent to poor. Source: authors' audit.

Fig. 6. Social Security. Frome left to right, examples of pedestrian path values, from excellent to poor. Source: authors' audit.

5 Conclusions

As highlighted in the introduction, promoting active mobility is crucial for achieving broader sustainable development goals. This underscores the need of improving walkability of infrastructures and urban areas. Despite the abundance of literature presenting methodologies for studying and assessing relevant pedestrian infrastructures and urban context characteristics for walkability, a universally recognized approach has yet to be established. Furthermore, public administrations and stakeholders often encounter challenges due to the intricate nature of data availability and collection when implementing such methodologies.

In this context, the aim is to develop a methodology for assessing several aspects pertaining to walkability through a set of KPI, using GIS analysis. The goal is to ensure the adaptability, reproducibility, and transferability of the methodology to other urban contexts. Additionally, this methodology could also guide the programming of public interventions and urban planning decisions. For instance, it could be employed to identify urban areas requiring priority regeneration interventions, enabling local authorities to allocate available resources more efficiently. Furthermore, it could be utilised to expand low-speed zones (30 zones), thereby contributing to improving road safety. Moreover, this methodology could be adopted as a standard protocol for ongoing projects, allowing for ex-ante evaluation and ex-post monitoring. This would enable the monitoring and evaluation of the effectiveness of actions taken to improve urban walkability over time, providing valuable empirical data to guide future interventions and enhance urban policies.

Thus, the paper presents the development of a methodology for calculating the defined KPIs of Safety and Security based on factors identified within the existing literature. These KPIs are developed to identify the major critical points of pedestrian paths and crossings from the perspective of these two complementary themes.

The methodology is applied to the case study of the station district of the city of Parma in the Emilia-Romagna region. Parma's station district, as explained in Sect. 3.2, is of particular interest for integrating urban and mobility aspects related to safety and security due to its localization within the city context and relevant flows that its station experiences. The results of the methodology application validated the consistency of road

safety and social security assessments with the assessed on-field situation. Furthermore, comparing the Road Safety KPI with actual road accidents involving pedestrians further underscored the effectiveness of this tool in evaluating road safety within pedestrian paths and crossings.

However, further research developments could refine the assessment system. Firstly, recalibrating the Road Safety KPI to consider road and pedestrian path typology as suggested. In fact, elements of protection from vehicular traffic may vary in importance depending on the classification of the road and pedestrian infrastructure typology (e.g. virtual footpaths or pedestrian lanes). In this scenario, it might be advantageous to consider these factors in their various combinations to identify optimal and critical conditions. Secondly, the Road Safety KPI could be further implemented through the assessment of wayfinding signage along the path. In fact, the presence of easy-to-understand directions indicated through wayfinding signage allows the user to orient himself in space and to reach different destinations through clear and safe paths.

Thirdly, there is potential to expand the Social Security KPI to encompass additional attributes derived from users' perception of security. This is crucial because areas that meet physical security criteria may still be perceived as unsafe by users. It is then possible to consider additional elements related to the quality of the urban context such as the presence of abandoned areas and buildings, litter, or other degradation elements.

Moreover, an additional development of this study could involve correlating these measurable aspects of pedestrian infrastructure security, as evaluated by the proposed methodology, with statistical data on petty crimes. Conducting a comparative study between infrastructure characteristics and adverse events could refine the model and help prioritize interventions.

Additionally, assessing how results change with varying selected station district areas could be valuable. There is no unique method for considering the station district area, and it would be interesting to explore how different calculation of the station district could add value to the model application.

In its future developments, the methodology plans to consider additional KPIs to cover aspects such as accessibility, enjoyment, and inclusive design, with appropriate datasets and audit protocols. Applying the comprehensive methodology in various case studies could provide support in formulating intervention strategies aimed at improving walkability and planning public space regeneration interventions in a complex interaction area like a station district.

Acknowledgments. This work was supported within the framework of the "Ecosystem for Sustainable Transition in Emilia-Romagna" (ECOSISTER) Spoke 4 and the "Sustainable Mobility Centre" (CNMS) Spoke 9.

Funder: Project funded under the National Recovery and Resilience Plan (NRRP), Mission 4 Component 2 Investment 1.5 - Call for tender No. 3277 of 30/12/2021 of Italian Ministry of University and Research funded by the European Union – NextGenerationEU. Award Number: Project code ECS00000033, Concession Decree No. 1052 of 23/06/2022 adopted by the Italian Ministry of, CUP D93C22000460001, "Ecosystem for Sustainable Transition in Emilia-Romagna" (Ecosister).

Funder: Project funded under the National Recovery and Resilience Plan (NRRP), Mission 4 Component 2 Investment 1.4 - Call for tender No. 3138 of 16/12/2021 of Italian Ministry of

University and Research funded by the European Union – NextGenerationEU. Award Number: Project code CN00000023, Concession Decree No. 1033 of 17/06/2022 adopted by the Italian Ministry of University and Research, CUP D93C22000400001, "Sustainable Mobility Center" (CNMS).

This manuscript reflects only the authors' views and opinions, neither the European Union nor the European Commission can be considered responsible for them.

Disclosure of Interests. The authors have no competing interests to declare that are relevant to the content of this article.

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Key Quality Criteria in an Integrated Multiple Transport Systems Scenario: A Systematic Literature Review

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Abstract. Sustainable mobility represents a paradigm widely shared within the international panorama. It aims to encourage mobility alternatives to private cars, which can reduce externalities associated with transportation, meeting the principles of innovation and efficiency close to the *Smart city* concept. These forms include public transport, non-motorized mobility (pedestrian and cycling) and electric micro-mobility. The quality of these transport systems is one of the main factors influencing the user's transport modal choice. It depends on several factors related to services, infrastructure and the surrounding urban environment. The quality evaluation of public transport has been widely investigated, while that of non-motorized mobility and electric micro-mobility still needs to be explored, especially considering their interaction. This paper presents a systematic literature review fitting into this research area, providing a general overview and a first list of key quality criteria, underlying research gaps to support possible research developments. The proposed approach focuses on the integration of multiple transport systems, trying to understand how to encourage multimodality through the assessment and improvement of the entire travel experience. At the same time, it aims to provide practical tools for triggering regenerative processes in the urban context, which can respond to the new needs of contemporary society referring back to the *Smart city* concept, increasingly oriented toward creating public spaces for people rather than cars.

Keywords: Transport quality · Key quality criteria · Transport planning

1 Introduction

The urban environment relates daily to multiple and unprecedented challenges due to high urbanization and growing population density [1]. These economic, social and environmental challenges highlight how the traditional urban growth model is inadequate to meet the needs of contemporary cities, increasing the pressure that urban centers face. Within the complex urban system, mobility plays a central role in managing these externalities and, in recent decades, has become increasingly associated with the concept of "sustainability". Given the heavy weight that the transport sector takes on in

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O. Gervasi et al. (Eds.): ICCSA 2024 Workshops, LNCS 14823, pp. 114–132, 2024.
https://doi.org/10.1007/978-3-031-65329-2_8

terms of externalities, the issue of sustainable mobility is one of the most debated topics in urban policies, aside from being an ace of the *Smart city* concept. Making cities "smart" requires providing a better quality of life [2] and finding environmentally sustainable urban mobility solutions. The development of sustainable urban transport systems depends on multiple factors and involves several transport modes, which include public transport, non-motorized mobility and newer forms of micro-electric mobility.

Public transport is considered an alternative to private cars, but it must provide quality services to be competitive. Knowing evaluation methods supported by quality criteria and indicators is essential for improving the quality of a transport system. Scientific research has been focusing on this issue for quite some time, making several contributions [3–6]. Some scientific interest has also developed toward pedestrian mobility quality assessment. Indeed, the development of a sustainable urban transport system also depends to a large extent on the propensity of users to consider "walking" an efficient transport mode for short-distance travel [7–10], which is closely dependent on their perception of the urban environment. Therefore, evaluating the quality of service (QoS) of infrastructures dedicated to pedestrian mobility, considering objective factors and the user's perception of the urban environment, is essential [11]. In addition, pedestrian mobility, as a conjunction between different modes of transport, strongly influences multimodality. Poor-quality pedestrian routes can discourage users from using public transport [12]. Consequently, more is needed to provide a good level of public transport quality to ensure its use by users. The quality of urban mobility must be considered, integrating different transport modes and land use [13, 14]. Cycling mobility can also contribute to developing a more sustainable transport system among these modes. Developing a set of assessment quality criteria and indicators to analyze the condition of existing bicycle lanes can be an effective tool for identifying infrastructure vulnerabilities and directing urban policies towards public space regeneration interventions [15, 16]. The same can be said of bike-sharing services [17–19] and electric micro-mobility [20, 21], which still need to be explored in the literature. Even these emerging forms of mobility offer the opportunity to rethink the urban space in which they operate, to build urban centers that are not only accessible and safe but also qualitatively attractive and "smart".

While there are numerous studies on the evaluation of urban transport quality, most of them focus on specific sectors. There is a significant gap in research that takes a holistic approach, evaluating the integration of various mobility systems and the urban environment. Therefore, this paper aims to fill this gap by investigating the key quality criteria and indicators that can assess the multimodality of an urban mobility system, going beyond the current segmentation between different modes of transport. The outcome of this research is crucial for deploying integrated solutions that enhance the quality of sustainable transportation services and infrastructures, from tangible implementations across networks to immaterial digital solutions like multimodal platforms and the development of quality indicators aiding in strategic planning [22].

Through a systematic literature review, this article provides an overview of how the concept of quality has been associated with transport systems. It identifies the most investigated forms of sustainable mobility and potential research gaps for future studies. The article also offers a preliminary set of criteria to assess the quality of urban mobility forms considered most sustainable and their integration. This identification of criteria

is crucial for improving the transport quality and its offer in terms of services, infrastructures and integration between several systems. It also enables the testing of effective urban policies in terms of public space regeneration and the management of conflicts linked to land use transformations.

The paper is organized as follows. Section 2 presents the methodology, including the search strategy and the type of analysis. Section 3 reports results with relevant descriptive statistics. Section 4 briefly reviews 49 publications, providing the current knowledge base and research gaps. Sections 5 and 6 present discussion and conclusions.

2 Methodology

The methodology applied to this systematic literature review is based on the technique PRISMA [23]. The PRISMA (Preferred Reporting Items for Systematic Reviews and Meta-Analyses) statement is a method for conducting systematic reviews and meta-analyses. It aims to collect all scientific evidence that meets predefined inclusion criteria and answers a given research question. This methodology consists of four stages: identification, screening, eligibility, and inclusion of collected articles (Fig. 1).

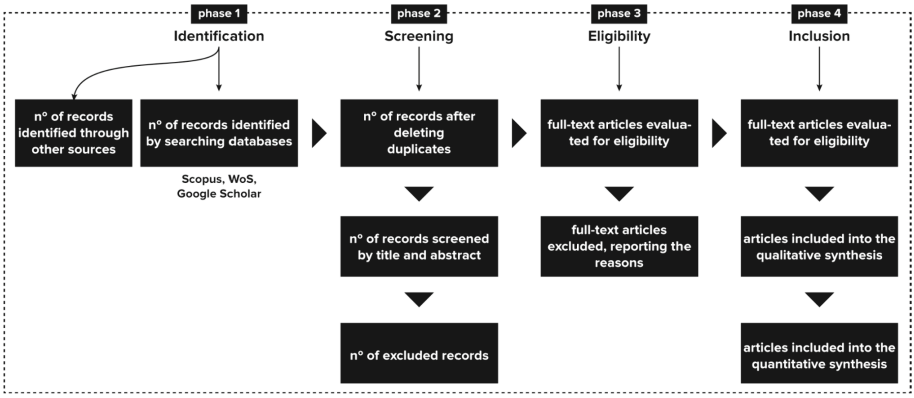

Fig. 1. Methodology flow chart. Source: personal elaboration based on [23].

The research question of this study focuses on the quality assessment of sustainable urban transport systems with a view to multimodality. An entire travel experience may include several transport modes, such as public transport, non-motorized mobility and electric micro-mobility, which may differ in terms of quality perceived by users. Given the research focus, private transport and studies relating to non-urban areas are excluded. The research aim is to identify key criteria for assessing the quality of a sustainable and integrated urban transport system.

3 Summary Results

3.1 Identification

The first phase of identification focused on identifying articles related to the quality of urban transport systems and infrastructure, starting with a keyword search conducted in three databases (DBs): Web of Science (WoS), Scopus, and Google Scholar. On Scopus and WoS the search was carried out on title, abstract and keywords, while on Google Scholar on title only, since the search system does not include the abstract and keywords. In all DBs, the same keywords were used to relate the quality assessment to the forms of urban transport mentioned above. After obtaining the search results, a single DB containing all scientific articles and their characterization was structured.

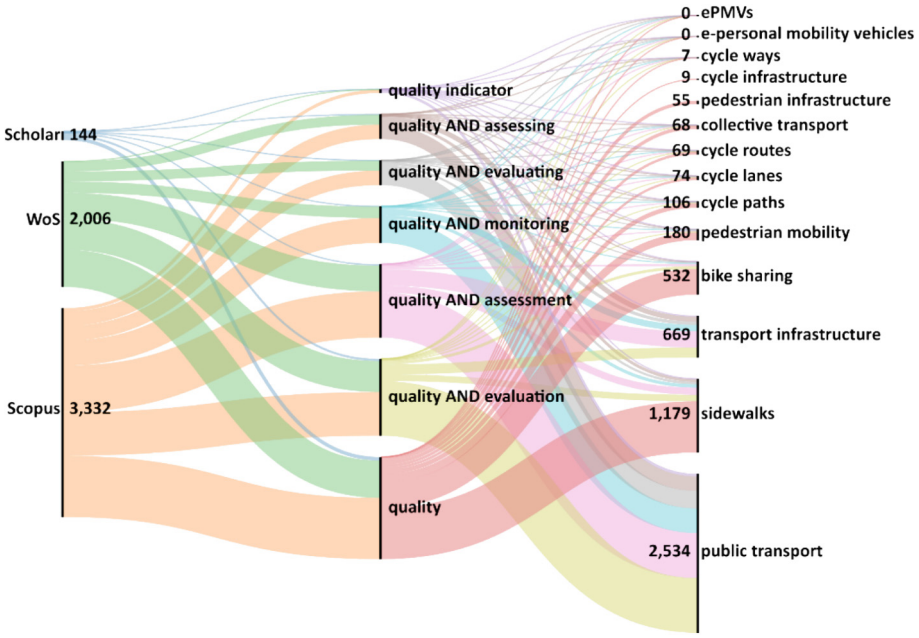

Fig. 2. Summary diagram of the results obtained from the first phase of the PRISMA statement. Source: personal elaboration adapted from Ferretto et al. (in press) [24].

Within the three chosen DBs, the keywords "quality" and "quality indicator" were cross-referenced with "assessing", "evaluating", "monitoring", and with "public transport", "collective transport", "sidewalks", "pedestrian mobility", "cycle lanes", "cycle paths", "cycle ways", "cycle routes", "bike sharing", "ePMVs", "electric personal mobility vehicles", "transport infrastructure", "pedestrian infrastructure", and "cycle infrastructure" for a total of 84 different combinations. Searching for scientific articles through these keyword combinations resulted in 5,482 records: 144 on Google Scholar, 2,006 on WoS, and 3,332 on Scopus. The records from Google Scholar are inferior because the search was only carried out by title, not by abstract and keywords.

Numbers in the first block of Fig. 2 represent the number of articles that emerged from the search in the three DBs, where the same keywords, given by the combination of the words in the second and third blocks, were searched. The width of the streams connecting the different blocks represents the number of articles that emerged from each keyword combination in each DB.

Therefore, the words in the second block were searched in association with those in the third block, corresponding to the mobility systems that were investigated. A first clear result, already at this preliminary level of analysis, concerns the prevalence of scientific studies focusing on public transport, rather than electric micro-mobility and non-motorized mobility systems (see Fig. 2). Indeed, 47.5% of the articles obtained come from the association with the keywords "public transport" and "collective transport"; 25.8% from the association with "sidewalks," "pedestrian mobility," and "pedestrian infrastructure"; 12.2% from the association with "transport infrastructure"; 9.7% from the association with "bike sharing"; finally, 4.8% from the association with "cycle lanes," "cycle paths," "cycle ways," "cycle routes," and "cycle infrastructure." There is no record of the association with "electric personal mobility vehicles" and its acronym "ePMVs," indicating that the most emerging forms of electric micro-mobility are still poorly explored in the literature from the point of view of their quality.

3.2 Screening

The second phase of screening is divided into three parts.

The first part involved the elimination of duplicates within each single DB and led to the removal of 1,516 articles; subsequently, the three DBs were merged, and another 1,099 articles present in more than one of them were eliminated, thus going from 5,482 to 2,867. This step led to a single DB containing the articles whose title and/or abstract contain one or more combinations of the chosen keywords. The DB is structured according to a matrix of rows corresponding to the articles and columns containing different information levels useful for characterizing scientific contributions.

The second part is based on the analysis of the relevance of the titles of the articles present in the overall DB with respect to the research topic. By analyzing the title of each article obtained from the previous step, 2,475 records were eliminated, going from 2,867 to 392.

Finally, the third part focuses on the relevance of the abstracts of the remaining 392 articles to the initial research question. From this further screening, 153 articles were removed, and 239 remained.

The screening phase guaranteed a restricted selection of articles and allowed the identification of more specific categories than those used in the identification phase. The 239 articles were then classified according to the different modes of transport (see Fig. 3) to facilitate the subsequent phases of analysis and to identify the focus of the scientific contributions more precisely. The clustering reveals a distribution aligned with the one identified in the preceding "Identification" phase. As depicted in Fig. 3, the distribution of scientific articles, categorized by transport categories and modes and represented as semicircles or concentric arcs across four distinct groups, predominantly features studies on the quality of public transport (specifically bus services), followed by research on

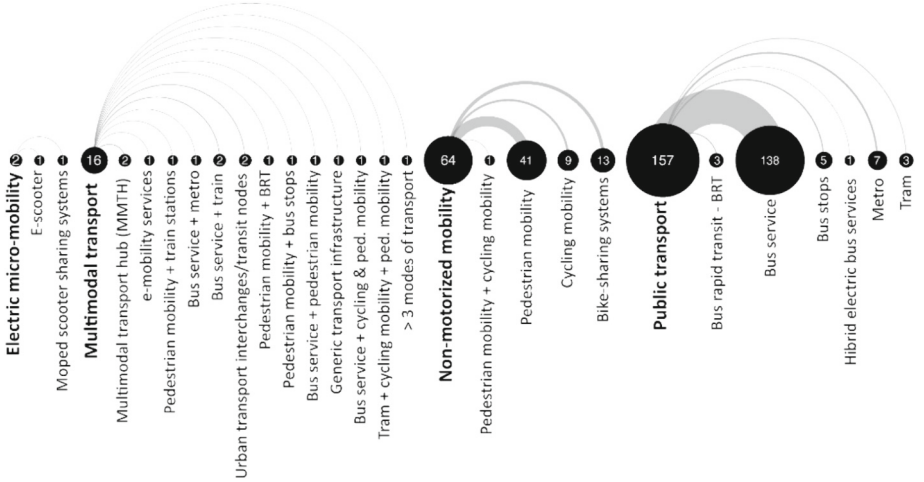

Fig. 3. Number of articles divided by transport categories and transport modes. Source: personal elaboration.

non-motorized (pedestrian) mobility. Research on the quality of multimodal transport systems is notably limited, as is the case with studies concerning electric micro-mobility.

3.3 Eligibility

The third phase of eligibility is based on the integral reading of the articles derived from the previous phase.

Before proceeding to the full reading of the articles, those concerning bus services have been excluded, except those focusing on bus stops. This choice is justified by the fact that there are already paper reviews that provide a viable methodology for defining a set of quality criteria and indicators for evaluating public transport services [25]. Infrastructural rather than service aspects of public transport have been less investigated and are strictly integrated with the infrastructures dedicated to non-motorized mobility, especially pedestrian mobility. For this reason, studies on bus/train/metro stops have moved on to the eligibility phase. The same goes for studies focusing on forms of mass transit such as trams, which have been far less investigative than bus service. Articles on the metro were also excluded, as it is a transport system that is not common in all urban centers but is typical of large cities/metropolitan cities. In light of this, 90 papers have passed the eligibility stage.

The integral reading of the articles led to further screening, identifying the scientific contributions that fully meet the criteria defined upstream of the development of the four phases of the PRISMA statement. At this stage, 23 articles were excluded because they did not fully meet the search criteria: (i) one was not strictly related to the urban area; (ii) one was specific to an exceptional situation (such as a sporting event), which implies a change in temporary transport demand, and its results could be difficult to apply to any urban context; (iii) one article considered the point of view of the service provider rather than the user; (iv) two were not in English; (v) two were of the same author and

reported the same indicators, and only one was considered; (vi) two provided general guidelines but did not include methods of evaluation of the quality of transport; (vii) 14 considered the transport quality only partially, and their evaluation was not coherent with the focus of this research. Another 18 articles were not available and/or downloadable. Consequently, 49 articles passed to the final inclusion phase.

3.4 Inclusion

The results of the 49 papers passed to the inclusion phase allow us to reconstruct a set of criteria and indicators for evaluating the quality of an integrated urban transport system, which includes multiple transport modes: pedestrian and cycle mobility, also considering bike-sharing, electric micro-mobility and public transport. Furthermore, this analysis enabled us to identify the geographical contexts, scientific journals and applied case studies that address the topic of the assessment of transport quality. A statistical summary of the main paper information levels that emerged from the systematic review is provided in the next section.

General Statistics About the Review

The selected publications reviewed comprised 35 articles, 9 conference papers, 4 conference proceedings, and 1 report. Therefore, 69% of the papers appeared in journals, whereas the remaining 31% were elsewhere. As for journals, 23% covered generically engineering, 17% business and economics, 17% transportation, 14% science and technology, 9% social science, 6% computer science, 6% green and sustainable science and technology, 3% urban studies, 3% earth and planetary science and 3% psychology. Recurrent journals were *Sustainability, Transportation, Transportation Research Record and Journal of Cleaner Production.* About 34% of the selected articles appeared in these 4 journals, the remaining 66% in the other 21. These different outlets showed the fragmentation of the journals addressing the transport quality assessment.

Concerning the geographical publications' distribution, the total number of authors is 144. Out of the total, 41% are affiliated with European institutions, 37% with Asian institutions, 22% with American institutions and 1% with Oceanian institutions. Europe has the largest coverage among the continents. In Europe, Italy constitutes 44% of the selected publications, followed by Poland (12%), Portugal (10%), United Kingdom (8%), Spain and Netherlands (7%), Croatia (3%), Austria, Belgium, Romania, France, Switzerland (2%). In Asia, China constitutes 42% of the selected publications, followed by India (17%), Malaysia and Bangladesh (9%), Taiwan (8%), Iran (6%), Turkey and South Korea (4%) and Iraq (2%). In America, Brazil constitutes 52% of the selected publications, followed by Colombia (32%), USA (10%) and Chile (6%). In Oceania, an author is affiliated with a New Zealand institution.

Figure 4 shows the geographic distribution by continents and countries of the case studies treated within the papers and the focus on the different categories and modes of transport analyzed. As with Fig. 2, the width of the flows connecting the different blocks represents the number of articles that have emerged in each continent/country, in association with different transport categories focused on service or infrastructure aspects. The analysis reports that 67 case studies were distributed as follows: 49% in Europe, 27% in Asia, 19% in America, and 4% in Oceania. 55% of the case studies

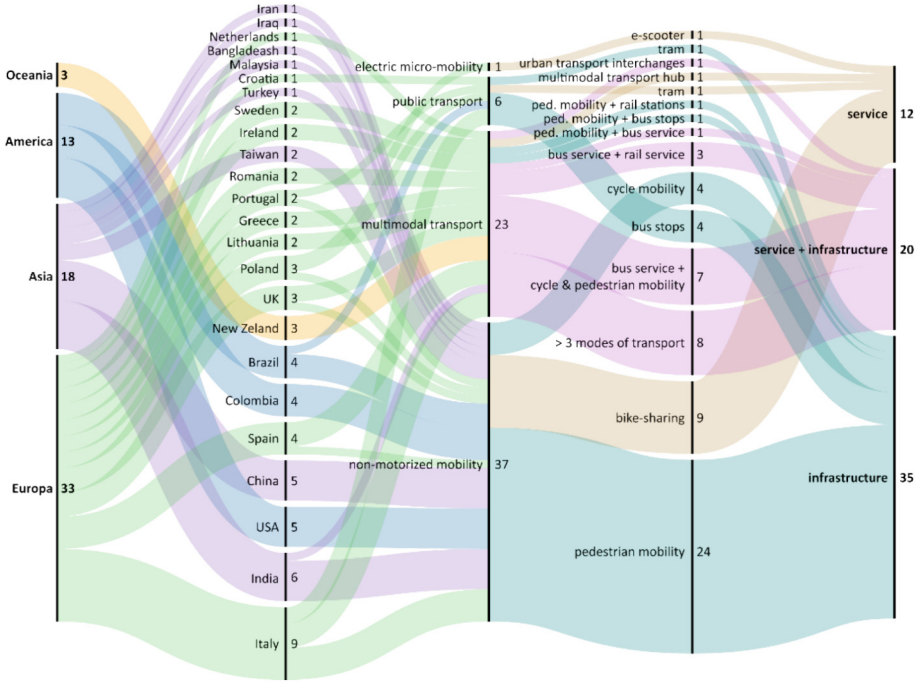

Fig. 4. Geographical distribution of the case studies divided by continent, country, transport category and mode. Source: personal elaboration.

concern non-motorized mobility, 34% multimodality, 9% public transport and 1% electric micro-mobility. The last flow of Fig. 4 shows how a reasonable part of case studies investigated the infrastructural aspects, especially concerning pedestrian mobility. It is interesting to note that in America and Asia there is a prevailing interest in non-motorized mobility. In Europe, interest is also largely in public transport, as well as pedestrian and cycling mobility. In terms of multimodality, most of the studies included non-motorized mobility and public transport services, which were investigated in Europe and Oceania.

4 Current Knowledge

This chapter presents the key quality criteria and indicators for evaluating urban transport systems, which have emerged from the literature review. In this phase, the quality criteria are divided into transport categories, as analyzed previously: electric micro-mobility, public transport, multimodal transport, and non-motorized mobility (see Fig. 5).

First, unique terminologies were identified to simplify the criteria that emerged from the systematic literature review. The chosen terminologies can represent parameters written differently but with the same (or similar) meaning.

The first list of parameters was picked up by [25], which provides eight service aspects articulated in 30 criteria and 103 indicators, based on the classification introduced by CEN/TC 320 (2002)[1]. The criteria derived from the last phase of the PRISMA methodology were partially associated with the classification terminologies provided by the European Norm. Therefore, the European normative recognition of the quality criteria presented in this paper, the involvement of international experts in their evaluation, and the review of relatively recent literature are the main reasons for choosing this paper. Many of the quality criteria associated with non-motorized or micro-electric mobility were consistent with those for public transport presented in [25]. In some cases, they found perfect coherence: for example, cleanliness is applicable for both buses and sidewalks. In other cases, they have been modified slightly while retaining the main meaning. For instance, in public transport, 'drive comfort' is associated with driving, for pedestrian mobility, it is associated with walking and for cyclists with cycling.

The quality criteria that emerged from the latest phase of PRISMA are 995 (which include duplicates): 17 for electric micro-mobility, 126 for public transport, 282 for multimodal transport, and 570 for non-motorized mobility.

"Comfort" was represented by indicators related to the pleasantness and amenities of the trip and environment. It included indicators related to the design of transport infrastructures and their practicability in moving and using urban space while waiting. Furthermore, it included the state of the environment, such as maintenance and cleanliness [26] and the presence of facilities, points of interest, and landscape [27]. Comfort was the most common criterion for all transport categories except for electric micro-mobility.

"Accessibility" included indicators related to access to a specific transport system and interface with others. It was second for both public, multimodal transport and non-motorized mobility. Differently, it did not appear to be relevant in micro-electric mobility.

A third relevant criterion for all transport categories was "Safety and security" [28–30], the second most frequent for non-motorized mobility, the third for public transport and electric micro-mobility, and the fourth for multimodal transport. It included criteria that provide personal protection (objective and subjective) from accidents (safety) and crime (security) experienced by users.

"Customer service" included indicators introduced to influence the closest practicable match between the standard service and the requirements of any individual customer/user. It represented the most important aspects of the bike-sharing and micro-mobility categories.

"Availability" included indicators in terms of service localization, area covered, operating timing, frequency, and characterizes all categories. Similarly, "Customer service" appeared in minor characterization compared to three previous ones.

"Information" included indicators related to the systematic provision of knowledge about the transport system to help the user before (trip planning phase) and during trips.

In contrast, "Time" includes indicators relevant to the planning and execution of trips in terms of length of the trip time and adherence to schedule. Both "Information" and "Time" were not associated with micro-electric mobility.

[1] CEN/TC 320 (2002) issued the European Norm EN 13816:2002 for the definition, targeting and measurement of transit service quality.

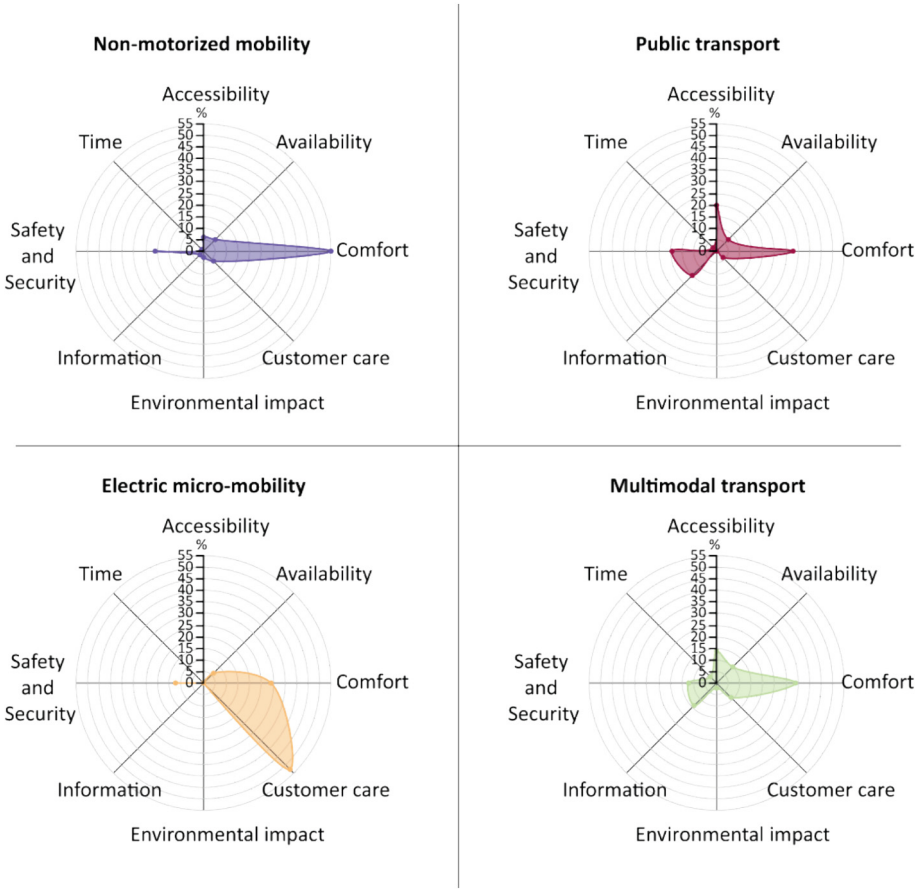

Fig. 5. The most common criteria in the categories of public, multimodal, non-motorized, and micro-electric transport (expressed in percentage) emerged from the systematic literature review.

Finally, "Environmental impact" included indicators related to the environment affected by the transport system analyzed and associated with multimodal and non-motorized transport.

Each of these criteria was represented by indicators that characterize specific aspects (see Table 1).

Some significant findings for research purposes emerged.

First, the result in "comfort" indicators demonstrated the high relevance of a transport system-land use relationship as a qualitative element of integrated travel experiences.

Second, although most indicators referred to a specific transport mode, several included the multimodality aspect as a key quality factor. It implicitly underscored the relevance of integrated quality, thereby reinforcing the research. For instance, [31] considered the type and distance of interchange opportunities with public transport. [32] considered the convenience of bike-sharing to connect to other modes of transportation.

Table 1. Criteria, indicators, and number of times they appear in papers (frequency) for assessing urban transport quality.

Criteria	Indicators	Indicator frequency
Accessibility	External interface	47
	External/internal interface	5
	Internal interface	25
	Ticketing availability	16
	Undefined	6
Availability	Dependability	4
	Network	37
	Operation	13
	Suitability	23
	Undefined	2
Comfort	Ambient conditions	109
	Complementary facilities	97
	Ergonomy	51
	Ride comfort	150
	Seating and personal space	23
	Usability for user facilities	17
	Undefined	7
Customer care	Assistance	5
	Commitment	5
	Customer interface	13
	Staff	18
	Ticketing options	32
	Undefined	2
Environmental impact	Infrastructure	2
	Pollution	20
	Undefined	4
Information	General information	60
	Travel information normal conditions	8
Safety and security	Emergency management	1
	Freedom from accident	108
	Freedom from crime	56

(*continued*)

Table 1. (*continued*)

Criteria	Indicators	Indicator frequency
	Undefined	12
Time	Adherence to schedule	13
	Length of the trip time	5

Accessibility was one of the criteria that most considered the interaction between different transport modes, represented by the indicator "external interface". The external interface was mainly concerned with accessibility to other forms of mobility than the one analyzed. Availability in some cases has also been related to multimodality, with indicators such as network-level distance between different transport nodes [33]. Safety and security, on the other hand, have taken on a negative valence when associated with multiple modes of transport. For example, the coexistence of pedestrians and cyclists in the same urban space was seen as critical from the perspective of user perception and accident risk [28]. The need to separate transport modes is expressed more clearly concerning active and vehicular mobility, with preventative design indicators such as barriers for pedestrian protection from vehicles or buffer zones between sidewalks and carriageways [12]. Information was mainly associated with individual modes of transport. Only in relation to mobility-restricted individuals does information about disabled-friendly interchanges (main terminals) assume the multimodal dimension [34]. Customer care and time have always treated a single transport mode.

5 Discussion

The literature review underlined different points of discussion on knowledge gaps that future research should focus on, especially concerning the specific modes of transport. Table 2 presents the knowledge gaps that emerged across the four macro-categories of transport. This overview provides a quick understanding of the areas that require further research and can guide future studies in filling these gaps.

In the domain of multimodality, a comprehensive array of quality indicators is imperative, especially focusing on the pre-travel, waiting, and walking phases. This is a complex area that requires in-depth exploration. An intriguing avenue for future research involves constructing a measurement model using structural equation modeling to assess how these indicators amalgamate to shape the overall traveler experience [54]. This approach will provide a more nuanced understanding of multimodality and its impact on transportation quality.

Moreover, recent research has tended to overlook the objective aspects of urban public mobility infrastructure. Studies should prioritize comparing objective mobility features, such as bus line quantity relative to population size, bus frequency, and incidents involving elderly pedestrians, with neighborhood quality indicators like shop density, green spaces, and attacks on the elderly. This research approach facilitates cross-validation between objective and subjective analyses, yielding comprehensive insights into mobility conditions [55].

Table 2. Knowledge gaps emerged for the four macro-categories of transport.

Transport categories	Source	Knowledge gaps
Electric micro-mobility	[21]	To replicate and improve the limited approaches to building theoretical frameworks for assessing quality
Public transport	[35]	To expand the analytical scope to encompass a broader array of services and parameters
	[36]	To conduct analyses during summer periods as well, considering that users' perceptions may be influenced by elevated temperatures and the influx of tourists during this time
	[37]	To differentiate between user demographics, as distinct groups, such as the elderly, may harbor varying perceptions
	[38]	To integrate environmental indicators into the analysis is essential for providing a comprehensive understanding of the subject
Non-motorized mobility//cycling mobility	[39, 40]	To provide additional details about the evaluation indexes and how to generate more suitable reconstruction projects to improve bicycle suitability of the road network by involving more resources
	[41]	To integrate the cycling network with other public transport and bike-sharing systems, considering its ability to serve urban places where mobility demand is concentrated
Non-motorized mobility//bike-sharing	[42]	To develop analytic methods, integrating information from social media with traditional data. Furthermore, for the regions where both dockless and dock-based bike-sharing systems, as well as reviews on both systems exist, it would be worth comparing these two different systems in terms of users' evaluations

(*continued*)

Table 2. (*continued*)

Transport categories	Source	Knowledge gaps
	[32]	To include both current users and non-users to foster loyalty among new users. Furthermore, comparative research should be carried out under different conditions and in relation to topography, weather, temporal, and cultural variables. Demographic characteristics of users should be accounted for: making bike sharing suitable for the elderly will be a valuable research direction
	[43]	Service operators should focus on retaining subscribers and addressing common priorities with users, like bike availability and totem operation
	[44]	To analyze local authorities' actions in co-designing public bike systems with residents
Non-motorized mobility//pedestrian mobility	[45]	To consider temporal variables and socio-demographic characteristics of users in future studies on pedestrian mobility is emphasized
	[46]	To evaluate sidewalks from the perspective of specific social groups such as the elderly
	[47]	To evaluate sidewalks from the perspective of specific social groups such as children
	[48–51]	To incorporate additional variables related to protection from climatic conditions and available services into evaluation models. Extending experiments to diverse case studies is necessary to understand how various factors influence user behavior
	[52]	To widen the sample and explore different statistical approaches
	[53]	To elements that impact user behavior and the role of Quality of Service (QoS) in route and mode choice

Finally, scholarly literature emphasizes the necessity to scrutinize the quality of transportation services and infrastructure across diverse locations, employing analyses through multiple case studies [56]. Prospective studies could investigate the effects on land use, accessibility, and congestion after the establishment of multimodal hubs. Furthermore, there is a demand to examine the correlations between socio-demographic

data and users' perceptions of the quality attributes of emerging services [57]. Finally, an interesting aspect of the research concerned the identification of indicators focused on vulnerable users. [58] provided several indicators for user groups, such as information about disabled-friendly interchanges for mobility-restricted travelers, provision of tactile information and clearly marked routes for communication-impaired, infrastructure design and information aspects for those older than 65 years, low-cost services for those younger than 24 years, design and quality on board for travelers with children. [59] considered the indicator "tactile paving" for sight-impaired, [12] included in transport quality the sidewalk slope to elderly people and wheelchair users, while [60] considered as a key quality indicator the sidewalk pavement for disabled people and handicapped.

6 Conclusions

Given the increasing complexity and density of urban centers under constant pressure from transportation demands, focusing on sustainable and smart mobility alternatives to cars is more crucial than ever. An important factor in incentivizing the modal shift toward less impactful forms of mobility and favoring integration of multiple transport systems concerns the quality of transport supply and its users' perception [51]. Its assessment is crucial both for understanding how to make existing services and infrastructure more attractive and for addressing urban policies toward urban space regeneration and smart mobility. Indeed, the perception of transport quality is strongly linked to the quality of infrastructure and services, surrounding public space, and land use. Route pleasantness is decisive when it comes to users' modal choice. Indeed, indicators such as the presence of urban design, elements of shelter from the sun or rain, green spaces, stores, services [12], and the type of pavement [59] are mentioned in the literature as factors that influence the quality perceived by users in non-motorized mobility [11]. Public transport can be perceived as more or less attractive, accessible, and safe depending on the aspects that characterize the context in which its stops are placed, such as the quality of sidewalks [60], the presence/absence of barriers [61], non-slip surfaces, lighting, ramps, and seating.

A recurring challenge for urban and transport planners is to comprehend how these interrelated parameters can be managed to create an urban environment that is responsive to users' needs and expectations [62]. The ultimate goal is to enhance the quality of existing infrastructure and services, thereby motivating users to adopt more sustainable modes of transport as a viable alternative to the car [63, 64]. The identification and assessment of these characteristics and their quality can provide valuable insights for planners, practitioners and policymakers, guiding them in designing public space, mobility infrastructure, and services. This approach fosters a full synergy between urban planning and transport planning [65, 66].

This paper has shed light on a significant gap in current understanding of quality assessment, which has been predominantly investigated in a sectorial manner. By identifying knowledge gaps and first- and second-level indicators, this study has laid the groundwork for evaluating an integrated urban mobility system in a multimodal transport scenario. This novel approach to quality assessment in the context of urban mobility represents a significant contribution to the field.

This research represents a first step towards addressing current knowledge gaps. Future development will delve into the indicators, providing a comprehensive understanding of their relationship with infrastructural and service aspects in each transport category. Furthermore, the research will focus on identifying key quality indicators that contribute to evaluating and improving integrated transport supply. The identification of these indicators will play a crucial role in strategic planning and mobility management, enabling the prioritization of smart sustainable mobility interventions.

Acknowledgments. This study was partially funded by the University of Brescia within the Grant "CUP: D75F21002920001" PON R&I 2014–2020 (FSE REACT-EU).

Disclosure of Interests. The authors have no competing interests to declare that are relevant to the content of this article.

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From Street Experiments to Planned Solutions (STEPS 2024)

From Spontaneous to Strategic: Integrating Street Experiments into Urban Planning Practices

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Abstract. In the pursuit of urban planning goals aimed at creating more liveable cities with enhanced public spaces, a crucial aspect to consider is the attention to vulnerable road users (pedestrians and cyclists) and their mobility and interaction within street space. This is also aligned with the principles of urban sustainability and inclusivity (Sustainable Development Goal n. 11). Extensive scientific literature supports the multifaceted benefits of this approach, encompassing not only environmental sustainability but also the enhancement of individuals' physical and mental well-being. These principles and models foster a communal approach to public space, thereby enhancing overall societal well-being and promoting sociability. A notable strategy to promote sociability is the adoption of experimental and temporary transformations of public spaces, such as tactical urbanism's street experiments. These initiatives often arise from community input rather than comprehensive urban planning analysis. Nevertheless, the literature illustrates how such interventions significantly contribute to increased social interaction, walkability, and ultimately the enhancement of quality of life within neighbourhoods where they are implemented. While many of these projects are initially temporary in nature, there is a growing interest in their potential integration into local plans and programs. Within this framework, the paper proposes the development of an analysis protocol for identifying optimal locations for street experiments interventions, focusing particularly on parklets, through a comprehensive examination of various components of the urban context. The protocol is then tested in the Oltretorrente neighbourhood in Parma, Italy. The adoption of such a localization protocol holds promise for enhancing the likelihood of successful interventions and advancing the integration of tactical urbanism initiatives into long-term urban planning strategies.

Keywords: GIS · Streets experiments · Parklets · Tactical urbanism · Sustainable mobility

1 Introduction

The issue of vehicular traffic in cities is increasingly apparent in modern urban environments. Not only does it pose significant environmental concerns such as air and noise pollution, but it also profoundly impacts the quality of life for urban dwellers [1–5].

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O. Gervasi et al. (Eds.): ICCSA 2024 Workshops, LNCS 14823, pp. 135–152, 2024.
https://doi.org/10.1007/978-3-031-65329-2_9

The dominance of motor vehicles over road space, often at the expense of other road users, notably vulnerable ones, is a striking feature of urban landscapes [6–10]. This dominance is exemplified by the prevalence of parking spaces, which consume a considerable portion of street space [11, 12]. This issue is even more evident within spaces such as historic centres whose morphology and intended use did not foresee the presence of vehicles within them and where the presence of on-street parking is even more impactful [13]. Numerous directives and planning policies advocate for the reduction of car-oriented spaces in favour of allocating more area to pedestrians, sociality, and active mobility, aligning with global agendas like the 2030 Agenda, more specifically Sustainable Development Goal n.11 [i.a., 14–17]. Moreover, several scholars have emphasised the integration of spatial planning and transport planning and explored strategies to assess and transform public space, making it more inclusive and adaptable to the needs of weaker users such as cyclists and pedestrians [i.a., 18–24]. Alongside these formal planning policies, interventions known as Tactical Urbanism (TU) [25–28] have emerged as alternative approaches, characterized by their temporary nature, community initiative, and cost-effectiveness. TU can be considered as an alternative and a challenge to formal spatial planning tools in response to the need for a more responsive planning system [29]. These temporary TU experiments have gained even more prominence following the recent COVID-19 pandemic, owing to their adaptability and rapid implementation capabilities [30].

Among the various TU interventions, Bertolini [31] draws out a specific group of interventions which he defines as "street experiments". In these experiments, the focus is on transforming streets from primarily serving vehicular traffic into spaces that prioritize active movement and socialization for people. Among the diverse array of TU interventions and street experiments, parklets can be deemed as the most suitable for repurposing parking spaces into areas conducive to social interaction and active mobility services. The concept of parklets was first introduced in 2005 in San Francisco by the Rebar Art and Design Studio, which transformed a parking lot into a temporary public space for two hours. This initiative eventually evolved into an annual event called "Park(ing) Day," designed to raise awareness about the shortage of green spaces in urban centres and stimulate discussions on the reclamation of urban space [32]. Since then, parklet installations have been legalized and widely embraced by numerous cities worldwide, with some interventions transitioning from temporary setups to permanent ones. Thus, while many of these projects are initially temporary in nature, there is a growing interest in their potential integration into local plans and programs.

Within this context, the paper aims to investigate parklet implementation by examining relevant criteria for identifying suitable spaces for their allocation. Subsequently, the paper defines a methodology to systematically determine the optimal pedestrian path segments for parklet localization within a neighbourhood. The methodology is then applied to the case study of the Oltretorrente neighbourhood in the city of Parma, Italy.

The innovation of this research lays on the gathering information on existing parklets and literature to create a location protocol applicable at the neighbourhood scale. This will make it easier for associations, citizens or eventually the administration to choose the location of interventions.

The paper is structured as follows: Sect. 2 describes a literature review focusing on the road optimal characteristics for parklets' location, Sect. 3 outlines the proposed methodology for identifying the segments of the pedestrian network most suitable for parklet installation. Section 4 introduces the case study neighbourhood and presents the results of applying the methodology. Finally, Sect. 5 provides conclusions on the application of the methodology to the proposed case study, highlighting its strengths and limitations, and suggesting potential avenues for further research.

2 Literature Review

Several guidelines have been formulated by cities worldwide, particularly those in America, in response to parklets' implementation. America, being the pioneer in parklet implementation, has played a significant role in shaping these guidelines. An essential factor in determining parklet placement is the presence of roadside parking along the street, a criterion supported by various sources, including the 2015 Philadelphia University City District report [33–35]. This criterion holds utmost significance in determining the location of these interventions, as the primary aim of parklets installation is to repurpose areas designated for private vehicles parking into spaces for communal interaction and active mobility related activities.

The table presented below (Table 1) summarizes the main characteristics of the urban context that the literature considers relevant for a more effective intervention, with the overarching goal of maximizing benefits in the surrounding area.

Amongst those, three main factors play a key role. Firstly, pedestrian traffic, which must already be significant, as emphasized in the manuals of Seattle [36], Philadelphia [33], NACTO [34], and UCLA [37]. Indeed, the Philadelphia University City District Report [29] underlines the high social function of parklets. Secondly, the presence of commercial activities along the street, as highlighted by the same manuals, but also by the cities of Watsonville [38], Boston [39], and Littke [40]. This aspect contributes to a livelier atmosphere, fostering increased pedestrian flow and facilitating greater social interactions. Moreover, parklet installations have been correlated with substantial sales boosts [29]. Thirdly, narrow sidewalks present a unique challenge. In such circumstances, where alternative solutions are limited due to various constraints, the installation of a parklet can significantly enhance pedestrian space, as highlighted in manuals such as Wellington city manual [41], Minneapolis city manual [42] and NACTO [30], as well as academic literature by authors like Campisi [32], Caymaz [43], and Peterson [44].

The 2015 Philadelphia University City District Report [33] proposes a categorization of the characteristics influencing the success of parklets in a specific area, offering useful guidance for planning and implementing such projects. It can be noticed, for example, that the aforementioned factors are strongly correlated, while proximity to bike lanes is considered a secondary variable.

Other factors to be considered include surrounding environmental and infrastructural conditions. For example, Watsonville [38] highlights the importance of reducing vehicular traffic speed near parklets to ensure user safety. Guidelines such as those provided by the Boston Tactical Public Realm [39] emphasize the importance of placing parklets in areas not provided with open public spaces (such as parks) or available seating, to maximize their use and attractiveness.

Regarding vehicular traffic flows, there exists a divergence of opinions among authors or manuals depending on the intended function of the parklet. While some advocate for placing parklets along streets with higher vehicular traffic volumes, as evidenced in the case of Divisadero Parklet in San Francisco [44], others suggest the opposite approach [33, 45, 46]. In this analysis, the authors consider streets with lower vehicular traffic flow. Indeed, the streets with high traffic often indicate high vehicle speeds or a lack of roadside parking and these conditions could conflict with other protocol requirements.

Finally, other aspects such as the street slope and proximity to bike lanes can influence the accessibility and use of parklets. The San Francisco Parklet Manual [47] recommends that parklets be built on streets with a slope of less than 5% to maximize accessibility for disabled users and minimize design challenges. Furthermore, although no direct correlation has yet been made between bicycle infrastructure and successful parklets, the Pavements to Parks movement [35] advises for parklets to be installed in areas that fall along bicycle routes to emphasize its goals of encouraging non-motorized transportation and enhancing pedestrian safety [48].

Table 1. Literature review about the best localisation of parklets.

Location	References
High pedestrian traffic	[33, 34, 36, 37, 43, 49]
Commercial activities	[33, 37–40, 43–45, 48, 50]
Narrow pedestrian paths	[32–34, 36, 37, 39, 41–44, 50, 51]
Lack of public spaces	[32, 39, 41, 44, 52, 53]
Slow speed streets (<25mph)	[37–39, 43, 54]
Narrow streets	[33, 45, 55]
Connected to cycle lanes	[33, 40]
Low rate of vehicular traffic	[33, 45, 46]
High rate of vehicular traffic	[44]
Presence of shade	[33, 37]
Areas that can improve pedestrian and bicycle safety	[53]
Presence of street lighting along the path	[37]

3 Materials and Methods

This section of the paper outlines the methodology developed to identify the most appropriate road segments for parklets locations. The methodology is structured into four stages:

- Classification of parklets based on their features;
- Development of a protocol encompassing relevant characteristics of the pedestrian infrastructure and urban context for parklet implementation;

- Evaluation of suitability for each type of parklet;
- Compilation of a comprehensive database detailing the current state of the area under analysis, followed by the application of the protocol to pinpoint potential parklet locations.

Subsequent subsections provide an in-depth explanation of the different stages of the methodology.

3.1 Parklet Typologies

The main feature of parklets implementation is the repurposing of areas originally designated for parking private motor vehicles into spaces intended for social interaction and active mobility. However, through literature analysis and case studies, it becomes apparent that parklets can serve various functions, including providing seating, green spaces, or bicycle parking facilities [31]. To understand this diversity, the research conducted an analysis of different parklet implementations documented in existing literature (including grey literature), categorizing them based on their intended purposes. Subsequently, these categories are used to identify different types of parklets, each associated with specific examples, as presented in the table below (Table 2).

Table 2. Typologies of parklet.

Location	Typologies	References
Public	Bicycle parklets	[56]
	Social parklets	[57]
	Pocket parks	[58]
Private or semi-private	Streateries	[36]

Through the literature analysis, four main types of parklets are identified. These can be grouped into two main categories based on their use. Specifically, there are parklets for public use and those for private or semi-private use. The latter consists of parklets located in close proximity to catering activities, such as restaurants, intended for patron use during their operating hours, and are defined by the Seattle guidelines [59] as Streateries. On the other hand, public parklets serve three primary purposes: bicycle parking and related services, pocket parks characterized by the inclusion of vegetation, and social parklets. The latter feature seating areas intended for passersby and community members. It is important to note, however, that this type often includes additional elements found in the previously mentioned categories, particularly bicycle racks and urban greenery.

3.2 Comprehensive Protocol for All the Typologies

This section aims to identify the relevant characteristics of public space for parklet placement, informed by a review of existing literature. To identify the most suitable

locations for parklet interventions, a protocol is developed to assess open public spaces and ascertain the presence or absence of critical characteristics. Instead of creating separate protocols for each parklet type, a unified protocol for evaluating urban space has been established. Thus, the protocol highlights the prevailing qualities and crucial aspects of urban space, aiding in the selection of the most suitable parklet type for installation in each identified area.

Each pedestrian path is then evaluated based on a set of factors, with values ranging from 1 to 0 assigned for each individual factor. A value of 1 indicates support for parklet installation, while 0 suggests that the characteristic does not favour parklet placement. Moreover, a value of 0 may indicate that existing conditions are sufficient, rendering parklet installation unnecessary.

The protocol considers various characteristics of the pedestrian path and surrounding urban context. Firstly, of primary importance is the presence of roadside parking, which, as previously emphasized, is crucial for determining the suitability of a segment for parklet placement.

Considering street characteristics, the protocol prioritizes streets with low vehicular speed limits, assigning a positive value to streets with a speed limit equal to or less than 30 km/h. Additionally, streets experiencing low traffic flows also receive a positive rating. Specifically, in the context of the paper's case study, located in Italy, suitable streets for parklet installation are those classified as E/F or F according to Article 2 of the Italian Highway Code [60]. Next, while the width of the street itself can be of significant consideration, the width of pedestrian paths becomes even more relevant. In fact, if the dimensions or the presence of obstacles cause the accessible width to be less than 90 cm, the installation of a parklet could address this limitation. Consequently, a value of one is assigned to pedestrian paths exhibiting this criticality, indicating their suitability for parklet installation. Other characteristics collected and assessed by the protocol, related to the pedestrian infrastructure, include the presence of shade provided by tree rows and the availability of street lighting. The presence of catering activities, i.e. bars and restaurants, along the path is also taken into consideration. To ascertain the presence of such activities along the pedestrian path, a 10-m buffer originating from the activity is employed. Additionally, the protocol assesses the proximity to cycle paths and green areas, i.e. parks and green squares. For cycle paths, a 100-m buffer is established, identifying segments within this radius as most suitable for parklet location. This is because parklets can also encourage active mobility and offer a convenient option to cyclists when equipped with services for bikes, such as bike racks or repair stations. For green areas, the protocol considers a 5-min walk time isochrone and segments outside this range are deemed favourable for parklet localization. This approach acknowledges that parklets can function as small pocket parks, providing access to green spaces where other parks may not be readily accessible.

In addition to the elements identified within the literature, the protocol also identifies as optimal characteristics for parklet localisation, including the presence of cultural buildings along the path. These buildings can contribute to creating a more enjoyable environment for walking, thereby promoting social interactions. Furthermore, the presence of urban seating along the path and proximity to bike racks within a 100-m radius, are considered favourable for parklet placement, as parklets can compensate deficiencies in

these amenities. Lastly, the protocol also considers the proximity of bike-sharing stations as a favourable element, following the reasoning applied to cycling lanes (Table 3).

For the protocol application to the selected case study, base maps and data for the analysis are collected from multiple sources. These include the Territorial Information System of the municipality of Parma and the Geoportal of Emilia-Romagna Region, which provide cartographic data on the street network, buildings, existing public services, and mobility services. Open data websites, i.e. Open Street Map, are used instead for the location of commercial facilities, notably bars and restaurants. Lastly, the remaining data, such as pedestrian paths and their characteristics, roadside parking, and urban furniture, are collected in situ by the authors.

Table 3. Values assigned to each characteristic of the paths.

Characteristic	Evaluation	Values
Roadside parking	Present Absent	1 0
Width	"<90" "90 < x < 150" + bottlenecks # null AND "90 < x < 150" + bottlenecks # absent Other	1 1 0
Cultural buildings	Present Absent	1 0
Proximity to cycle lanes	Present Absent	1 0
Proximity to sharing services	Present Absent	1 0
Proximity to urban green areas	Within a 5-min walk Beyond a 5-min walk	0 1
Speed limit	"30 km/h" Other	1 0
Shading	Present Absent	1 0
Lighting	Present Absent	1 0
Presence of catering activities	Present Absent	1 0
Vehicular traffic	"E"or "E/F" or "F" Others	1 0

(*continued*)

Table 3. (*continued*)

Characteristic	Evaluation	Values
Urban seating	Present Absent Present without protection	0 1 1
Bike racks	Present Absent	0 1

3.3 Suitability Evaluation

Once the protocol is defined, data collection for evaluating the pedestrian infrastructure and the immediate urban context is initiated. Values are then assigned to individual segments of the pedestrian network. To identify the most suitable type of parklet to be located along the various segments, specific conditions for each type are then defined as follows:

- **Social parklets**: Roadside parking + Speed limit + Vehicular traffic + Width + Shading + Lighting + Urban seating + Cultural buildings + Proximity to cycle lanes + Proximity to sharing services;
- **Pocket parks**: Roadside parking + Proximity to urban green areas;
- **Bicycle parklet**: Roadside parking + Proximity to urban green areas;
- **Streateries**: Roadside parking + Presence of catering activities.

4 Results and Discussion

4.1 Case Study: Parma's Oltretorrente Neighbourhood

The case study used to test the methodology is the Oltretorrente neighbourhood in the city of Parma. Situated to the west of the Parma River, it constitutes part of the city centre along with its eastern counterpart (Fig. 1). The neighbourhood covers an area of 1.1 km^2 and is home to 8,496 inhabitants (as of 2023 [61]). Bordered by urban boulevards to the north, west, and south, and the Parma River to the east, the district can be divided into two main areas along the east-west axis, represented by via Emilia. The northern area is primarily designated for services and amenities, which includes the Parco Ducale park, while the southern area is predominantly residential. The neighbourhood is equipped with green and blue infrastructures, including small parks in the inner areas, health facilities such as clinics and hospital services, and various commercial activities. Furthermore, a notable presence of secondary schools, constituting most of such institutions in the city of Parma, is observed within the neighbourhood. These schools are primarily situated along the eastern border, facing the Parma River. Additionally, some of the University of Parma premises are also located within the neighbourhood, particularly in close proximity to the Parco Ducale park. In terms of mobility, the district is predominantly accessible to vehicular traffic, apart from Via Emilia and the surrounding area until Ponte di Mezzo, the bridge that crosses the Parma River along Via Emilia. Indeed, this area of the neighbourhood included within the LTZ (Limited Traffic Zone). Active

mobility infrastructure is limited, partly due to the mainly narrow configuration of the neighbourhood streets. However, extensive pedestrian paths are prevalent throughout the area. The local public transport network is extensive and offers convenient access along the main streets of the neighbourhood. Additionally, numerous bike-sharing stations are identified within the Oltretorrente neighbourhood.

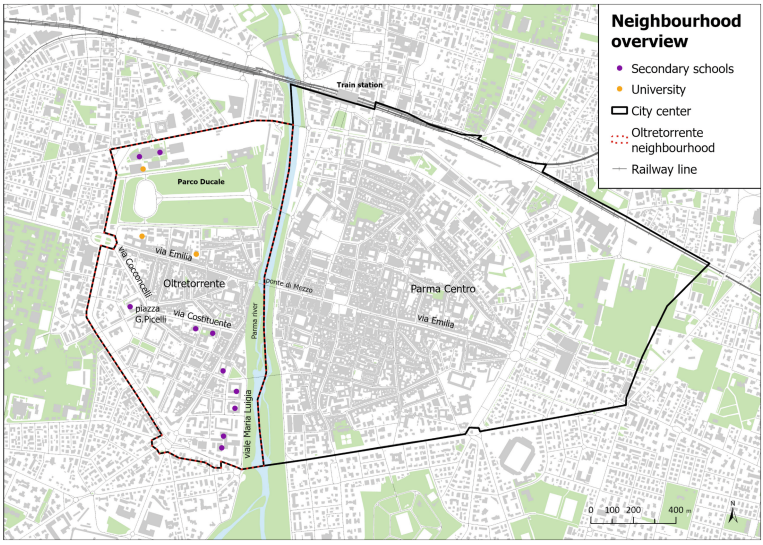

Fig. 1. Framework of the Oltretorrente neighbourhood in relation to the historic city centre. Secondary schools and University poles, as highlighted, characterise this neighbourhood. Source: authors' elaboration.

The neighbourhood was selected as the case study of this paper due to its previous inclusion in studies on sustainable mobility [62], including the recent European project Thriving Streets - URBACT III 2014–2020, where the city of Parma played a central role as lead partner. Furthermore, in 2023, the neighbourhood was chosen for the installation of a parklet along Viale Maria Luigia, the street which accommodates most of the area's high schools. The parklet initiative is temporary and stems from a bottom-up approach initiated by a group of teachers and students from one of the schools situated along the street. Thus, given the complexity and diversity of the neighbourhood, it can be interesting to study where and which typology of parklet could be located.

4.2 Protocol Application Results

The primary criterion established in the methodology chapter for parklet establishment is the availability of roadside parking spaces.

Within the Oltretorrente neighbourhood, the analysis (Fig. 2) indicates the inner residential streets with reduced traffic flows are depicted as the most suitable areas for parklet installation, as they typically offer roadside parking. In contrast, the ring roads, and main thoroughfares, particularly in the southwest portion of the area, characterized

by higher traffic flow and faster speeds present parking spaces of different types that are not aligned along the roadside, thus making them unsuitable with the selected criterion. Consequently, a preliminary selection of suitable streets for parklet localization is conducted based on this criterion.

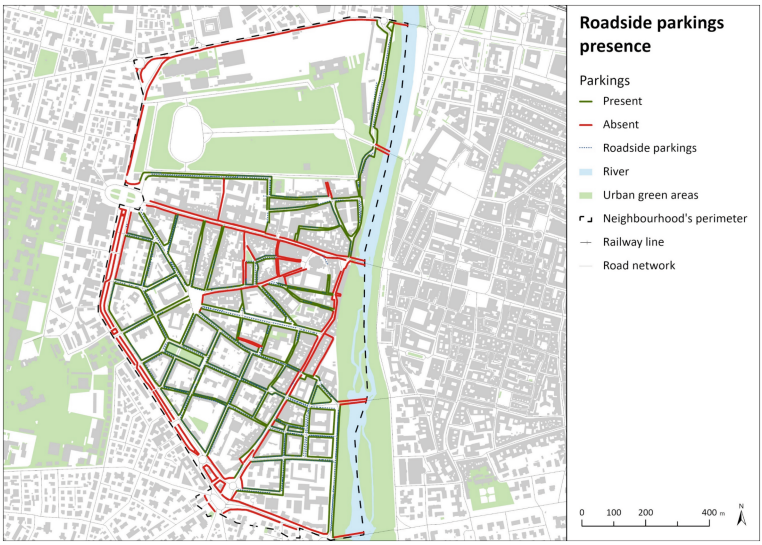

Fig. 2. Streets suitable for parklets due to the presence of roadside parking. Source: authors' elaboration.

The case study assessment, using the protocol, unveiled that the neighbourhood features numerous cultural buildings, shared mobility services, and tree-lined main routes. However, one of the protocol factors considered seems to hold little relevance for this study area. In fact, the vehicular speed limit throughout the neighbourhood remains uniformly limited to 50 km/h, with very few exceptions. As a result, the rating for almost all streets regarding this feature are 0.

The following figures (Figs. 3, 4, 5 and 6) illustrate the identified suitable streets for each parklet typology previously defined: social parklets, bicycle parklets, pocket parks and Streateries.

Those segments are primarily located along the perimeter of the Parco Ducale park and in the southwest area of the neighbourhood. Conversely, the majority of segments achieves a sufficient rating. Those segments are primarily located within the inner streets of the district, concurring with the previous observation made through Fig. 2. Particularly noteworthy are the main streets with high pedestrian traffic, such as Via della Costituente, Via Cocconcelli, Viale Maria Luigia, and their intersecting streets.

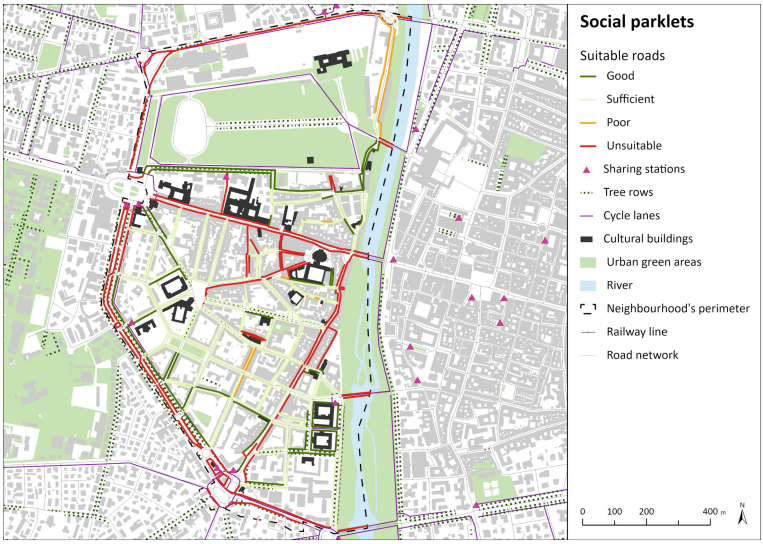

Fig. 3. Streets suitable for parklets as meeting places, i.e. to enhance sociality. Source: authors' elaboration.

In terms of bicycle parklet typology, Fig. 4 highlights the widespread presence of bike racks throughout the neighbourhood, especially near public facilities such as schools. Nevertheless, these amenities frequently appear insufficiently sized in relation to demand, suggesting a potential need for additional bike racks. Suitable locations for

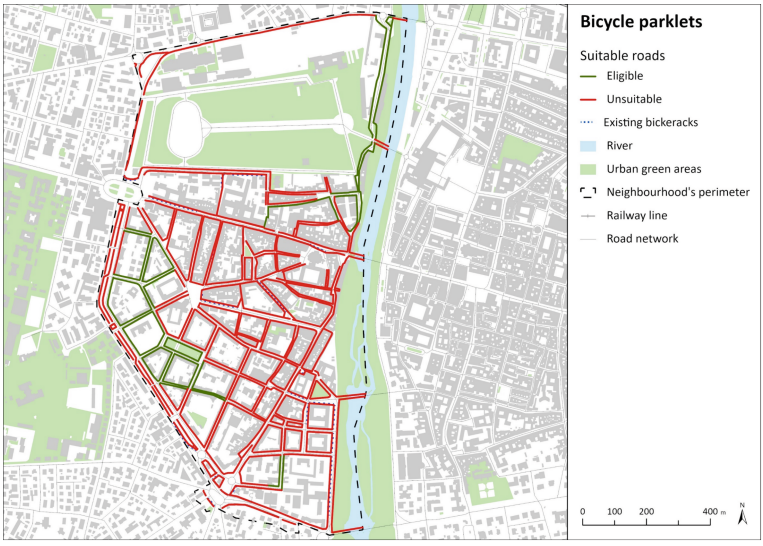

Fig. 4. Streets suitable for parklets as bicycle racks. Source: authors' elaboration.

such installations are observed primarily in the western and northern parts of the district, including areas adjacent to the Parco Ducale park.

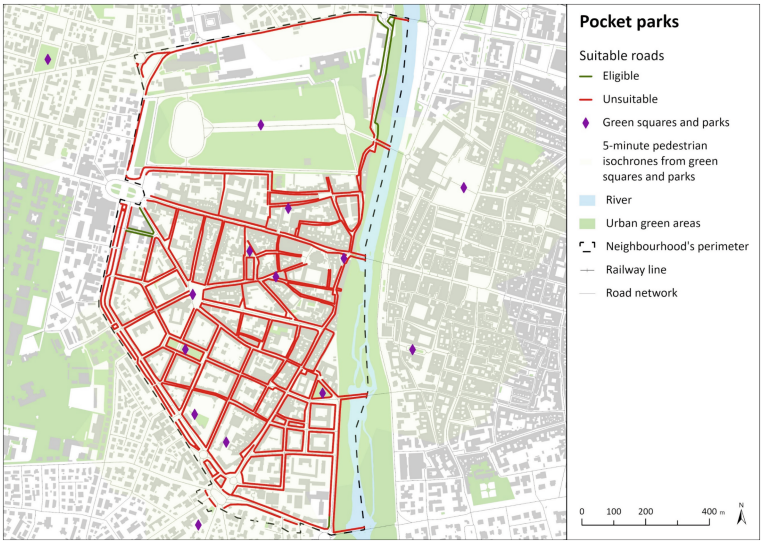

Fig. 5. Streets suitable for parklets as pocket parks. Source: authors' elaboration.

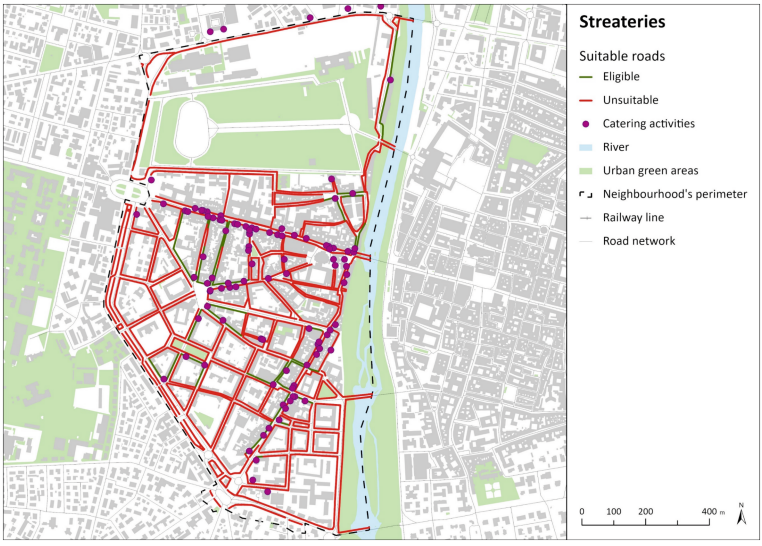

Fig. 6. Streets suitable for parklets as Streateries, for catering activities. Source: authors' elaboration.

Figure 5 depicts the pedestrian path segments deemed suitable for pocket park installations according to the protocol assessment. A closer examination of this figure reveals

the neighbourhood's abundance of public green spaces, both within its boundaries and in the surrounding areas. Consequently, the demand for pocket parks in the case study neighbourhood appears to be minimal. Indeed, nearly the entirety of the area falls within the 5-min walk isochrone generated from the identified green spaces, ensuring convenient access to these areas for the neighbourhood population. Thus, only two streets, located to the west of Piazzale Santa Croce, are identified as potential locations for pocket parks.

On the contrary, identifying suitable segments for Streateries (Fig. 6) interventions poses challenges, primarily due to the concentration of catering activities along the main streets of the neighbourhood. These streets coincide with those identified in the initial analysis to determine the presence of roadside parking. As a result, only specific inner streets are capable of effectively accommodating this parklet typology.

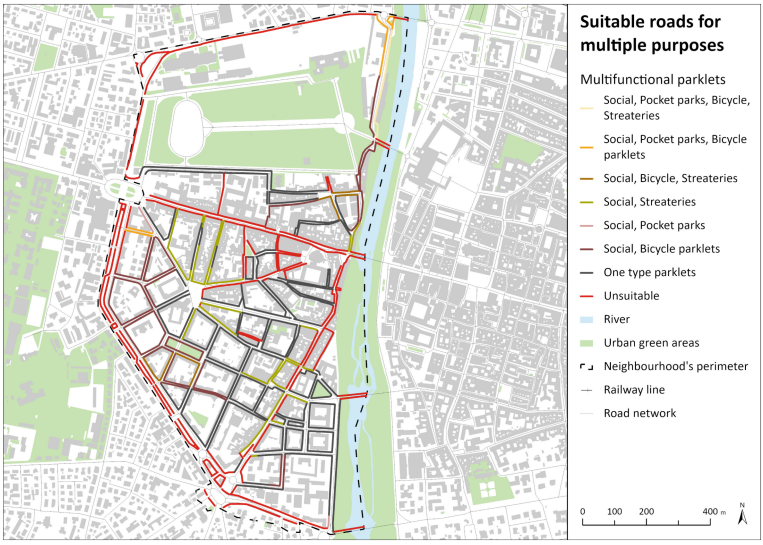

Fig. 7. Streets suitable for parklets with multiple purposes. Source: authors' elaboration.

Lastly, an additional analysis is conducted to evaluate the suitability of pedestrian path segments for various types of parklet installations (Fig. 7). This analysis makes it possible to not only identify the most suitable locations for street experiments but also to determine the most appropriate typology of intervention. The findings indicate that the two most pertinent typologies and thus most suitable for the neighbourhood under study, are social parklets and Streateries. This observation aligns with the neighbourhood's primarily residential character and the abundance of catering activities in the area.

5 Conclusions

Tactical urbanism interventions, as emphasized by the authors, play a crucial role in promoting sociability, enhancing social interaction, improving walkability, and ultimately enhancing quality of life. However, these interventions are typically bottom-up in nature

and are characterized by their temporary implementation. Nevertheless, while many of these projects are initially temporary in nature, there is a growing interest in their connection with local plans and programs.

In this context, the aim of this study is to introduce the initial results of the development of a localization protocol, which seeks to integrate parklet interventions into local urban planning plans and programs. One potential application of this tool could support public administrations, where it could help conduct preliminary assessments to identify suitable locations for parklets interventions. This process could facilitate dialogue with citizens, who are often the advocates for such interventions. In fact, by providing a list of suitable locations based on desired functions, the protocol could promote more interventions and offer alternative options in cases where proposed locations are deemed unsuitable by public administrations, thus becoming a toolkit for community engagement.

Thus, the paper outlines a methodology to identify potential locations for street experiments, specifically parklets, through the development of an assessment protocol based on characteristics of pedestrian paths, streets, and the surrounding urban context, identified in the existing literature. This underscores the importance of focusing attention on the specific needs and vocation of the neighbourhood, which can be partially addressed through these interventions.

The results of the methodology application revealed that not all of the identified typologies of parklets are suitable for the area. Additionally, it is evident that improving walkability cannot solely rely on the installation of parklets. For instance, the presence of adequate public lighting along paths is essential, as parklet installation alone may not compensate for this deficiency. Therefore, to truly enhance walkability and sociability, parklet implementation must be complemented by targeted interventions along pedestrian paths and the surrounding urban context. Conversely, the inverse holds true: the more favourable the conditions of the urban context and the route where the intervention is situated, the greater its likelihood of success of parklet implementation. Consequently, at this stage, the methodology focuses on areas where such specific street experiment interventions can effectively contribute to an overall improvement of people's quality of life and walkability.

While the developed protocol presents certain limitations, it could be refined in future iterations to further enhance its effectiveness and applicability. In particular, the most important limitations can be summarised as follows:

- the protocol focuses on pedestrian and street infrastructure characteristics, neglecting environmental and social aspects of the area, including the need to engage the local population in constructive dialogue;
- the protocol considers cultural buildings, it does not take into account other public buildings that could serve as significant focal points for promoting sociability, such as schools or neighborhood primary services;
- the methodology identifies suitable areas for intervention, but it does not consider the potential challenges of specific streets that may make them less suitable for such interventions. This condition is exemplified by the case of via Kennedy, located south of the Parco Ducale park, which the protocol assesses as suitable for the localization of social parklets. However, both pedestrian paths along the street are bordered by fences:

one belonging to the park itself and the other delimiting the university premises. Thus, even if relevant buildings and services are present along the path, it would be advisable to also investigate their degree of permeability and openness towards the street;

- many of the investigated features require on-site collection, due to their unavailability on institutional portals or in public geodatabases. Therefore, it is essential to collect and constantly update this data to ensure the validity and reliability of the methodology;
- need for additional data reported in the literature, including the identification of the neighborhood's most frequently visited areas and the monitoring of traffic flows. The latter is particularly useful for conducting pre- and post-installation analyses of the parklet to assess its impact on the presence of people in the surrounding area;
- the methodology doesn't take into account the calculation of parking spaces lost due to the installation of parklets. This is relevant in order to possibly determine where parking spaces can be replaced.

Lastly, future developments of the work will consider refining the methodology, specifically the evaluation protocol, to promote the inclusion of parklets in sustainable urban mobility plans, thus making them a structural measure. The refinement of the evaluation methodology and protocol aims to address these limitations.

Acknowledgments. This research was granted by PNRR-M4C2- I1.1 – MUR Call for proposals n.104 of 02-02-2022 - PRIN 2022 – ERC sector SH7- Project title: MOVING StEPS - MOVING from Street Experiments to adaptive Planned Solutions - Project Code 2022BLK9TS - CUP Code D53D23011060006 - Funded by the European Union – NextGenerationEU.

Finanziato dall'Unione europea NextGenerationEU

Ministero dell'Università e della Ricerca

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This manuscript reflects only the authors' views and opinions, neither the European Union nor the European Commission can be considered responsible for them. Participation of G. Pellicelli and L.J. Marinelli was also supported by the projects ECOSISTER (ECS00000033) and Sustainable Mobility Center (CN00000023) respectively.

Disclosure of Interests. The authors have no competing interests to declare that are relevant to the content of this article.

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User-Centered Policy Interventions for Future Cities

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Abstract. Rising societal demands are a direct result of the exponential rise in urbanization and technological development. Addressing these needs in a way that is sustainable, inclusive, and user-friendly is a problem for policymakers. Citizens' participation at every stage of a policy's development is critical to the user-centricity concept's success in policymaking. By involving the citizens in this collaborative effort, we can make sure that policy interventions are specific to each community's needs, which will increase their acceptability, relevance, and longevity. In the long run, this can make cities better places to live by making them more resilient, citizen-centric, and focused on the needs of ambitious inhabitants. Overall, this paper presents a range of user-centric policy initiatives that might help policymakers better understand the varied requirements, preferences, and urban experiences of city dwellers.

Keywords: Cities · Citizens · Policy · Urban development · User-centered approach

1 Introduction

Urban areas are experiencing rapid population expansion and better economic prospects as a result of people moving from rural to urban areas [1,2]. Especially, in the developing nations an increasing number of people migrating to metropolitan areas in search of better job opportunities, easier access to a wider range of services, and an overall higher standard of living [3–5]. There will be numerous obstacles to relocating people to cities, therefore politicians should consider funding multi-modal transportation networks, building accessible and affordable housing, and pursuing smart city initiatives to meet the needs of the population and their expectations [6–9]. Green infrastructure based urban development and

© The Author(s), under exclusive license to Springer Nature Switzerland AG 2024
O. Gervasi et al. (Eds.): ICCSA 2024 Workshops, LNCS 14823, pp. 153–167, 2024.
https://doi.org/10.1007/978-3-031-65329-2_10

mixed-use zoning are also prioritized in the pursuit of environmentally conscious and liveable urban environments [10]. This will allow us to claim that these cities will be more technologically advanced, robust, and able to foster innovation from a social and economic standpoint [11]. These modern urban centers have a leg up when it comes to resource planning and environmental impact reduction thanks to cutting-edge smart technology like intelligent building management, smart grids, and autonomous vehicles [12–15]. Sustainable development, community innovation, and citizen-centric development are all areas where policy interventions are crucial [16,17]. It is critical to determine how to incentivize the schemes in order to meet the demands of resilient and ecologically friendly urban infrastructure. Sustainable and accessible transportation, energy-efficient housing construction, and renewable energy applications all benefit from this [18–20]. The advantages of urban development can be dispersed fairly if decision-makers prioritize inclusive and egalitarian policies [21].

Under the current regulatory framework, lawmakers face significant challenges when trying to implement the numerous policy-based decisions at the grassroots level [22,23]. Various government institutions' aversion to change and the present bureaucratic lethargy pose serious challenges to the implementation of progressive policies that would improve citizens' lives. There is also the matter of the city's development budget, which involves complicated funding procedures and the involvement of the central and state governments [24]. Working jointly, public and private entities may build the city's infrastructure, which solves the budget problem. But with all the responsibility, openness, and sharing of best practices among recipients, it's not as simple as it seems [25]. In order to address these types of problems, community involvement is crucial. Through inclusive and effective decision-making processes, we can address the concerns related to public-private partnerships and governance [26,27].

One game-changing factor that could influence the design of cities of the future is user-centered policy interventions. Incorporating citizen feedback into policymaking can help make cities better places to live by making them more adaptable, welcoming, and enjoyable for everyone [28–30]. The different needs and aspirations of urban people should be carefully considered when crafting policies. Only then can these policies be expected to tackle the real-world difficulties that communities face and provide actual benefits. The numerous approaches that can be employed by policymakers to effectively obtain and utilize collaborative information, such as user research, co-creative workshops, and iterative prototyping, can ultimately benefit communities [31–34]. The chances of effective implementation and long-term sustainability are enhanced through this collaborative approach, which guarantees that policies are based on urban life's reality and encourages individuals to feel ownership. By implementing user-centered policy interventions, we can pave the way for future smart cities, find creative solutions to the current problems of urban congestion, and spark new forms of innovation [35,36].

The structure of the paper includes, Sect. 2 covers the numerous approaches to user-centered policy intervention. The level of improvisation for user-centered

policy interventions and future problems associated with city growth are described in Sect. 3. In the final section of the paper, which is Sect. 4, the conclusion is presented.

2 User-Centered Policies

The present state of urban development is inadequate to meet the requirements of its inhabitants. A lot of things come into play here; for instance, cities often grow to accommodate industrial demands rather than those of their residents. Improving the quality of life in future cities is an urgent matter that requires the active participation of citizens. Various methods can be employed to implement policies that prioritize users, as shown in Fig. 1.

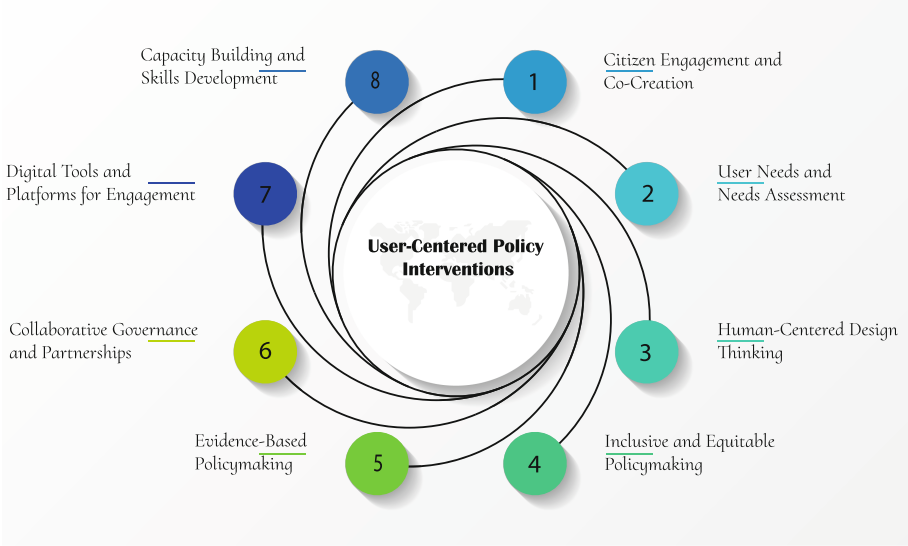

Fig. 1. Various methods for user-centered policy interventions

2.1 Citizen Engagement and Co-creation

When citizens actively participate in shaping policies, their unique perspectives, knowledge, and experience will shape emerging norms. Citizens will be happier and more engaged in the process of establishing policies as a result of this. The consultations were conducted through the use of public-private partnerships, a variety of community workshops, and participatory design methodologies [37,38]. In addition to exploring additional objectives of urban dwellers, this type of partnership guarantees that policies are made based on the grassroots experience

of occupants. Within the policy on citizen involvement and co-creation, feedback techniques may also be considered. The policies can be redesigned or revised based on the feedback that is gathered from online platforms, citizen dialogues at different venues, etc. [39–41]. By actively engaging citizens (as decision-makers), these processes cultivate a sense of ownership and trust, making the city a more liveable and equitable place for everyone.

2.2 User Needs and Needs Assessment

It is critical to understand and assess citizen demands in order to create future cities that are joyful. There are a plethora of resources available to help determine the user's requirements and conduct timely assessments. In order to receive social advantages from the government, policymakers often use qualitative data segments among different user groups, many of whom are disadvantaged and socially stigmatized [42]. Focus groups, user-focused interviews, ethnographies, surveys of the most vulnerable members of society, and in-depth interviews with members of the target community are some of the additional methods that contribute to this evaluation of user needs [43]. Data collected from the aforementioned resources helps lawmakers meet constituents' demands and objectives [44–46]. It suggests that user-centered policies and better laws could help with city life's pressing problems while also improving the quality of life for everyone involved [47].

2.3 Human-Centered Design Thinking

If you want to revolutionize service development and draft new laws to ensure that everyone can reap the benefits, try design thinking, an approach to design that puts people first by listening to and responding to their preferences and needs. To get insight into how users perceive city design, researchers can employ methods such as empathy mapping, ethnographic research, and user group interviews [48,49]. To accomplish the goals of user-centered design thinking, it is necessary to first cultivate an ideology among people regarding the creation of new designs; subsequent co-creation workshops might help with this [50,51]. Policymakers should reevaluate the entire lifecycle evaluation process of policy interventions to nurture the human-centered attention. Certainly, this paves the way for a human-centered design thinking approach while also bringing up the attractiveness, viability, and feasibility of citizens' various benefits to create future cities more liveable [52].

2.4 Inclusive and Equitable Policymaking

One of the most important weapons in the arsenal of the future city development plan is the inclusion and fairness of policymaking. Including those that have been excluded from the flow of progress up until this point is absolutely necessary in order to make the policy more inclusive. To ensure that the policy is both

inclusive and equitable, there have been modifications made to the legislative process wherever it was feasible to do so. These modifications have included the inclusion of individuals or groups of young citizens, families with low and middle incomes, people with disabilities, and various ethnic minorities [53].

Furthermore, inclusive policymaking requires anticipatorily evaluating the distributional effects of policy interventions on a variety of user groups. This is part of the process of inclusive policymaking. When legislators conduct comprehensive impact evaluations and equity analyses, they have the ability to identify potential disparities or unanticipated effects and then take steps to mitigate those concerns. For the purpose of achieving equality, it may be important to establish evaluation and monitoring systems in order to keep track of how far we have progressed, to distribute resources in a fair manner, and to adapt projects in accordance with the requirements of underprivileged groups [54]. Equal and inclusive policymaking also requires us to acknowledge the interdependence of urban issues and work toward a holistic solution. We need to break down barriers and work together across sectors if we want to make sure that economic, social, and environmental prosperity are all considered when formulating policies. When cities rule with equity and inclusion in mind, they may improve life for all city dwellers, level the playing field, and advance social justice [55].

2.5 Evidence-Based Policymaking

In most cases, lawmakers use data gathered from administrative records, social media, sensor networks, and crowd-focused polls to reach final decisions on policy-related issues [56,57]. Legislators can gain a deeper comprehension of urban systems' complex dynamics and user segments' diverse needs by utilizing data analytics and user insights. By utilizing this evidence-based framework, policymakers may zero in on the most effective initiatives and distribute funds appropriately. Policymakers can also improve results by conducting thorough evaluations and impact assessments to determine how effective policy interventions were and then adjusting those measures based on the facts [58].

Government transparency, accountability, and trust are all improved by adopting policies based on evidence. Making policy thinking and evidence clear can boost stakeholder support for user-centered initiatives and build consensus. And this approach encourages a growth mindset by giving lawmakers leeway to change regulations based on public feedback and scientific discoveries. Moreover, in addition to depoliticizing the decision-making process, evidence-based policymaking guarantees that policies are formulated on the basis of objective, data-driven insights, as opposed to being solely influenced by political expediency or intuition. Future cities can cultivate user-centric policies that are responsive, efficacious, and firmly rooted in the practical necessities and ambitions of their inhabitants by adopting an evidence-based methodology [59].

2.6 Collaborative Governance and Partnerships

Governments are increasingly recognizing the efficacy of collaboration as an instrument for formulating user-centric policies pertaining to future cities. This encompasses not solely the government-to-government (G2G) approach, but also collaboration between governments and citizens (G2C), resulting in enhanced inclusivity for the populace. A multitude of sectorial communities, including educational institutions, ethnic community organizations, non-governmental organizations (NGOs), small and medium-sized enterprises (SMEs), and large business houses, can participate in this approach's integration in order to identify holistic solutions [60].

Collaborative governance instruments, such as multi-stakeholder platforms, public-private partnerships, and community-based coalitions, can be utilized by politicians to foster dialogue, the exchange of information, and collective problem-solving. Additionally, collaborative governance enables the mobilization of resources, knowledge, and innovation to develop more effective, sustainable, and scalable user-centered policies through the utilization of the strengths and capacities of numerous partners [61–63]. Through the active engagement of communities and inhabitants as participants rather than passive recipients of services, collaborative governance fosters an environment that is more inclusive and conducive to participatory policymaking [64]. Collaborative governance that fosters a sense of ownership and shared responsibility appears to provide an opportunity for all stakeholders, including grassroots ethnic groups and local actors, to participate in policymaking. Thus, we will be able to design future cities more effectively in accordance with the desires and requirements of the communities that have previously inhabited them [65,66].

2.7 Digital Tools and Platforms for Engagement

The utilization of digital tools and engagement platforms is crucial for the development of user-centered policy interventions for future cities. Legislators may be able to facilitate more opportunities for citizens to share their thoughts and collaborate on solutions that address their needs and objectives by leveraging technology [67]. Nowadays, citizens can easily communicate through a variety of media platforms, such as interactive webpages/websites, many online forums, smartphone apps, and, of course, social media [68–70]. In order to better understand the demands, requirements, preferences, experiences, and expectations of users, legislators can make use of a variety of machine learning and data analytics methods. You can easily see how people are feeling about the development process, as well as what the current trends are. Politicians have been known to gauge public opinion through the use of design sprints, online workshops with participants of varying ages, and hackathons [71].

When it comes to future city policymaking and keeping track of citizen participation, one of the biggest benefits of digitalization is the increased openness and accountability it brings to the government process [72]. Consideration of collaborative participative approaches to urban development must also take into

account the needs of individuals who are not technologically adept, so it is imperative that they find a way to participate. Such citizens should be provided with both traditional methods of cooperation and the flavour of technology. In order to better comprehend the demands and desires of the people in relation to their future expectations of cities, this would undoubtedly enhance the efficiency of the system [73].

2.8 Capacity Building and Skill Development

The foundation of the cities of the future rests on enhancing human capacity and acquiring new skills. Because young people in metropolitan areas are increasingly tech-savvy and have lofty goals for their own skill sets, etc., future policy interventions should focus on the needs of these individuals. One way to address this is through user-centered policy interventions, which help identify needs and then inform decisions about how to best support their professional growth. Both official channels and citizen-led initiatives will contribute to this capacity-building process [74,75].

One of the components that will make future cities smart and its inhabitants smarter than today is education and training. With the use of residents' insights and experiences, lawmakers will be able to formulate new legislation and shape

Table 1. Design approach differences between the various methodologies.

Method used	Specific design approach
Citizen-Engagement and Co-Creation	Public-private partnerships, community workshops, participatory design methodologies
User-Needs and Needs Assessment	Collection of qualitative data through focus-group, user-focused interviews, ethnographics, surveys of vulnerable ones
Human-Centered Design Thinking	Empathy mapping, user-group interviews, workshops
Inclusive and Equitable Policymaking	Group interview of young and old citizens, low- and middle-income families, people with disability
Evidence-Based Policymaking	Data from administrative records, sensor networks, crowd-focused polls
Collaborative Governance and Partnerships	Government-to-government (G2G) and government-to-citizen (G2C) approach, non-government organizations (NGOs), small and medium-sized enterprises (SMEs), local actors
Digital Tools and Platforms for Engagement	Online forums, websites, smartphone-based apps, and machine learning and data-analytics methods
Capacity Building and Skill Development	Digital literacy through tinkering labs, civic centers

city development in response. There should be a number of initiatives aimed at skill development, such as community-based workshops, citizen involvement in different projects, improving digital literacy, and creating new civic centers to help the less fortunate with their digital literacy [76].

Building capacity also includes creating an environment where policymaking institutions value experimentation, creativity, and ongoing learning. The cities of the future offer fresh chances, places to learn, and comprehensive methods of development that allow us to reflect on and improve upon our previous successes and failures [77]. The establishment of tinkering labs for new discoveries across streams, the implementation of policy rewards systems, and the promotion of cross-departmental cooperation are all viable options.

Overall, we are able to provide a tabular representation of the differences between all of the methodologies, as shown in Table 1.

3 Challenges in Deployment of User-Centered Policies

Using the knowledge and experience of the people, user-centered policy methods are responsive, inclusive, and effective in improving city life. This is particularly true when it comes to accountability. Even if there are many challenges ahead, the user-centered policymaking approach to future city development is still in its early stages. There are numerous other challenges, but the most important ones are:

1. *Diversified user needs:* It can be somewhat challenging to provide an accurate assessment of user demands at times because they change over time. Policymakers will face a formidable challenge in conducting further explorations of this area with a user-centered approach [78,79].
2. *Inequality in access and digital division:* The digital revolution has brought numerous benefits, but it has also brought certain drawbacks, such as the fact that only very tech-savvy individuals can understand and respond to digital platforms [80–82]. As a result, other low-income families, those with disabilities, or others unfamiliar with digital services will be unable to take part in the groundbreaking user-centered collaborative movement.
3. *Data security and privacy concerns:* Concerns about data security, who holds the data, and the level of security for acquired data make data collection a challenging procedure. Persuading the public to uphold data security and privacy standards is an arduous task for legislators [83,84]. Because it raises both legal and ethical questions, maintaining faith in the process is a major challenge.
4. *Balancing competing interests and priorities:* One typical difficulty in user-centered policymaking is striking a balance between the diverse and, at times, conflicting needs and desires of numerous user groups. As lawmakers try to settle these disputes, come to compromises, and reach accords, it is critical that they do not ignore the needs of oppressed or underrepresented groups [85].

5. *Policy silos and institutional resistance:* There are a number of things that need to alter in order to adopt user-centered policies, including the institutional working culture, different power centers, and traditional policymaking processes [86]. Policymakers need to develop plans for different types of cooperation, management techniques, and accountable leadership if they want to solve these problems [87].
6. *Scalability and resource constraints:* Prior to incorporating user-centered techniques into policymaking decisions, it is crucial to verify the budget for user research, capacity building, resource development, and citizen involvement [88]. Among the most pressing issues facing lawmakers is the question of how to increase the magnitude of financial support.
7. *Accountability and impact measures:* The ability to make a final choice in policymaking processes depends on accountability and openness. Any policy's success was defined by its robust and well stated framework for evaluation and other policy metrics. Concurrently, user-centered interventions will suffer from lengthy and complicated decision-making procedures leading to effects that are hard to assess [89,90].

4 Conclusions

When creating a smarter city than the one we currently have, it is important to give careful consideration to the implementation of policy interventions that are user-centered. The strategies in question are superior in terms of their responsiveness, inclusivity, and potential for sustainability. Due to the fact that the "user" is an essential component of the development process as a whole, it is also simple to give priority to the preferences, requirements, and various experiences of individuals. The effect of interventions that create a sense of ownership and empowerment among residents is the creation of urban places that are collaborative, intelligent, co-creative, innovative, responsible, resilient, and people-centric. At the same time that user-focused group interviews provide information on the needs and desires of citizens who are not proficient with computers, digital resources guarantee that we will have complete transparency about policies. Overall, user-centered policymaking will result in an increase in the magnitude, timeliness, and priority of people's dreams for the future.

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A Preliminary Analysis on Parklets: Can They Contribute to the Realisation of a Walking Friendly City in Italy?

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Abstract. The most current city models banish the concept of a car-oriented city by promoting a series of actions and strategies that allow users to choose more sustainable solutions aimed at walking and cycling, and contemporarily promoting the concept of proximity city. In recent years, parklets have played a crucial role among the different strategies found in the literature to reach this goal. Parklets are built on equipped public areas used for parking cars and can also be an extension of the sidewalk. In this way, they become meeting places where you can stop drinking, eating, or relaxing. The present work focuses on a review of European and non-European literature on the implementation of parklets and the estimation of SWOT analysis in various contexts, emphasising the purpose of these interventions and considering the peculiarities of Italian urban areas where parklets have already been built or where they could be in the coming months. An analysis of the literature on mathematical modelling for vehicular traffic is also included, to enrich the paper with a rigorous description of the vehicle and pedestrian interactions in a street and to predict the impact of the actions of urban planning by evaluating the most suitable way to model the phenomena arising from the previously discussed urban interventions. These results can serve as a basis for local administrators to improve strategic planning and sustainable mobility in Italian cities.

Keywords: Parklets · SWOT analysis · Walking city · Urban and sustainable mobility · Tactical urbanism

1 Introduction

Since the end of the nineties, various tactical urban planning interventions such as the introduction of different technologies, sensors, and sustainable mobility have been carried out to encourage smarter and happier urban mobility and to reduce pollution [1, 2].

In particular, various urban planning actions have aimed towards models of proximity cities, where all services are within fifteen minutes walking distance and therefore consider a substantial modification to the scale model in the neighborhood. However,

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O. Gervasi et al. (Eds.): ICCSA 2024 Workshops, LNCS 14823, pp. 168–183, 2024.
https://doi.org/10.1007/978-3-031-65329-2_11

other interventions aim more specifically at the reconversion of spaces, especially after the recent pandemic phase [3, 4]. The latter, together with the need to make urban spaces more usable, have allowed the spread of some space reconversion actions, such as parklets [5, 6]. A study conducted by [7] underlined how parklets are solutions capable of supporting urban development and mobility planning in the post COVID-19 phase by improving the quality of public space and social distancing near shops and activities, benefiting from this micro-regeneration urban. This study also highlighted features for identifying and planning spaces where parklets can be deployed to improve sustainability and support post-pandemic recovery. They can be defined as a simple, low-cost tool for the recovery of public spaces as well as traffic-calming functions. The creation of parklets is a useful tactic for structuring a strategy aimed at reducing vehicular traffic for the benefit of mobility on foot and by bicycle. The explosion of the pandemic has highlighted the importance of managing public spaces in terms of both physical and social resources [8–10]. This is a way to raise awareness among citizens about the value of the road space currently used for parking. An increasing number of studies have highlighted how cars remain stationary and unused for 95% of their life cycle. These data require a reflection on how much precious space in our cities is dedicated exclusively to the parking of private cars, taking it away from other uses [11].

The design of a parklet varies depending on the wishes of partners or applicants. Designs may include seating, greenery, bike racks, or other features but should always strive to become a focal point for the community and a welcome gathering place.

Parklets involve the conversion of two or more parallel parking spaces, or three or four angled parking spaces. The configuration varies depending on the site, the context, and the desired character of the installation. Parklets can be installed on streets with a high pedestrian volume and local commercial activities but without public spaces for pedestrians. In cases where on-street parking is frequently obstructed owing to dispersed street activity, the city may permit the rezoning of one or more parking spaces through a permitting process, requiring the spaces to remain open and accessible to the public. These urban acupuncture initiatives have experienced remarkable success. Furthermore, they generate the opportunity to revitalise roads that were previously exclusively traffic axes [12]. Parklets can obviously have temporary characteristics and thus fall within the great voice of tactical urbanism, or they can have a definitive character to highlight the vision of public administration towards the management of urban space. Parklets, as small-scale, short-term urban interventions, can be the result of studies on urban improvement efforts often led by citizens and, in some cases, incorporated into more formal planning processes [13]. In Italy, such urban planning interventions are still struggling to spread due to various regulatory, economic, and social critical issues. What comes closest to the idea of parklets are dehors, structures with tables, and umbrellas, typically linked to the ownership of private catering establishments, while parklets maintain their characteristics of a public place. The following paragraphs provide an overview of the space-time diffusion of parklets in the world, outlining the benefits and critical issues, and defining a series of strategies and recommendations developed starting from the first interventions in the city of San Francisco. Subsequently, attention was paid to the importance of analysing test pilots and preparing SWOT analysis applied in various contexts and then defined in the Italian context.

A SWOT analysis required for the approach allowed to try to understand the opportunities that arise from the implementation of the aforementioned urban planning interventions according to the aspects of public or private actions, define the parameters for a better spatial-functional, economic, and social definition of the ecological and environmental well-being of populations; highlight the need for a multidisciplinary approach to the study of such interventions. Furthermore, the analysis of the mathematical models presented in the literature provides a wider perspective. Indeed, the issue of parklets installation can also be considered mathematically as an optimization problem in which the variables of the optimization are the position and shape of the parklets in a street. Trying to capture the features of the phenomena arising from the installation of parklets, we can choose the most realistic and suitable model to describe in a rigorous way the urban planning interventions previously discussed. Mathematical modelling also has the advantage of having on one hand a predictive function and on the other hand a fitting role, in the sense that by collecting data from street experiments, a mathematical model could be a perfect tool to analyse the data and from that, to create a function depending on the time, to analyse the macroscopic variables describing the dynamics of vehicles and pedestrians and the interactions between them.

2 The Spread of Parklets in the World

The first parklets were born in San Francisco in 2010 inspired by various Park(ing) Day initiatives [14, 15]. Such tactical urban planning interventions are having great success in numerous cities around the world [16], from New York [17] to London [18], passing through the most recent case of Bern, Switzerland [7]. To date, the largest number of studies on parklets has been conducted in the Americas. In particular, cities such as New York and San Francisco have introduced pop-up interventions on the streets and the reconversion of spaces such as car parks and squares [19]. A parklet pilot program began in Vancouver in June 2013, mapping and comparing the aforementioned case studies with those first implemented in San Francisco. Research has revealed that parklets begin as corporate-sponsored projects and evolve into community partnerships over time. Therefore, recommendations need to be developed for emerging and established programs in North America [17]. In the same context, the study addressed by [20] attempted to define which factors influence the feasibility and success of implementing parklets and public squares, and to define what the social and environmental outcomes of building parks and public squares are at a site-specific level and on larger urban scales. Research has emphasised promoting a wide range of uses and can serve as localised nodes. On a larger scale, design considerations can be used to change the perception of an area or neighbourhood development and have the potential to create a connected system that provides widespread circulatory and ecological improvements. Furthermore, creating programs that facilitate the installation of parklets and conversion of squares offers cities and communities the greatest value for money because they provide low-cost flexible spaces. Therefore, it is possible to state that parklets and public squares are feasible projects for providing green spaces and promoting pedestrian circulation within neighbourhoods and communities. In California, a series of studies have been carried out to define a series of advantages and disadvantages, as well as the common and different

characteristics of the "flex zone" and the parklet, to understand replicability in different contexts. In particular, the study conducted by [21] on three Californian roads provided ideas for the implementation of parklets in Japan.

The research clarified the common characteristics and differences between them relating to flexible zones and parklets and then explored their advantages and disadvantages such as their uniqueness as methods of producing outdoor spaces for eating and drinking. As regards the methods of implementation in Japan, the research underlined the importance of considering specific implementation methods in accordance with the purposes and existing conditions of the target area, responsibilities, systems and measures to ensure pedestrian safety, consistency with the relevant ordinances and their necessary revisions. Furthermore, in 2023, a study conducted in Southern California made a series of recommendations from the perspective of landscape designers, urban planners, and municipal officials interested in creating infrastructure for parklets and extended sidewalks, underlining the need to modify the permitting process and ensure that these interventions are long-lasting for the future design of the commercial street landscape [22]. Finally, the diffusion of such interventions and the creation of a network of multiple intervention points has been proven in the suburban landscape of Bryan, Texas, to have not only an impact on the economy and sustainability of transportation but also an impact on public health by increasing walking/reducing driving to obtain daily food. In fact, increasing the spaces used for walking and decreasing the propensity to use cars reduce the negative impacts of a sedentary lifestyle on residents. These interventions are related to low-capital investments and tactics that can be used by design professionals in collaboration with neighborhoods, local governments, and service organisations to begin to reverse the trend against sedentary lifestyles associated with the spread of chronic, costly, and debilitating diseases [23]. In Australia, similarly to the mapping of Vancouver, research was conducted in Melbourne, observing its spatial distribution, and identifying numerous urban design factors that provide capacity for parklets or inhibit them. The research also highlighted how smaller side streets can provide parking capacity, but many design conditions prevent this [24]. The study conducted by [25] has analysed the spread of parklets in Australia since 2005, outlining how these urban planning interventions have adapted to rapidly evolving social needs and priorities for economic activity, health, safety, socialisation and on-street parking, as well as changes in road function. Parklets have been absorbed into institutional urban planning practice since 2008 as a strategic tool to improve community engagement, test possibilities, and gain support for long-term spatial transformations. Since 2012, Australian commercial parklet programs have been developed to encourage local businesses to expand into street parking, to calm traffic, and improve pedestrian amenities. In 2022 the study conducted by [26] focused on the deployment of Melbourne's parklets reveals both the potential both obstacles to convert automotive space on streets to new uses, placing particular focus on the spread of hundreds of café parklets that have incrementally transformed Melbourne's streetscape to cater the new needs of hospitality businesses to provide socially distanced outdoor dining. The research revealed little dislocation where streets are devoid of pedestrians, including commercial areas such as indoor shopping centres, which have different urban morphologies that largely separate streets and cars from pedestrian spaces. They lack business-to-street interfaces in which parklets can intervene. In parallel in the city of

Melbourne and Stonnington in 2024 a study conducted by [27] outlined the evolution of the design, programming, approval process and reception of a "playful park", available for free public use, which was transformed and relocated between four urban contexts in Melbourne as an action of tactical urbanism. An analysis of its playful, portable, and flexible design points out three areas of innovation: testing new possibilities for governance and engagement post-COVID; incorporating adaptability and incremental adjustment into parklet design; serving as a platform for new social and spatial game modes [28]. On the Asian continent in 2023, a study focusing on the Japanese city of Higashi-Hiroshima was released. The behaviour of people who parked in street parklets was studied by analysing the data relating to the attributes and duration of people's stay in street parklets based on surveys of traffic volume, surveys on the measurement of comfort levels, and images from fixed-position cameras. The results showed that the number of pedestrians doubled during the experiment and that the attractiveness of the street space as a "fun place to spend time" was clarified [29]. On the African continent, the study conducted in [30] Jazan City was fundamental as a reference for all cities in the Saudi Kingdom, as it outlines parklets as a new idea with the simplicity of solutions capable of solving some social and environmental problems at the same time. Starting from theoretical investigations and rethinking the approach of future road design as a new redistribution of safer and more comfortable spaces for all users, as well as places of conviviality for communities. In the European and English contexts, several studies have been conducted over the last decade. In London, the transport company Transport of London (TfL) financed two parklets, and these interventions are aimed at street innovation, including one on a very busy commercial street in central London. In particular, the flexible design of the installation allowed it to be easily dismantled and/or moved to another site, while the flexible management of the project helped respond to feedback quickly. The basis for this intervention was a potential study of users, including the possibility of antisocial behaviour, which could have helped overcome objections to the project [31]. A study conducted by [32] analysed the "street experiments" (SE) and evaluated aspects related to upscaling, acceptability by the public or professionals and underlined that to date there are few studies that openly explore the value that citizens attribute to SE in context of daily life on the street. To fill this gap, this research analysed four different parklet and square interventions in three neighbourhoods of London, Munich, and Bologna. The results show that in all three cities, the majority of citizens evaluated the public life dimensions of these interventions to a greater extent than the benefits for active mobility, including the attractiveness of the streetscape, the provision of public spaces for stationary activities, and the creation of opportunities for social and civic interaction within neighbourhoods. A study conducted by [33] highlighted how such interventions and parklets, in particular, have been criticised when their installation leads to the long-term loss of parking spaces. This research has revealed substantial divisions of thought related to these interventions, underlining that they undermine small actions in support of decarbonising futures and healthcare infrastructures, which are the basis of broader and more urgent social and environmental gains. Another research conducted in Edinburgh, was carried out through the dissemination of an online questionnaire whose results underlined a considerable interest on the part of the community in the concept of parklet and its design and implementation. At the same time, a clear

division of support also emerged, and a statistically significant correlation emerged for people under the age of 45 and for residents who do not own a car who feel a strong sense of belonging to the community and are in favour of being present of parklets in their neighbourhood. In contrast, older and car-owning respondents were not in favour [34]. The city of Berlin has promoted the spread of tactical strategies such as parklets to facilitate and make possible active mobility integrating street observations and brief surveys in different neighborhood streets. This research has also revealed that parklets contribute to creating liveable streets, replacing car parks with public, green, and multi-functional spaces for active mobility users. Furthermore, parklets alone do not directly influence active transportation behaviours. However, in combination with traffic calming interventions, parklets facilitate active mobility by prioritising pedestrian needs to rest and walk on a safe and lively street. Overall although parklets are not great motivators in themselves, they can be strong facilitators of active mobility if combined with sufficient greenery and placed on slow-moving neighbourhood streets [35]. In recent decades, many European and non-European municipalities have temporarily closed roads for vehicular traffic to open them to people and promote the community.

3 SWOT Analysis

SWOT analysis is a simple and effective strategic planning tool that is useful for highlighting the characteristics of a project, a program, an organisation, and the consequent relationships with the operational environment in which it is located, offering a reference framework for the definition of strategic orientations aimed at achieving an objective. SWOT analysis allows us to think about the objective to achieve while simultaneously considering both internal and external variables. The internal variables are part of the system and on which it is possible to intervene; the external ones, not depending on the organisation, can only be kept under control, to exploit the positive factors and limit the risk factors that compromise the achievement of the set objectives. The SWOT Analysis was constructed using a matrix divided into four fields, in which we have Strengths, Weaknesses, Opportunities and Threats. The advantages of an analysis of this type can be summarised in three points: the in-depth analysis of the context in which one acts, made possible by the preliminary observation and collection of data and their skillful interpretation, translates into a precise delineation of strategies; the continuous comparison between the needs of the organisation and the strategies adopted leads to an enhancement of the effectiveness achieved; it allows greater consensus on strategies to be reached if all parties involved in the intervention participate in the analysis. The limits linked to this type of analysis are essentially: the risk of describing reality in a too simplistic way; the risk of subjective procedures by the valuation team in stock selection; the requirement of a context of partnership that, if not achieved, leads to the risk of a disconnect between the theoretical and the political and pragmatic level. This type of analysis can therefore only be a good starting point for the evaluation of a potential feasibility study of the aforementioned interventions. For the definition of the SWOT analysis related to interventions on urban spaces, a critical analysis of the literature relating to emblematic case studies of interventions on urban spaces, such as those conducted in the city of Santa Monica through the pilot case study for main roads carried out in 2019, is fundamental [36].

3.1 SWOT Analysis Applied to Parklets

Cities vary greatly in size, history, development pattern, design, shape, and citizens' attitudes towards public spaces. Parklets fall under the classification of emerging infrastructure because, rather than being planned and imposed from the outside, parklets emerged from within as a response to people's needs. The study conducted on an American urban scale has revealed some indications on how to improve the implementation processes of both parking lots and parklets [37]. The means of communication and dissemination of these interventions are also fundamental, as demonstrated by the study conducted by [38] applying a case study approach and considering social network analysis to investigate the diffusion of parklets, an innovative way of transforming car parks into green and public spaces on Twitter. The results of this research demonstrate the complexity of the responses deriving from the diversity of the participants and their activities, as well as from the variety of relationship structures and at the same time underline the importance of the technologies and possibilities offered by Web 2.0 to address urban challenges through collaborative models of urban governance. Likewise, the dissemination of digital tools relating to basic information, a map of the parklet's potential, a design tool and a form for requesting the necessary permits were fundamental for the diffusion of such urban planning interventions in Vienna, especially since a dissemination campaign among citizens' organisations and through social media channels [39]. In the same city the study carried out by [40] highlighted that while such tools could inform people about the possibilities in the city, other aspects, such as previous involvement, play an essential role in the perception of new tools and their potential adoption. Over the years, SWOT analysis has been performed to define the pros and cons of implementing parklets in various parts of the world. For example, a study conducted on the city of Lubumbashi in the Democratic Republic of Congo (Africa), which has recorded strong demographic growth and a large, rapid and anarchic urban spatial expansion, has underlined how important the streets are in the urban context, underlining their role as a place of transition and first-rate social diversity [41]. The study conducted by [36] in the city of Toronto released a SWOT analysis underlining the importance of spreading a collaborative approach between citizenship institutions and associations for the temporary development of urban interventions with reference to the transformation of the car parks of a suburban shopping centre into a meeting place. The results of this research outline a reference framework that facilitates the evaluation of the impact of public spaces, while providing a tangible and real application through the implementation of a parking redevelopment project. The study conducted by [42] in Vancouver aims to expand the parklet deployment program to new locations in North Vancouver with the goal of addressing the complex issue of social integration within the city. The research outlines through a SWOT analysis a series of recommendations to help policy makers guide the City of North Vancouver through the process of community development and partnerships. In particular, the study promoted an analysis of the interested parties and the environment which includes SWOT and PESTEL analysis indicators on the feasibility of such interventions [42]. Starting from these studies it was possible to construct Table 1 with a SWOT analysis divided into 3 macro areas, namely landscapes and resources (connected to regulatory and legal aspects in the field of urban planning

and mobility and use of resources), economic and social aspects (relating to the different types of parklet users) and health.

Table 1. Comparative SWOT analysis related to the study of various parklet interventions implemented.

Strengths	Weaknesses	Opportunities	Threats
Landscape and resources			
– Reduction of car spaces and promotion of soft mobility – Increase in poles of attraction for food and beverage – Increase in poles of attraction for recreation and wellness – Increased liveability of street spaces – Improved planning of parking areas (especially near the historic centre)	– Lack of town planning regulations – Lack of functional geometric standards for roads – Need to define actions to contrast private transport and improve walking and local public transport – Seasonal use due to weather – Potential dissatisfaction from residents and city users	– Improved urban development – Increased meeting places – Creation of places for various segments of the resident and non-resident population – Improvement of pedestrian and cycle mobility infrastructure – Increase in the number of seats in the area concerned – Presence of temporary covers for annual use – Creation and definition of standards and guidelines for planning, design and management – Analysis of past case studies to gain experience	– Overestimation of the expansive phenomenon when planning city development – Reduced demand for the settlement of economic activities – Limited synergy with associations and entrepreneurs – Risks of transformation of some areas into less utilised districts – Weaknesses of public transport and school system in the examined area
Economic and social aspects			
– Increased proximity trade as opposed to large-scale distribution – Balanced integration between the productive economic system and the social system – Definition of a commercial and proximity network for the urban area and beyond – Increased community involvement – Very low-cost operation for the city with corporate sponsorship	– Reduced number of interventions in proportion to population density – Lack of financial resources (budget constraints) that may prevent the necessary interventions from being carried out	– Redevelopment of disused urban spaces – Creation of new urban cultural spaces – Improving the safety of pedestrian traffic – Greater liveliness of citizenship and spirit of hospitality – Enhancing and relaunching the establishment of businesses in the area – Redevelopment of the built heritage and use of urban spaces to reduce housing density	– Rainwater management and irrigation systems – Security, damage and vandalism – Disputes between small businesses and the city – Loss of parklet benefits – Misuse of space

(*continued*)

Table 1. (*continued*)

Health			
– Reduction of sedentary lifestyle and related diseases – Reduction of vehicular traffic emissions	– Reduced presence and use of parklets and thus reduced psychological well-being and health	– Improvement of psychophysical well-being – Increasing green or equipped spaces to increase walking and/ or also encourage sporting activities	– Possible injuries in outdoor areas near parklets

The above table therefore highlights how different sectors are connected to the benefits and critical issues produced by the implementation of parklets. If on the one hand the lack of legislation or the lack of regulatory homogeneity between the various states creates critical issues of implementation in a continuous version and not only as temporary installations, on the other hand the need to increase social spaces and spaces for complement of the economic life of cities for general benefits. To promote the diffusion of these installations on a continuous basis, it will be necessary to carry out greater training and information campaigns for citizens to make them understand not only that their installation has the advantage of being reversible and, therefore, they can also be tested for predetermined periods, to verify its effectiveness and any critical issues. Finally, the idea that the parklet can be understood as a simple, low-cost tool for the recovery of public space, also with traffic calming functions, must be promoted.

Therefore, of fundamental importance is the study on the actual and project status of the areas and infrastructures to be donated to parklets together with a study of the demand for transport and diffusion of services present in the analysed area, both current and potential. The study also reveals that the key issue also in the Italian context is to guarantee the introduction of parklets in appropriate places that will encourage their use as demographic data and possible users change (citizens, tourists, commuters).

The SWOT analysis preliminarily highlights positive and negative aspects of previous interventions and suggests improvements for new installations. At the same time, it is essential to correlate SWOT analyses with more in-depth studies on transport supply and demand and current regulations in the transport and transport sector, considering individual case studies.

Furthermore, evaluating the relative correlations between factors is very important and useful.

In fact, a more in-depth study of the literature relating to the mathematical models that describe user behavior and the discretization of mobility infrastructures and services is necessary to better describe the analyzed contexts.

Furthermore, it is essential to be able to calibrate the equations and therefore describe the phenomena from a mathematical point of view, giving a more robust justification to the preliminary results or to the results deriving from actions such as data acquisition campaigns through surveys and questionnaires or even the drafting of calculated preventive scenarios through dedicated software or even the comparison of results between case studies.

4 Mathematical Modelling Literature

In order to help with the analysis of the different interventions possible in an urban context, bibliography research about mathematical modelling is also presented in this section. First attempts at developing the mathematical models for traffic flows were undertaken by Lighthill and Whitham [43], Richards [44], Greenberg [45], Prigogine [46]. More details about the results obtained could be found in Whitham 's book [47].

The mathematical models more used in literature can be grouped into the following categories: cellular automaton approach, mean field game theory, a microscopic approach given by the force-based models, a macroscopic approach devised by the hydrodynamical models, and the kinetic approach that could be considered in a mesoscopic scale, between the two previous mentioned models. Cellular Automaton simulation [48, 49] is based on a mathematical idealisation in which space and time are discrete and physical quantities are evaluated on a set of discrete values. Cell state is also an important parameter. Every cell has one certain state value from a finite set of possible states. Consequently, the continuous variables like length, speed and time have to be discretized for the sake of effective modelling. The idea is to divide the simulation domain into cells. These cells must be regular, so that they form a regular grid. The grid structure can form different patterns depending on the performance of each to a particular simulation. The basic forms are triangular grid, rectangular grid, and hexagonal grid. Mean field game approach [50–52] is a mix between the game theory and the mean field theory. The game theory part enters because each agent (vehicle or pedestrian in our case) is considered as a player in the sense of game theory and each player behaves in order to reach a Nash equilibrium, that is to say that he is rational, and he tries to take the best decision for himself but also for the other agents (players). Mean field theory enters in the sense that one starts from a microscopic formulation and then one passes by the limit for N that tends to infinity, where N is the number of the agents, to a mean field formulation in which mean and average macroscopic quantities are considered. The approach is like that of stochastic or classical mechanics.

Another approach used to describe pedestrians and vehicles movements is the force-based one [53]. In this case, the idea is to represent each pedestrian or vehicle like a particle that obeys to the Newton laws of dynamics. Most of the force-based models describe pedestrian dynamics qualitatively fairly well but there are only poor quantitative descriptions of these phenomena. Usually, implementations of the repulsive force require additional elements to guarantee realistic behaviour, especially in high density situations. Sometimes strong overlapping of pedestrians or negative and high velocities occur as artefacts of the force-based description. This kind of model has the limitation that it doesn't consider the anisotropy of the space around a pedestrian, because we usually consider only the people in front of us and not behind; furthermore, the physical contact doesn't product a repulsion strength like for two particles, therefore this kind of model sometimes can lead to an unrealistic choice of parameters. The Centrifugal Force Model (CFM) is an attempt to overcome these issues. In this case the force is anisotropic since its range of influence is reduced to the range of vision of pedestrians, which is 180°, furthermore it describes clearly "collision detection technique" to deal with the problem of overlapping pedestrians and succeed in managing collisions among pedestrians, which can be interpreted as a failure of the avoidance-mechanism expressed in the form of

repulsive forces. Therefore, under some additional assumptions, this kind of model could be improved. A totally different approach with respect to the previous is the macroscopic approach. These kinds of models are based on fluid dynamics [54–57]. They try to describe complex systems, i.e. interactions between particles in a dynamic context. The name comes from the analogy with the equations used in the fluid dynamics field. The idea is to see each pedestrian or vehicle like a particle in a fluid and therefore to use the same equations used for fluids moving in a pipe for example, to describe the dynamics of people or vehicles in a road or in a room. The feature of this approach is to deal with variables that are macroscopic like local average of density, velocity, flow, and the equations used are partial differential equations (PDEs) like continuity equation (for the first order models) with suitable initial conditions and boundary conditions or constraints in order to take into account the limitation or the obstacles present in a road or in a room. Sometimes also the moment equation is included and therefore the velocity variation, for second order models.

The last model analysed is based on the kinetic approach [58, 59]. The idea for the modelling of vehicular traffic is based on the choice of an intermediate representation scale between the macroscopic and the microscopic ones, technically called mesoscopic. Rather than looking at each single car or pedestrian of the system, like in the microscopic approach, a distribution function is introduced depending on the microscopic state of the vehicles. The distribution function represents a measure of the number of vehicles at a certain time, position, and velocity. The knowledge of the distribution function enables one to recover the usual macroscopic variables of interest as local averages over the microscopic states of the vehicles. Then, the macroscopic and microscopic approach are mixed here. In this case we deal with the Partial Differential Equation like continuity equation or Boltzmann equation, depending on the specific application to simulate. All the previous models describe essentially the dynamics of vehicles and/or pedestrians in a street or in a closed room, but also the variables of position and shape of the parklets on a street could be included in this kind of models, by reformulating them in a suitable way.

4.1 Analysis of Advantages and Disadvantages for Each Mathematical Model

Advantages and disadvantages for each mathematical models analysed are summarised in the following:

- Cellular automata: In this case the approach is based on rules behaviour and not on equations and this aspect could be considered an advantage because it could simplify the description of the phenomena occurring in the streets. On the other hand, they furnish a discrete idealization of the PDEs (Partial Differential Equations) and through this idealisation the description could be less realistic.
- Mean field games: In this kind of model, the mean field limit is used to obtain nonlinear PDEs, so that some average quantities are deducted from complex nonlinear PDEs, and this is the advantage of this approach. Contemporary the hypothesis of rationality considered from the game theory is restrictive and not realistic. One of the criticisms of game theory, as applied to the modelling of human decisions, is that human beings are, in practice, rarely fully rational.

- Force based model: This kind of models are detailed but they do not consider the chaotic description of the street phenomena and vehicle and or pedestrian movement. Furthermore, they are computationally expensive, because they describe the dynamic of each pedestrian or vehicle by ODEs (Ordinary Differential Equations) and for this reason the number of equations could be very high to be simulated in a short time.
- Fluid dynamics models: These models have the advantage of being computationally not expensive, but they lose something in terms of a detailed description of the situations. Indeed, they deal with macroscopic quantities, it is to say, mean or average quantities that don't take into account the nature of the single vehicle or pedestrian in the vehicle flux.
- Kinetic models: This last model is a mix of the previous two models and takes the advantages of both. On one hand the continuum hypothesis (the idealisation of vehicle flux like fluid flux in a continuum) is a bit strong and not realistic, because the cars or pedestrians are not particles in a fluid, but their movements are discrete, with spaces between the elements that take part in the street's phenomena and interactions.

On the other hand, this kind of model can be improved by introducing a granular nature of the flux that mathematically corresponds to the introduction of some class of velocities which the vehicles belong to. In this way we can be more detailed about the description of vehicle fluxes and at the same time, we can overcome the disadvantage of the huge amount of time to simulate a microscopic model.

The aim is to reach a realistic mathematical model describing the vehicles/pedestrian dynamics in a case study in order to simulate traffic components evolution in time as well as how it changes with surrounding environment. It allows to support the SWOT analysis in the investigation of an optimal plan and design of parklet implementation for adaptive and durable transformation of spaces.

5 Conclusions

In this study, the analysis of literature on the space-time diffusion of tactical urbanism interventions such as parklets is carried out as the first step of research analysis. Subsequently, this work shows a comparison of case studies, highlighting the limited presence of parklets in the Italian context and providing some specifications relating to the potential and critical issues of implementing such interventions through the definition of a SWOT analysis. Specifically, the research focused on this type of analysis to outline in a general and local (Italian) way the potential of the territory with particular reference to the small urban scale and at the same time underline the weaknesses and threats generated by users. A first analysis shows that the advantages would be for everyone: for shops since a city re-designed on a human scale improves everyone's life, increasing the feeling of well-being, optimism, and propensity to shop; for apartment owners because urban villages become quieter and less invaded by cars and smog, they automatically enhance everything they contain, starting with the apartments which rise in value; for citizens because a tidier, cleaner, and safer city constitutes a natural invitation to live it to the full; furthermore, the presence of controls and attention to detail favours social relationships which are more open and constructive with a strong reduction in vandalism and petty crime. This research underlines the need to disseminate greater

challenges and for strategies not only of tactical urbanism but also of a legal and regulatory nature and finally also connected to the development of digital placemaking and how these strategies can contribute to broader smart city initiatives. A new generation of commercial "parking cafes" has emerged during the COVID-19 pandemic, facilitated by American and Australian local governments to support the hard-hit hospitality sector. Their design and construction show continuous innovation, growing scalability and professionalism, but also standardisation. Such examples could be particularly useful in the Italian national context and could be useful for the definition of national recommendations and guidelines reiterating the strong similarities in spatial contexts, needs, risk factors and technologies that have defined this practice in different global contexts. Through this document, the benefits and critical issues arising from the implementation of parklets instead of car parks are researched, analysed, and evaluated. The creation of parklets must be based on a series of problem definitions and possible scenarios considering a process of small-scale interventions scale and from bottom to top. Starting from the problem of car-centric urban areas, it is necessary to analyse the national and local regulatory limitations as well as structural and infrastructural ones.

Of fundamental importance is the analysis of the pedestrian context and the possibility of greater pedestrian use and valorisation as well as a cycle path. To help with this analysis, mathematical modelling literature is also included, underlining the advantages and disadvantages of each type of model considered. This last analysis brings us to prefer a kinetic model approach to describe the insertion of parklets in a street and the consequences of this intervention in vehicular traffic. Indeed, in a kinetic model we can also consider the capacity of the street and a possible narrowing of the street, by varying the maximum capacity and density of vehicles and/or pedestrians. In this way, a parklet installation could be simulated and consequently the effect on the traffic could be analysed and described. Furthermore, an in-depth study on the user demand present in the area will allow us to attract a greater number of people of all ages to socialise through the establishment of these car-free spaces. This article therefore demonstrates that tactical urban planning can be an effective methodology to improve the use of urban spaces or their reconversion in the short term, underlining the need to carry out more in-depth and multidisciplinary studies.

This research confirms, through a literature and comparative analysis of different case studies in different global contexts, how the SWOT analysis is an effective operational tool for context analysis and therefore allows us to highlight the strengths of the project an event in the territory, its weaknesses, opportunities, and threats. This allows us to carry out an assessment of the utility/disutility of creating parklets and therefore allows us to make the "optimal" decision to achieve one or more strategic planning objectives.

The research also underlines the need to resort to a mathematical approach in continuation of the SWOT evaluation to better correlate the factors that describe the demand and supply of transport connected to the implementation of the interventions and therefore be able to simulate a series of scenarios as the aforementioned changes factors and their correlations.

Acknowledgments. This research was granted by PNRR-M4C2- I1.1 – MUR Call for proposals n.104 of 02-02-2022 - PRIN 2022 – ERC sector SH7- Project title: MOVING StEPS - MOVING from Street Experiments to adaptive Planned Solutions - Project Code 2022BLK9TS - CUP Code D53D23011060006 - Funded by the European Union – NextGenerationEU. The authors A. R., M. R, G. V. acknowledge the support by G.N.F.M. of I.N.d.A.M.

Disclosure of Interests. The authors have no competing interests to declare that are relevant to the content of this article.

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A Literature Review on Street Experiments: A Preliminary Step Towards Adaptive Planned Solutions from Bottom-Up Experiments

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Abstract. From the first parklet established in 2005 in San Francisco by Rebar, an art-design-activist organisation, to the latest urban experimentations launched during the Covid-19 pandemic, street experiments are an established trend in the tactical urbanism. During these experimentations, city streets become key spaces not only for testing alternative form of transportation, integrating various urban activities, such as commerce, recreation, social interaction, and leisure, but also for suggesting innovative models for environmentally friendly public spaces. These reversible and temporary practices often originate from a bottom-up approach and seek to raise public awareness about current and widely debated issues such as sustainable and active mobility, as well as improving quality of life. The increasing understanding of their beneficial impacts is supported by numerous research and studies proposed by the scientific community. However, cutting-edge framework for street experiments has not been developed. This paper is part of an ongoing research and it seeks to address this gap through a systematic and critical literature review. In particular, the research examines the potential of street experiments, specifically parklets, with the aim of proposing operative process able to change these temporary experimentations in adaptive planned solutions, to transform and enhance the urban landscape sustainably, to promote active mobility, and enhance accessibility.

Keywords: Accessibility · Bottom-Up Approach in Urban Planning · Parklets · Participatory Planning · Sustainable and Active Mobility · Tactical Urbanism

1 Introduction

The transformations of the streetscapes have been significantly influenced by the aims of the current urban agendas (i.e. active and sustainable mobility and liveability of city). Over the last two decades, several cities throughout the globe have seen changes in their streets, adopting a 'tactical urbanism' strategy that involves temporary experimentation.

These transformations have been often object of criticisms, but, at the same time, they have been widely recognised with great optimism by public opinion. Nowadays, perhaps due to the impact of Covid-2019 epidemic limitations, there has been a rise in

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O. Gervasi et al. (Eds.): ICCSA 2024 Workshops, LNCS 14823, pp. 184–196, 2024.
https://doi.org/10.1007/978-3-031-65329-2_12

street experiments aimed at raising public awareness about pressing and highly discussed issues like sustainable mobility, as well as improving quality of life. Furthermore, they serve as a vital element in the field of urban planning.

Within this framework, city streetscapes lose their primary purpose as places for vehicular traffic and instead transform into pivotal areas that serve many functions and accommodate diverse users. These spaces are used for experimenting with alternative modes of transportation and facilitating a range of urban activities, including commerce, recreation, social contact, and leisure. In this context, these concepts are regarded as unique prototypes for environmentally conscious communal areas.

City street experiments, as described by Bertolini, refer to «intentional, temporary change of the street use, regulation and/or form, aimed at exploring systemic change in urban mobility, away from "streets for traffic", and towards "streets for people"» [1, p. 735].

Therefore, within the realm of tactical urbanism, street experiments have become a well-established trend, with Parklets being the most well recognised instances [2–6].

In 2005, Rebar, an art-design-activist organisation, made a payment to a parking metre in downtown San Francisco for a duration of two hours, thereby creating the first parklet. The roadway was adorned with a seat, a tree, and some sod. This action later resulted in the establishment «of an official planning programme in San Francisco and the yearly international event Park(ing) Day», which seeks to stimulate a significant discussion on the importance and on desire for a different public space [2, p. 165].

Parklets, along with other street experiments, exemplify the complex issues that modern cities must deal with, such as financial limitations, fast urban growth, and increased population density. These urban initiatives place additional demands on the availability of public space. Furthermore, parklets serve as economical and semi-permanent projects that align with the need of finding new models for public space. These projects are established via a public-private partnership model [2, p. 165].

This has facilitated their swift global dissemination and an increasing achievement of their implementation. Moreover, other instances were introduced in response to the need for social isolation during the Covid-19 epidemic [7].

Research on tactical urbanism, street experiments, reorganising of the public spaces [8–11], and parklets have shown significant growth and diversification in the last decade. They include several disciplines, ranging from social science to environmental science. Some researchers contemplate the evolution of phenomenon and its actual potential to revolutionise urban mobility [1]. Other scholars scrutinise the idea of formalising these temporary experiments into a permanent framework via systematic planning, considering the significant positive reaction they received during the worldwide epidemic [12–15]. Furthermore, many academics have engaged in the task of cartography, emphasising the distinctive environmental characteristics of these events on a worldwide scale [7], while others have examined the progress and transformation within more limited settings to highlight the strengths and vulnerabilities [16]. However, cutting-edge framework for street experiments has not been developed.

Starting from these considerations, this study proposed is part of an ongoing research that examines the potential of street experiments, specifically parklets, with the aim of

proposing operative process suitable and able to change these temporary experimentations in adaptive planned solutions, to transform and enhance the urban landscape sustainably, to promote active mobility, and enhance accessibility.

Specifically, the objective of the study is to address this gap by identifying relevant literature and establishing a comprehensive understanding of the current state of knowledge in the field. In order to achieve this aim, the paper is organised into four sections: After the *Introduction* (1), the *Methodology* is described (2), before going in a depth detail by defining *The state of art on street experiments* (3). The *Conclusion* (4) discusses the results obtained from the literature evaluation, as well as the main findings of the study, and the research agenda.

2 Methodology

The study aims to analyse the existing literature on street experiments in order to create an innovative framework through a methodical and evaluative literature review.

Following the prevailing approaches and methodologies [17, pp. 4–11], the literature review is conducted in five steps, described in Fig. 1: 1. Problem formulation; 2. Data collection; 3. Data evaluation; 4. Analysis and interpretation; and 5. Public presentation.

The primary step, *Problem formulation*, aims to identify and define previously the research questions to guide the literature review, and then, to determinate the criteria for inclusion and exclusion. In particular, the literature review goals are to establish the phenomenon of the street experiments in the current context, to frame its evolution, to highlight its strengths and weaknesses, and to understand its role in the cities' transformation and in the urban planning.

For these goals, the literature review starts at first clearly defining the topics necessary to delimit the research, and then, selecting keywords to further filter search results. The first are Tactical Urbanism, Street experiment and Parklet/parklets; while the second are Active Mobility, Built Environment, Street experiments, Sustainable Mobility, Urban design, Urban planning, Walkability.

The second phase, *Data collection*, begin with the choice of Scopus as a search database among the many currently available [18].

The queries utilised for the research of the relevant literature on Street Experiment contained into the Scopus Database are: Tactical [and] Urbanism, Street [and] experiments, parklet/parklets.

In the early search, a considerable number of results has been selected [19]. Thus, subsequently, the search has been delimited by filters.

It considers the chronological range 2012–2024 (first trimester) as time span. The 2012 was chosen as the starting year of the survey because it was observed that before this date the contributions of the different topics are rather sporadic and not continuous.

Then, the subject area taken into consideration are Social Sciences, Engineering, Environmental Science, and Art and Humanities. While Article, Book chapter, Book, Conference paper, and review, in English language, are the document types selected.

In order to further delimit the field in the street experiment topic, the selected keywords have been searched in the title, abstract and between the authors' keywords.

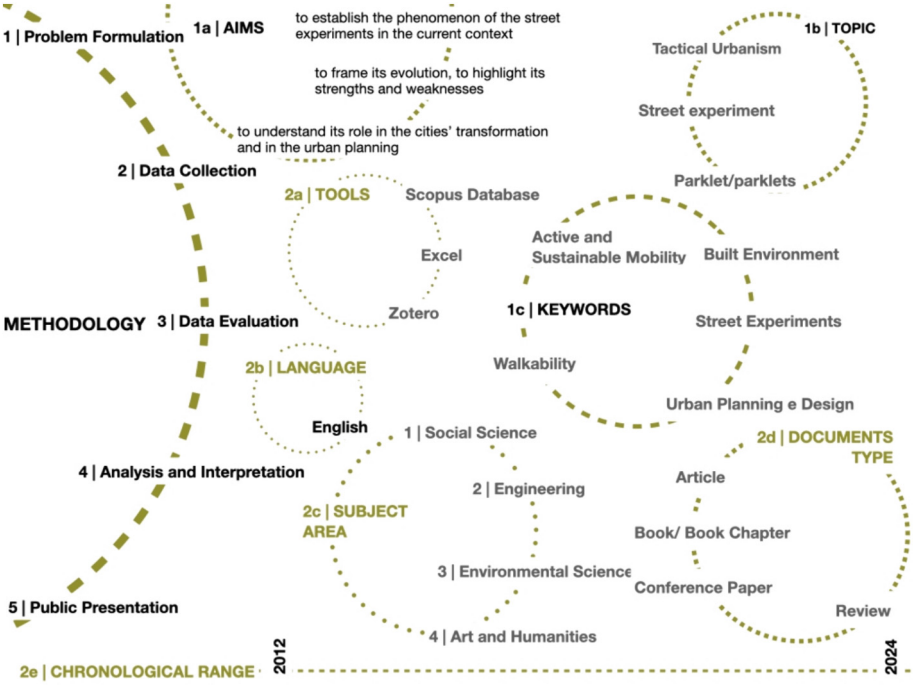

Fig. 1. Methodology's Scheme (MSP).

Ultimately, 485 is the total number of contributions selected. The different and numerous data and information of the several contributions was collected in an Excel sheet. In addition, all contributions were recorded in a Zotero library dedicated [20].

The study has been then carried out in the next phase, *Data evaluation*, through reading the abstracts to evaluate the usefulness of the sources found. After discovering a valuable article, the mentioned sources were examined to include further sources in the bibliography. Subsequently, the evaluation procedure of the sources is conducted with the objective of determining the ones that are most pertinent to be included. Lastly, the analysis and the interpretation of the data has been conducted using a thematic approach. Identifying patterns in literature, such as recurring themes, ongoing debates, and research gaps, has shown to be especially important.

This paper presents the initial findings of a study that focuses on contributions related to street experiments and parklets. It specifically examines contributions that mention "street experiment" in their title, text, author's keywords, as well as contributions that refer to parklet/parklets.

3 State of Art on Street Experiments

3.1 Quantitative Synthesis

The research of the relevant literature on street experiment contained into the Scopus Database has selected about 485 contributions, in English language, divided into Article, Book chapter, Book, Conference paper, review. As mentioned above, it has been investigated the chronological range from 2012 to 2024 (first trimester) as time span.

As shown in the Fig. 2a, from chronological point of view, it is possible to note a significant increase of the contributions in reference to the topics, from 2018 (from a distribution of 2–3% between 2012 and 2017 to 8% in 2018, a peak of 18% in 2022).

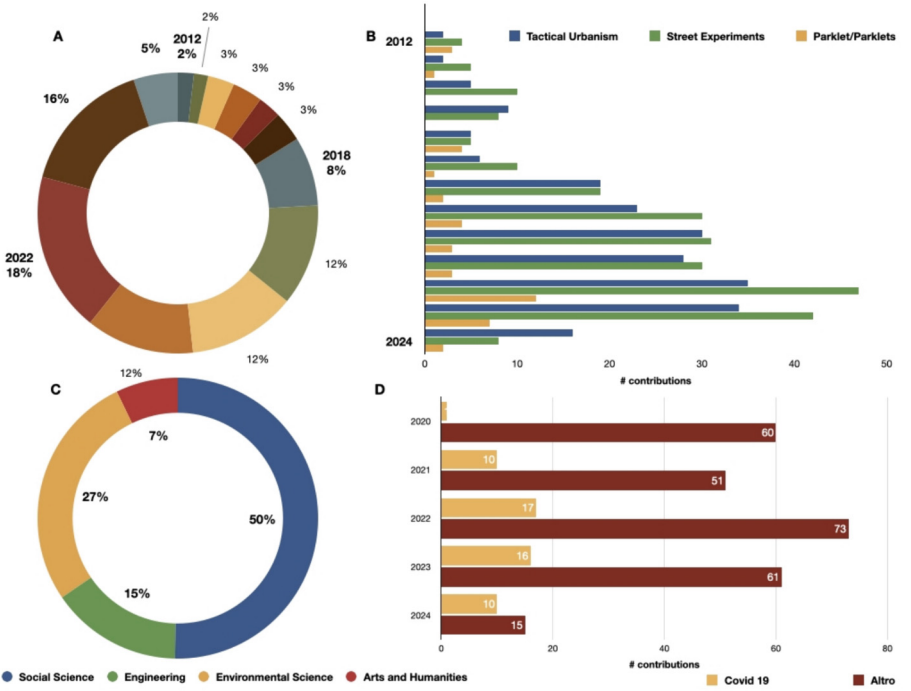

Fig. 2. Graphitisation of the research results. Distribution of the relevant literature selection from a point of view: A. Chronological; B. Topic; C. Subject Area; and regarding Covid 19 pandemic (MSP).

Moreover, as shown in Fig. 2b, among the three topics, the contributions focused on street experiments are considerably higher, especially in 2022. As for the references to Parklets, the first years are infrequent and of little number, while there has been a consistent increase since 2016, with a significant increase in 2022 (about three times more than 2016). As previously said, the chosen themes are the focal point of investigation in several disciplines. The planned study primarily focuses on the fields of Social Science, Environmental Science, Engineering, and Arts and Humanities.

The distribution of the relevant literature selection is shown in Fig. 2c and is as follows: Social Science (50%), Environmental Science (27%), Engineering (15%), and Arts and Humanities (7%).

Another finding that arises from this quick quantitative assessment is the dissemination, starting in 2020, of research that investigates street trials generated by the Covid-19 pandemic (11%).

The geographical situations under investigation are different. Europe, Canada, and the United States are the primary areas of investigation, with further exploration of other settings including Latin America, Asia, and Australia.

3.2 Towards a Thematic Framework

The early analysis and the interpretation have been carried out for the contributions related to street experiments and parklets, previously selected because they mention "street experiment" in their title, text, author's keywords, as well as contributions that refer to parklet/parklets.

This phase, characterised by a thematic approach, allowed us to identify recurring themes, ongoing debates, and research gaps.

In particular, from the contents of the contributions, it is possible to identify 5 general themes, later explained and here summarise: 1. The phenomena of street experiments and its connection to urban mobility; 2. Legislation, conflicts, and criticism; 3. Involvement of stakeholders and communities, and assessment by citizens; 4. Street experiments prompted by the Covid-19 pandemic; 5. Ensuring safety.

3.2.1 Street Experiments Phenomenon and Its Relationship with the Urban Mobility

Numerous scholars investigate the phenomenon of street experiments. Furthermore, Luca Bertolini has the highest number of citations. In 2020, he conducted research to define street experiments and to identify the different intervention types, considering their specific environment and characteristics. The aim was to determine whether street experiments can effectively contribute to the improvement of urban mobility [1, 21].

These purposes are essential in the special issue of *Journal of Urban mobility*, entitled *Street experiments*, edited by Enrica Papa (University of Westminster), Benjamin Büttner (Technical University of Munich School of Engineering and Design) and Luca Bertolini (University of Amsterdam). It is an open reflection on the phenomenon of street experiments, their connection to urban mobility, and their potential as catalysts for transformative change in urban mobility.

Many studies focus on the dynamic development, programming, permission procedure, and public acceptance of street experiments, particularly parklets, frequently using real case studies as examples [5, 22–26].

Krity Gera and Peter Hasdell's research aims to comprehensively analyse street experiments and their impact on mobility and on access. They specifically focus on the influence of gender on the social-spatial environment [27].

Simultaneously, another study seeks to investigate the use of street experiments to enhance gender-specific movements and design urban landscapes that prioritise the

requirements of women in enhancing their access to public transportation, which in turn enables them to engage in many aspects of city life. The researchers critically evaluate the Topuk project, which aims to enhance women's access to public transit in Maltepe, Istanbul. The analysis focuses on assessing different methods of people involvement used in the street tests [28].

A very widespread and debated issue in ongoing research is the possibility of processing the street experiments from temporary events to permanent changes [12, 29].

3.2.2 Street Experiments: As Matter of Policies?

The transition capacity of street experiments often can be limit by institutional barriers. Thus, their success or their failure are certainly connected to the specific policies and planning instruments of the examination contexts, as well as the deep conflicts and criticism. Thus, many researchers offer a reflection about the regulation [3, 30–33], the criticisms and the conflicts that arise between different street users [34, 35].

Some research reports the positive example of the Living Street program of in Ghent (Belgium), where the municipalities have played a crucial role in the street experiments, improving their transitional capacity [36, 37].

Others research, by contrast, examine failed street experiments in order to address planning and governance policies in similar contexts. An example of this is the Asian area, characterised by a high-density urban environment with highly intensive use of streetscape, and conservative and prescriptive planning. Specifically, the researchers Caterina Villani and Gianni Talamini examine Hong Kong context, its policies and planning instruments, and illustrate two representative cases failed due the competing roles and pratical uses [38].

3.2.3 Stakeholder and Community Participation and Citizens' Evaluation

Other aspects investigated in the research are the stakeholder and the community participation in the street experiments process and the citizens' evaluation of the street experimentations. On the one hand, actively engaging the stakeholders and the community, sharing the aims, and the phases of the street experimentation process with them, understanding their needs, is decisive for success of the street experiments. On the other, exploring what the citizens value about the street experiments allows to propose a more effective and inclusive design.

For these purposes, for example, Karyn Scerri and Maria Attard created Virtual Urban Living Lab (VULL), a virtual platform to engage the local community, for a street experimentation process in Malta. Here, it can access in an interactive space where it is possible identify the barriers, explore, and evaluate the street experimentation proposes [39].

Smeds and Papa offer inductive and qualitative survey method for understanding citizens' qualitative evaluations of street experiments, considering both use value and the social meanings of streetscape changes. Specifically, they analyse the citizens assessment of five street experimentation, parklets and plazas, in three neighbourhoods of London, Munich, and Bologna [40].

It is particularly interesting what emerges from the investigation of four case studies in Sweden, where many temporary street experiments realised with the aim to create public spaces that enhance social inclusion and quality of life. The investigation has been carried out through an interdisciplinary approach, based on the exploration of the physical parameters and psychosocial processes that concern people's acceptance and place usability during car-free initiatives. In addition, the four case studies have been analysed from an environmental psychological, landscape architectural, urban transport and planning point of view. This put in evidence how, in the residents' perception of street experiments, acceptance and usability of the street experimentation depend on the perceived qualities of the physical urban settings and on interceding psychosocial processes such as, neighbourhood attachment and perceived quality of life [41].

At the same time, others research are addressed to the knowledge of the users 'perceptions (city centre residents and street users) with the aim to improve using interim design strategies. This approach has been proposed for a *Complete Street* in Norwegian [42].

As well as investigative methodologies, also the tools used to analyse the evaluation of street experiments are diversified. In particular, it is interesting the analytics approach, based on deep learning video, for the assessment of temporary street experiments, and for evaluate the effectiveness of intervention. This has been experimented on a tactical urban planning and participatory design, realised in Bologna in March 2022 [43].

3.2.4 Covid 19 Pandemic-Induced Street Experiments

As mentioned above, the street experiments have been really numerous in worldwide cities during the Covid-19 pandemic. They have been highly recognised and accepted by public and authorities, allowing the communities to live safety in the streetscapes and the urban spaces, according to physical distancing requirements. Some researchers have explored these pandemic-induced street experiments in order to demonstrate that these offer an efficient solution, to specific challenges to mobility and public space [15, 44]. Others research analyse and map the pandemic-induced street experiments on global scale. On the hand, 539 street experiments in 333 cities have been registered through a geospatial database (PISE Database) developed with a standardised template, characterised by built environment indicators and quantitative approach, able to facilitate comparisons between different cities [7]. On the other hand, the *Shifting Streets Database* has interested 524 cities around the world, for understanding the processes, their implications [14].

Others still study the phenomenon of Covid 19 Pandemic-induced Street experiments in a more restricted context [45–47]. For example, the research of Meredith Glaser and Kevin J. Krizek observes the street-focused emergency response measures from 55 largest cities in the US through a rubric to understand if these measures can trigger a transformation in the transport system [16]. The series of street experiments realised in Chilean intermediate cities during the global pandemic have been analysed by the research group led by Luis Vàsquez. The aim is to understand which measure has been most frequent, which area has been most interested, what type of funding or fund has been used, and the public perception associated with the street experiments [48].

In addition, the Covid-19 pandemic has conducted many studies to address a reflection on the need of change the public spaces, rethinking the urban green spaces as sensitive places for physical exercise and mental recreation [49–52].

3.2.5 Ensuring Safety

The street experiments, as is known, determine a reduction the number of vehicular through lanes and, consequently, these can be reallocated to other uses such as bicycle lane, parking, sidewalks, transit use, turn lanes, curb extensions, parklets or pedestrian refuge islands. This circumstance greatly enhances safety both pedestrians and vehicles. In this sense, the searches address both to the evaluation of the safety effectiveness of these spaces [53, 54] (i.e., The case of an intervention in Virginia using the empirical Bayes method) [55, 56]; and to the investigation for ensuring adequate ventilation of exterior and interior urban spaces for essential for safety and comfort of inhabitants, with the aim to share the result for the design for urban structures such as parklets [57].

4 Conclusions

Implementing a 'tactical urbanism' approach, which involves street experimentation, is of the utmost importance for addressing the issues of active and sustainable mobility and transitioning towards a liveable city, as outlined in current urban agendas.

For the last two decades, streetscapes in many cities across the globe have been undergoing temporary experimentation, sometimes welcomed with great enthusiasm by the street users. These experimentations improve the safety of the streets and the cities, and the quality of life. The Covid-19 pandemic has led to widespread street experiments that have quickly gained global traction and achieved significant success. This has prompted consideration of the potential for these experiments to become regularised via systematic planning.

This aspect is essential subject for the ongoing research, of which this study is part. Specifically, the research examines the potential of street experiments, in particular parklets. The research aim is to propose operative process suitable and able to change these temporary experimentations in adaptive planned solutions, to transform and enhance the urban landscape sustainably, to promote active mobility, and enhance accessibility. In order to achieve this aim, for the research is essential the analysis of the context in which the interventions will take place, and the synergy and participation of all the actors involved (administration, experts in mobility and planning, citizens and various users of the spaces, object of study).

The first step is to develop a cutting-edge framework for street experiments. The goal of the literature review is to establish the phenomenon of the street experiments in the current context, to frame its evolution, to highlight its strengths and weaknesses, and to understand its role in the cities' transformation and in the urban planning.

As mentioned above, due to the multitude of contributions found on the research object, the research achieves the first results from the investigation of the contributions related to the street experiments that include 'street experiment' in their title, in the text and author's keywords and a part of those referring to parklet/parklets.

The next phase will focus on the exploration of the literature review of tactical urbanism with the aim to highlight the relationship between this approach and the street experiments.

Acknowledgements. This study has been supported by the MUR through 2 projects: SMART3R-FLITS: 1) SMART Transport for Travellers and Freight Logistics Integration Towards Sustainability (Project protocol: 2022J38SR9; CUP Code: F53D23005630006) and 2) MOVING StEPS: MOVING from Street Experiments to adaptive Planned Solutions (Project protocol: 2022BLK9TS; CUP Code: F53D23005550006), both financed with the PRIN 2022 (Research Projects of National Relevance) program.

This research was granted by PNRR-M4C2- I1.1 – MUR Call for proposals n. 104 of 02-02-2022 - PRIN 2022 – ERC sector SH7- - Funded by the European Union – Next GenerationEU.

This manuscript reflects only the authors' views and opinions, neither the European Union nor the European Commission can be considered responsible for them.

Authors' Contributions. This paper is the result of the joint work of the authors. 'Abstract', and '2. Methodology', '3.1 Quantitative synthesis', and '3.2 Towards a thematic framework' were written jointly by the authors. CG wrote '1. Introduction'. MSP wrote '3.2.1 Street experiments phenomenon and its relationship with the urban mobility', '3.2.2 Street Experiments: As matter of policies?', and '3.2.3 Stakeholder and community participation and citizens' evaluation', FP wrote '3.2.4 Covid 19 Pandemic-induced Street experiments', 3.2.5 Ensuring safety', and '4. Conclusions'. CG and FP coordinated and supervised the paper.

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A Digital Twin Simulation Framework to Assess the Impact of Street Experiments: Transforming Urban Mobility in Acireale (Italy)

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Abstract. Urban mobility policies focus on several strategies and actions towards sustainability, among them the implementation of street experiments schemes to discourage high-polluting vehicles entering in urban areas. The increase in vehicular traffic generates numerous externalities, including high congestion levels, polluting emissions and a worsening of the quality of life, especially in urban centers. To reduce these critical issues, one can refer to experimental Low Speed Zones (LSZs) or Limited Traffic Zones (ZTLs). These vehicular traffic restrictions can be of several types: spatial (i.e. territorial extension), permanent or temporary (i.e. variation in duration over time); partial or total (i.e. reserved only for specific categories of vehicles).

This work presents a methodology to evaluate the impact of traffic restriction configurations through a digital twin implementation based on microsimulation models to perform scenario analyzes and evaluate quantitative variables (e.g. service levels, queue lengths, delay times). Different scenarios have been simulated and assessed within the municipality of Acireale (Italy): (i) permanent ZTL with limited extension to the central area of the historic centre; (ii) temporary restricted traffic zone extended to the entire historic center; (iii) permanent ZTL extended to the entire historic center (assuming a modal shift in travel demand); (iv) 30 km zone extended to the entire historic centre.

The obtained results, associated with the northern area of the city at the entrance to the historic centre, show that the spatial extension and temporal duration of these street experiments can generate critical issues on alternative roads. Future research developments will include the integration of emission models to assess the environmental impacts deriving from the proposed sustainable mobility actions.

Keywords: Sustainable Mobility · Transport modelling · microsimulation · Low Speed Zones (LSZs) · Limited Traffic Zones (ZTLs) · urban regeneration

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O. Gervasi et al. (Eds.): ICCSA 2024 Workshops, LNCS 14823, pp. 197–210, 2024.
https://doi.org/10.1007/978-3-031-65329-2_13

1 Introduction

Vehicle congestion in cities causes several disruptions compromise the livability of urban areas [1]. The impact of pollutants generated by vehicles in cities is significant [2]. In 2021, 24% of total greenhouse gas emissions were caused by transport sector, whereby road mobility is the main driver, accounting for approximately 92.9% [3]. The emissions are primarily carbon dioxide (99.0% in 2021), a gas determined by fuel consumption, which has significant direct health impacts, contributing to respiratory illnesses, cardiovascular diseases, and other ailments, ultimately resulting in premature deaths [4]. The effects of vehicle congestion are remarkable not only in large cities, but also in small and medium-sized cities, especially those with a historic urban fabric, because they are characterised by a road network with reduced capacity and narrow cross-sections [5]. Therefore, to face these issues it is essential to identify and adopt strategies and actions promoting sustainable mobility within urban areas and assess their impacts [6–10]. The need to make sustainable cities [11], emphasizes the role of planning for accessibility that is at the core of all sustainable urban planning policies [12, 13]. In this regard, a strategic European legal tool is the Sustainable Urban Mobility Plan (SUMP), introduced in Italy as "Piani Urbani della Mobilità Sostenibile" (PUMS) by Ministry of Infrastructure and Transport Decree No. 397 of 4th August 2017 [14]. Among its contents, it foresees actions and strategies to achieve the objectives that each municipality must pursue to promote the sustainable mobility for citizens [15, 16]. To foster a holistic and comprehensive vision of the PUMS, also in coherence with European guidelines, four of its areas of interest and related mandatory minimum macro-objectives to achieve balanced and sustainable development are the following: 1. Effectiveness and efficiency of the mobility system; 2. Energy and environmental sustainability; 3. Road mobility safety; 4. Socio-economic sustainability [17]. Among the strategies and actions envisaged by this planning tool there is the possibility of introducing limitations to vehicular circulation as street experiments [18, 19], to encourage active mobility as the main means to access services within a neighbourhood [7]. Specifically, there are several types of vehicular traffic restrictions, including Limited Traffic Zones (LTZs), linked to the type of vehicle, and Low Speed Zones (LSZs), linked to travel speed.

LTZs are areas in which restrictions are enforced on motorized traffic or specific types of vehicles, including 'traffic calming' infrastructural measures [20]. In Italy, LTZs are called "Zone a Traffico Limitato" (ZTL) and they are regulated by the "Linee Guida sulla regolamentazione della circolazione stradale e segnaletica nelle zone a traffico limitato" of 28/06/2019 [21] according to Presidential Decree No. 250/99 [22]. Within LTZs, restrictions may be of different types: spatial (i.e. territorial extension), permanent or temporary (i.e. inter- or intra-day variations); total or partial (i.e. concerning only certain categories of vehicles).

Whereas LTZs are areas or roads where strict speed limits are imposed on motorized vehicles, either through the placement of appropriate prescription signs, or through proper infrastructural interventions for speed moderation (i.e. punctual, along the road axis or coordinated interventions) [23].

The impact of these strategies does not only concern the intervention areas but also the surrounding neighborhoods. In fact, it is quite recorded a decay in level of services

within the areas immediately adjacent to the traffic calming intervention, due to the re-routing of vehicles which generate an increase in vehicle traffic considered (i.e. parasite traffic) [24, 25].

In this regard, there are different methodologies for assessing the impacts of LTZs and LSZs. Some studies focus on pre- and post-intervention speed and volume assessment using measures of central tendency and dispersion, [26]; other studies focus on analyzing the effects of LTZs on air quality and the environment [27]. However, these approaches require the intervention implementation and then measuring the impact.

The impact of a traffic closing should be assessed before implementing temporary or permanent interventions; this can be done through simulations that could provide a detailed representation of the system, i.e. digital twins [28], a set of virtual information constructs that fully describe a potential or actual physical system [29]. This allows to suggest the implementation of traffic restrictions that are more suitable for existing traffic conditions, thus increasing the likelihood of their being maintained over time.

Based on this premise, this work applies a methodological approach described in Sect. 3, for evaluating the impact of different traffic restricted zones, through the implementation of microsimulation models to perform scenario analysis and evaluate several variables (i.e. service levels; queue formation; time loss) [30]. Before, Sect. 2 describes the case study where this methodology has been applied, i.e. to the case study of the city of Acireale (Italy), characterised by a poor public transport supply and a high motorisation rate. The effects of four different vehicle traffic restriction scenarios have been evaluated: (o) Current status; (i) permanent LTZ with reduced extension; (ii) temporary and extended LTZ; (iii) permanent and extended LTZ with modal shift; (iv) 30-km and extended LSZ and the results are discussed in Sect. 4. Finally, Sect. 5 concludes the paper by presenting future developments of the research.

2 Case Study

2.1 Territorial Framework

The examined case study in this work is the city of Acireale, a municipality of approximately 50,000 inhabitants located in the metropolitan city of Catania (Sicily), located in the east of the island, north of the capital of the metropolitan city (Fig. 1).

Acireale is, after the capital city, the most populous municipality in the metropolitan area of Catania [32]. Its relations with Catania are very straitened, characterised by complementarity in terms of tourism and commuting for university studies and work. For these reasons, streets are often characterized by congestion phenomena. Acireale is known for its narrow streets, winding alleys and crowded squares, which make vehicular circulation often tricky and potentially hazardous for pedestrians. In fact, within the historic center of Acireale, the interaction between vehicles and pedestrians presents several critical issues related to the urban characteristics and traffic dynamics, as shown in Fig. 2.

This case study has been proposed as the city of Acireale has been subjected to a spatial planning and management tool to regulate its transport mobility. Specifically, the Municipality of Acireale has a General Urban Traffic Plan (in Italian “Piano Generale del Traffico Urbano” – PGTU) [34] as regulated for municipalities with a population of

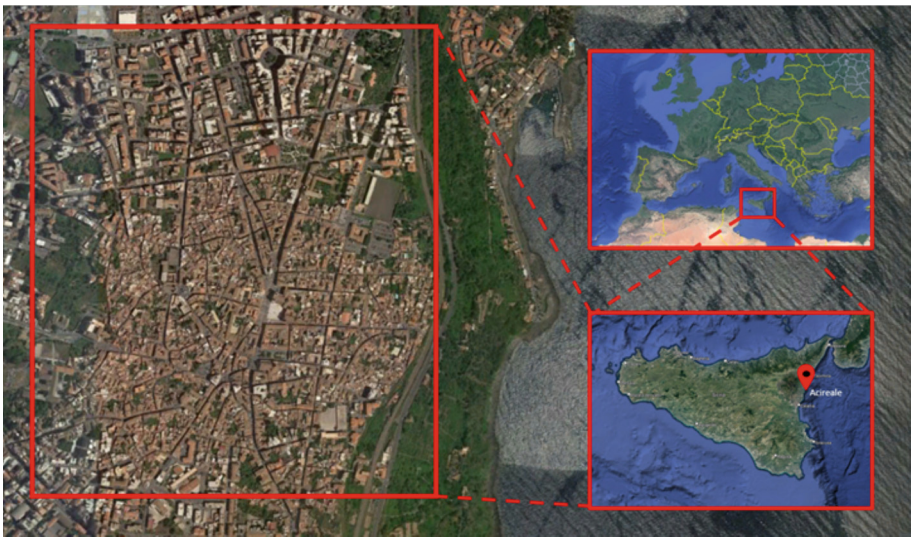

Fig. 1. Study area. Source: Author elaboration [31]

Fig. 2. Interaction between pedestrians and vehicles within the historic center of Acireale. [33]

more than 30,000 inhabitants. It is an urban planning legal tool that defines the guidelines for the territorial development of the city and defines targeted interventions on traffic and mobility to improve the safety, environmental and efficiency conditions of the urban

system, addressing issues related to the territory, the transport supply, the demand for mobility and their interaction. One of the main aims of this plan is to promote widespread and sustainable urban accessibility, referring to the three dimensions of sustainability: environmental, economic and social.

The PGTU revealed the need to limit motorized vehicle traffic and travel speeds in certain areas of the city center (i.e. the historic center) through the implementation of measures to improve the quality of cycling and walking and thus raise the livability indexes of the urban context, i.e., through the spatial and temporal definition of the LTZs and the identification of traffic calming areas (i.e. LSZs).

For the PGTU the temporal implementation of traffic restriction interventions is envisaged in the following four phases:

- phase 1: LTZ with minimum spatial extension (ZTL - 1st step) and 30-km Zone with minimum spatial extension (Zone 30 - 1st step);
- phase 2: LTZ with minimum spatial extension (ZTL - 1st step) and 30-km Zone with maximum spatial extension (Zone 30 - 2nd step);
- phase 3: LTZ with minimum spatial extent (ZTL - 1st step), 30-km Zone with maximum spatial extent (Zone 30 - 2nd step) and access regulation of the most polluting vehicles ("Zona 30 Ambientale");
- step 4: LTZ with maximum spatial extent (ZTL - 2nd step), 30-km Zone with maximum spatial extent (Zone 30 - 2nd step) and access regulation of the most polluting vehicles ("Zona 30 Ambientale").

The objectives to be pursued through the above-mentioned phases (temporally sequential) are mainly:

- to permanently eliminate motorized vehicular traffic in specific areas, subject to special exceptions (i.e. mainly related to residents);
- to reduce pollutant emissions in the central areas of the city;
- to make the historic center more livable;
- and to minimize the number and severity of traffic accidents.

LTZs, like other initiatives involving the temporary transformation of public spaces, e.g. streets or squares, to test new solutions or improvements in the urban environment, can have several impacts on the urban environment, the local economy and the quality of life of residents. The need arises to evaluate the effects of implementing these initiatives impacts on urban traffic.

The application of traffic micro-simulation to model at different level these vehicular restrictions may be an effective approach to evaluate their impact and optimize traffic management for different scenarios (Fig. 3).

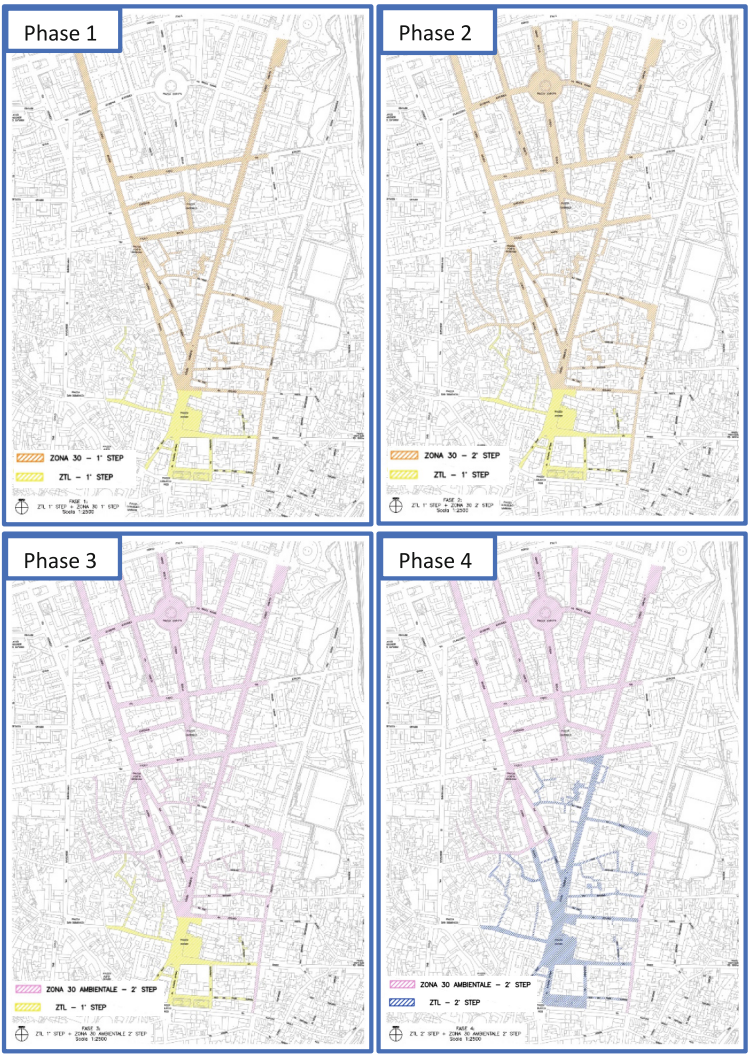

Fig. 3. Phases of traffic limitation interventions [34]

2.2 Traffic Survey Campaign and Scenario Analysis

Analyzed scenarios have been hypothesized and modelled through microsimulation software (i.e. PTV Vissim) to assess the impact that these interventions would have in the northern part of the city, with traffic flows entering the historic center.

It has been first necessary to determine the mobility demand through proper traffic survey campaigns. Traffic surveys were carried out at specific time slots of the day to record critical flows affecting the study area. The duration of each individual survey time slot was 15 min and was recorded during the following peak hours: morning (8:05–8:20 a.m.), midday (12:55–1:10 p.m.), and evening (5:35–5:50 p.m.).

In this work, in addition to the current scenario, four alternative scenarios have been considered:

- (o) current status at the time of traffic surveys; an assessment of this scenario is made in order to compare the indicators calculated for other scenarios;
- (i) permanent LTZ with reduced extension to the central area of the historic center, with closure of the road from Duomo Square to Porta Gusmana Square;
- (ii) temporary LTZ extended to the entire historical center: the hypothesis is made of extending the LTZ up to Savoia Road;
- (iii) permanent LTZ extended to the entire historical center (assuming a modal shift in the travel demand); following the total closure of the historic center, a reduction in the vehicular flow is assumed;
- (iv) 30-km zone (i.e. LSZ) extended to the entire historical center. This alternative is considered for a short time.

These scenarios have been identified based on the various vehicular restrictions phases in the PGTU with a view to intervening in the entire historic center and making it a permanent LTZ. Thus, the choice of scenarios is geared toward maximizing the long-term benefits of the extended LTZ, while attempting to mitigate any transitional problems through temporary measures such as 30-km Zone.

3 Methodological Approach

The procedural steps of the proposed methodological approach are described as follows (Fig. 4):

- Definition of the study area;
- Implementation of the transport demand, both vehicular and pedestrian;
- Node evaluation and calculation of the level of service of the current scenario.

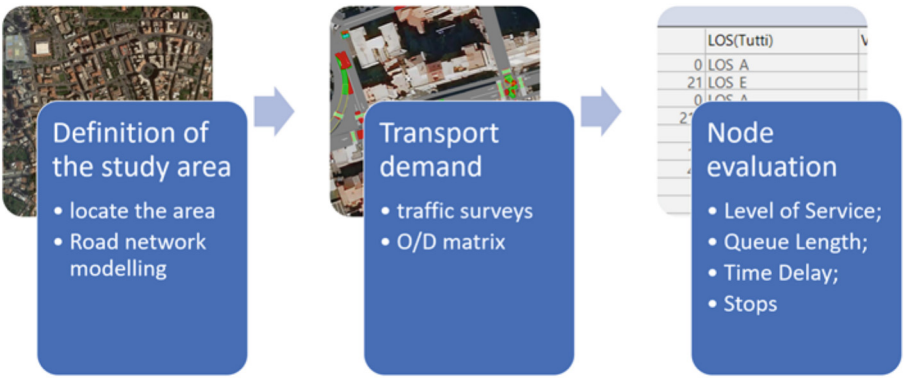

Fig. 4. Methodological framework. Source: Authors elaboration.

For the first phase, the study area has been identified, coinciding with the area in which the LTZ is planned and where data are collected, e.g. topography, existing road network,

priority and access rules to the LTZ, travel speeds, crossing times at intersections and other factors influencing the movement of vehicles. This network has been modelled through the design of links with the corresponding lanes and priority rules.

For the second phase, the characterization of transport demand has been carried out by means of special fixed operator traffic surveys carried out at specific times of the day, to record the critical flows that affect the areas under study, specifying the vehicular composition (consisting of cars, motorbikes, heavy vehicles and buses). From these measurements, an O/D matrix was drawn up with reference to the critical flow of the morning time slot, which was used during the assignment procedure to distribute transport demand through flows and routes within the simulated model. The vehicular flows were assigned to the incoming connected network link so that the vehicles in the network were in operation at the beginning of the simulation. Once the flows were assigned, the vehicular routes were defined, of static type, specifying for each of them the origin and destination arc, assigning to each of them the corresponding flow and considering some maneuvers not performed by certain categories of vehicles.

In the third phase, a node evaluation of the network's level of service and other calculated quantities has been carried out for several alternative scenarios.

The Level of Service (LOS) of a road section is a measure of the quality of vehicular flow on that section. These levels are distinguished by six letters, i.e. from A to F, in descending order of traffic flow quality. In general, for roads with uninterrupted flow, the vehicle running conditions at the various LOS can be defined as follows:

- A: free circulation, i.e. each vehicle moves without any constraints and in absolute freedom to maneuver within the current: maximum comfort, stable flow;
- B: circulation can still be considered free but there is a modest reduction in speed and manoeuvres begin to be affected by the presence of other users: acceptable comfort, stable flow;
- C: the presence of other vehicles causes increasing constraints in maintaining the desired speed and freedom to maneuver comfort is reduced while the flow remains stable;
- D: the range of speed choice and freedom to maneuver is restricted; there is high density and disturbance problems arise: comfort is lowered and the flow may become unstable;
- E: flow approaches the limit of compatible capacity and speed and freedom to maneuver are reduced: flow becomes unstable as even moderate disturbances can cause congestion;
- F: Forced flow: the disposable vehicular volume decreases along with the ve-location; unstable flow conditions easily occur up to the onset of severe queuing phenomena.

Other important performance measures that have been evaluated are queue length, number of stops and vehicle delay:

- Queue length: in each time step the queue length is measured and then the mathematical average is calculated for each time interval;
- Stops: number of vehicles stops linked to interference experienced on their journey;
- Vehicle delay: the time delay of a vehicle is obtained by subtracting the ideal travel time from the real one. The ideal one is what would be obtained under free flow conditions.

In the results of implementing microsimulation model, at the node level, indicators can also be displayed that measure exhaust gas emissions, referring to a typical North American vehicle fleet their node rating is used to compare the emissions of different scenarios. These indicators are:

- Emissions CO: Quantity of carbon monoxide [grams];
- Emissions NOx: Quantity of nitrogen oxides [grams];
- Emissions VOC: Quantity of volatile organic compounds [grams];

By evaluating these indicators for different traffic micro-simulation scenarios, it has been possible to gain an in-depth understanding of the effects of changes in traffic conditions, enabling informed decisions to be made to improve the efficiency and safety of the road system. In this work, these indicators have been calculated for the existing state scenario and for the 4 redevelopment scenarios.

The adopted methodology stands out for its replicability and innovation. Using models based on users' behavior, it enables accurate reproduction of road conditions and traffic flow in virtual scenarios. Its replicability derives by clear processes and algorithms used, that can be implemented at different levels. At the same time, the innovative approach is evident in the use of advanced data analysis and predictive modeling techniques to simulate traffic dynamics in complex contexts, thus providing valuable insights for improving urban planning and road infrastructure management.

4 Application and Results

Regarding the application of the methodology to the study area, i.e. the historic center of the municipality of Acireale, the area north of the historic center has been considered to carry out the simulation analysis.

Information have been collected on the network geometry, i.e. number of lanes characterizing each road, width, traffic flows, traffic directions, parking, presence of priority and stop rules, horizontal and vertical signs, etc. This analysis was used to implement the modelling on Vissim microsimulation software of the entire area under study.

As a first modelling phase of the road network, the individual lanes have been modelled using the link command, characterised by information regarding the geometry and relative connections, taking care to calibrate the conflict areas generated by the intersections between various links. This calibration has been carried out respecting the priority rules that regulate the road network in the study area.

The mobility demand has been reconstructed by means of traffic surveys as described in the previous section. This mobility demand was modeled through the inclusion of vehicular flows and routes.

For the evaluation of the level of service it has been necessary to insert a node enclosing the area under study as shown in figure (see Fig. 5).

The indicators have been calculated using a special command, the time of each simulation is 3600 s, for a total of 5 different simulations. Table 1 shows the simulation results in terms of vehicle parameters (i.e. Level of Service, Queue Length, Time Delay and Stop) and environmental parameters (i.e. CO, Nox and VOC emissions).

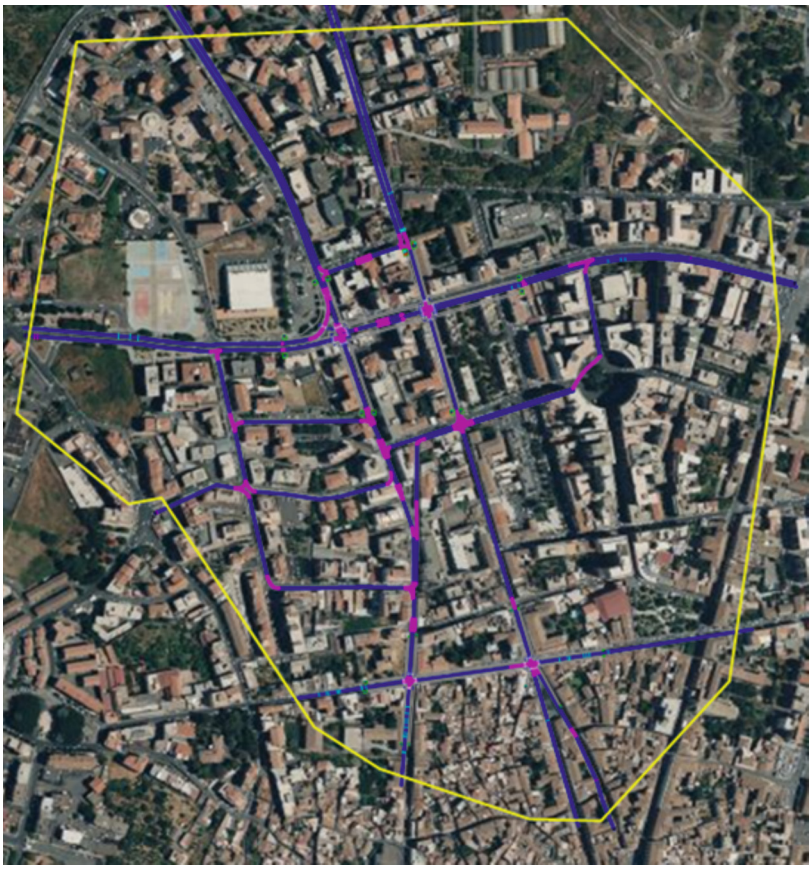

Fig. 5. Network of arcs and connections made in the model and node for evaluating the service level. Source: Elaboration on PTV Vissim

Table 1. Scenario evaluation Source: Elaboration on PTV Vissim

Scenario	LOS	QLEN [m]	VEHDELAY [s]	STOPS	EMISSIONS CO [g]	EMISSIONS NOX [g]	EMISSIONSVOC [g]
o	B	0,99	13,02	1,05	4677,34	910,04	1084,02
i	D	1,73	28,91	2,04	5593,68	1088,33	1296,39
ii	E	3,38	46,50	3,59	6618,24	1287,67	1533,84
iii	C	0,59	14,97	1,29	3689,87	717,91	855,16
iv	C	1,11	15,27	1,31	4919,06	957,07	1140,04

For the Current State scenario there is a rather good situation with an average service level of B. If street experiments implementation is considered, the results significantly change. From the LTZ relating to the historic center with closure in the section between Piazza Duomo and Piazza Porta Gusmana, the situation worsens (i.e. LOS is equal to

D). If the area is extended in the section between piazza Duomo and Corso Italia, as described in scenario ii, the level of congestion increases further (i.e. LOS equal to E). This worsening of LOS in the areas surrounding the LTZ entails multiple benefits, e.g. improved walkability, decreased accidents, improved local economy, etc.

Considering this, it is assumed that following a permanently extended LTZ in the long term there will be a component of vehicle traffic that will choose other modes of transport to travel to the center. Therefore, a scenario is calculated, where a reduction in vehicle flows of 20 per cent is assumed, resulting in a LOS C. Thus, a long-term extended LTZ has better effects than a LTZ restricted to the city center alone. It is assumed, however, that the transition period between the activation of the extended LTZ beyond the historic center and its full operation is the one that will generate traffic problems. Therefore, a further scenario has been assumed for this phase, namely that of a 30-km Zone in the short term. From the results of this scenario, the impact of a 30-km has on traffic, compared to that of an LTZ reduced to just the historic center, is less, since a LOS C is obtained.

The calculated emissions are related to the service level values, because they have been calculated through an emission model based on vehicular traffic flow. Thus, same consideration can be highlighted: for scenario o, the calculated pollutant emissions are quite significant. With the implementation of vehicular restrictions, there is a significant increase in congestion levels, resulting in a substantial increase in pollutant emissions. In this regard, considering the scenario in which a reduction in vehicular flows is assumed for the long-term scenario, emissions become lower than in the most congested scenarios.

5 Conclusions and Future Research

This study highlighted the central role of some kinds of street experiments, through a synthesis of empirical data and traffic modelling techniques. We evaluated the impacts of implementing different LTZ scenarios (i.e. both temporary and permanent) on traffic flow, air quality and, thus, overall urban livability.

The results underline the potential of traffic experiments as valuable tools for policy makers and urban planners seeking to create sustainable, people-centered cities.

Furthermore, the application of microsimulation allowed for a qualitative and quantitative examination of LTZ interventions, revealing insights into their effectiveness on various spatial and temporal scales. In fact, by entering input data (e.g. number and width of lanes, vehicular and pedestrian flows and routes, etc.), it has been possible, thanks to the simulation process, to measure the changing behaviour of drivers. By simulating different scenarios and assessing their real-world implications through the implementation of a digital twin model, we gained a deeper understanding of the complex interactions within urban environments. The implemented model allowed us to calculate and compare the reference parameters (i.e. LOS, delays, emissions and fuel consumption) for the various alternative scenarios.

Going ahead, this research emphasizes the importance of collaboration between urban and transport planning and decision-making supported by data and models in shaping the future of urban mobility. Future research developments will include the integration of emission models to assess the environmental impacts deriving from the

proposed sustainable mobility actions. It is also intended to implement this methodology on other contexts, which can be a significant step toward more efficient and sustainable urban planning and traffic management.

Acknowledgements. This research was granted by PNRR-M4C2- I1.1 – MUR Call for proposals n.104 of 02–02-2022 - PRIN 2022 – ERC sector SH7- Project title: MOVING StEPS - MOVING from Street Experiments to adaptive Planned Solutions - Project Code 2022BLK9TS - CUP Code D53D23011060006 - Funded by the European Union – NextGenerationEU.

This manuscript reflects only the authors' views and opinions, neither the European Union nor the European Commission can be considered responsible for them.

The work of Vincenza Torrisi related to the realization of digital twin model and further indicators analysis is funded by the European Union (NextGenerationEU), through the MUR-PNRR project SAMOTHRACE (ECS00000022).

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Sustainable Development of Ports (SUSTAINABLEPORTS 2024)

AIS Data for Building a Transport Maritime Network: A Pilot Study in the Strait of Messina (Italy)

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Abstract. The maritime transport of goods enables economic exchanges at a global level. Containership, sea routes, port systems and relative performances (e.g. times and costs) influence the quality and quantity of these exchanges. For these reasons, it is necessary to develop quantitative methods for evaluating the main performances of maritime container services. At the same time, ICT (e.g. Automatic Identification System, AIS) enable the acquisition and collection of information and data for supporting Transport Simulation Models (TSM), useful for calculating the performances. In this context, this paper presents a method for building a supply transport network model of container maritime services. The method is based on the acquisition and elaboration of data deriving from the AIS. The supply model allows the calculation of indicators for evaluating the main performance of containership services at the international level. The proposed method is applied to developing a pilot study of maritime containership services in a portion of the Mediterranean Sea. The results of the pilot consist of the representation of a transport network obtained from the available AIS data. The obtained results show the main potentialities of the proposed method for developing TSM from the fed by the AIS data. The method and results obtained are of potential interest to public and private decision-makers and takers involved in the maritime transport sector.

Keywords: TSM · maritime transport · AIS data · containerships · big data · sustainability

1 Introduction

Maritime transport plays a relevant role because it enables economic exchanges at a global level. Containership, sea routes port systems and relative performances (e.g. times and costs) influence the quality and quantity of these exchanges. For these reasons, it is necessary to develop quantitative methods for evaluating the main performances of maritime container services.

This research focuses on the Transport System Models (TSMs) supported by data deriving Information and Communication Technologies (ICTs). The good use of transport supply maritime networks has great potential for evaluating the performances of

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O. Gervasi et al. (Eds.): ICCSA 2024 Workshops, LNCS 14823, pp. 213–226, 2024.
https://doi.org/10.1007/978-3-031-65329-2_14

container lines. This implies the necessity to adapt the existing modelling approaches to the maritime sector by using the potentialities offered by ICT [1]. With the correct use of small and big data, by considering their volume, velocity and variety, the consolidated formalizations can be enhanced to improve the modelling representation of the maritime networks. In other contexts, the combination of different sources is experimented to support the implementation of TSM, about supply, demand [2, 3] and their interactions for measuring performances [4].

This paper focuses on the potentialities offered by the Automatic Identification System (AIS) used in different research fields of interest in the maritime industry. This paper focuses on the use of AIS data to extract maritime transport networks. The works available on this topic propose different methodologies to extract maritime transport networks by elaborating AIS data [5]. However, there is a limited use of AIS data for building transport supply network models. This paper explores the possibility of using AIS data for implementing the graph approach generally adopted in terrestrial transport systems [6]. With this aim, the paper offers the following research contributions:

- an overview of methods and models to build a maritime transport network, starting from the acquisition and elaboration of AIS data with a specific focus on the containership sector;
- an approach to formalize maritime transport supply modelling according to TSM;
- a first pilot for building a network in a specific case study.

The paper represents the first step of a wide research aimed at analyzing intermodal transport at the global level and transport network performances that influence economic exchanges.

After this introduction, the paper has four sections. Section 2 recalls the main approaches available in the literature for building a maritime transport network by using the AIS data. Section 3 proposes a TSM approach for building maritime transport supply models empowered using AIS data. Section 4 describes the main results obtained by the pilot study relative to the study area. Section 5 discusses the results with final remarks and further developments of the research.

2 The Use of AIS Data for Maritime Transport Networks

Scientific literature presents works about the AIS characteristics (Sect. 2.1), the possible applications for building maritime transport networks (Sect. 2.2) and calculating transport performances (Sect. 2.3).

2.1 AIS Data Characteristics

According to the International Maritime Organization (IMO) rules, ships must be equipped with an Automatic Identification System (AIS), shipborne monitoring that provides ship voyage and navigational status information. AIS provides updated information about vessels information in different times. The information and data can be classified on [7]:

- static, by considering the structural data about the ships (e.g. ship name, characteristics and international identification); collected data regards physical and functional information about the ships (e.g. capacity);
- dynamic, by considering the registered data about the movements (e.g. spatiotemporal positions) and navigation status of the ships; collected data regards the historical and real-time vessel sailing information (e.g. speed) referred to different time intervals.

There are different commercial platforms (e.g. AISHub, Elane, ExactEarth, FleetMon, IHS Markit, and Marine Traffic) that collect and provide AIS data that can be available in a row or elaborated formats.

More details about AIS data and relative application are reported in [8].

2.2 AIS Data for Building Maritime Transport Networks

Different frameworks and methodologies for building maritime traffic networks by using AIS data are available in the literature [9]. The proposed approaches regard the extraction of maritime transport networks from AIS data.

A great part of the scientific works available in literature regards the automated extraction of maritime networks from AIS data [5, 9]. Several of these studies are based on geospatial clustering techniques aimed at grouping a set of objects identified by geographic and temporal positions. The elements belong to the same cluster with different criteria, for instance, the degree of similarity measured by spatial, temporal and non-spatial attributes [10]. Lee et al. [11] propose a clustering algorithm aimed at identifying maritime routes starting from the ship trajectory pattern. The method is based on a spatial clustering methodology (DBSCAN) performed to identify the waypoints of vessels that are connected to the individuated routes. Similar patterns constitute the result of a kernel density estimation analysis (KDE), becoming a cluster that represents a specific maritime route.

Yan et al. [12] propose a method based on the graph theory for extracting maritime routes. AIS massive data are used for reconstructing the historical spatiotemporal positions of a ship and relative trajectories [13], where each ship trip is represented as "stop-waypoint-stop" trip object. The result is a directed maritime traffic graph where nodes and links allow the extraction of the shipping routes.

The maritime transport network extractions from AIS data are used for different applications. The more common application is to the identification of previous trajectories, or paths taken by a vessel, obtained elaborating data about the vessel's positions in space and time. Ship trajectories obtained from the historical AIS data can be elaborated for automatic route analysis and the extraction of the maritime shipping network. Some authors used AIS data to analyze the influence of COVID-19 Pandemic, on international container liner ports [13]. The maritime network allows analysts to evaluate the transportation efficiency of the supply chain at a global level [14]. The possible evolution of this common application concerns vessel trajectory prediction and sailing optimization by modifying speed to enhance energy efficiency [15]. In other applications, AIS data are useful for estimating externalities, for instance, the estimation of gas emissions deriving from maritime transport lines. The elaborations apply "bottom-up" methods that use static (e.g. power engine) and dynamic (e.g. kinematics characteristics) information of

vessels. This approach is more accurate concerning the "top-down" methods based, for instance, on fuel consumption or fuel-based emission factors. Other AIS data applications regard maritime safety, concerning the possibility of supporting the avoidance of vessel collisions [16].

In synthesis, according to Yan et al. [12], the methods for extracting maritime transport networks can be classified into:

- grid-based methods, based on a reorganization of the original data by grid index; by counting the traffic data in each element of the grid, it is possible to individuate the maritime traffic characteristics (e.g. nodes); this method is simple, but it is not suitable for large areas;
- vector-based method, based on the elaboration of data for representing maritime routes as a combination of points and segments needed for individuating the main traffic patterns in large regions; one representative method is the Traffic Route Extraction and Anomaly Detection (TREAD) proposed by Pallotta et al. [17];
- statistics-based method, based on statistical modelling for individuating the ship maritime traffic patterns from data; spatial and temporal cluster analysis is commonly used in the methods belonging to this class; for instance, ship tracks are grouped into different line clusters for individuating the main patterns of maritime traffic Yan et al. [12].

2.3 AIS Data for Calculating Transport Network Performances

Maritime transport networks allow the calculation of performances relative to different aspects of the maritime sector.

Ducruet [18] proposes a critical review of different studies on maritime flows and networks producing more insights about the possible evolutions of maritime network analysis, in geography and other sciences. The main evolutions regard three issues: the managerial implications of maritime flows from a business point of view; maritime flows and networks as markers and vectors of wider geo-economic structures and dynamics; maritime networks as parts of territories and chained systems, similar to urban or regional networks. The results of the review show the necessity to cover other scientific fields (e.g. complex network analysis).

Kanrak et al. [19] review the principal applications of the network theory and models in the maritime sector. The focus is on the methods of calculations of indicators (e.g. centrality, density, degree distribution, …), of the maritime transport networks, where ports are nodes linked by shipping services. The implementation of the existing theories and models of network analysis in the maritime sector requires further investigations.

The traditional applications concern the route design or navigation planning to support navigators by considering weather conditions such as wind or sea currents. Other applications regard the calculation of energy consumption concerning the maritime route and then its planning for increasing efficiency [20].

Some authors analyzed the competition between roll on–roll off (ro–ro) and lift on–lift off (lo–lo) services inside the Short Sea Shipping (SSS), regarding the Mediterranean Sea [21, 22]. Sometimes, these maritime network services offer a possible alternative to terrestrial transport producing relevant impacts on social, economic and environmental sustainability. Then, it is necessary to analyze maritime passenger transport to evaluate

the centrality of the national maritime services networks [23]. In other research contexts, approaches based on maritime networks support investment decisions aimed at increasing reliability and resiliency in a port system for facing the effects of multiple disaster scenarios [24].

A limited quantity of research applies classical analysis approaches adopted for transport systems. For instance, Kang et al. [25] study the speed-density relationships that characterize ship traffic. The final aim is to estimate the fundamental diagram of ship traffic in the Singapore Strait by elaborating AIS data.

In synthesis, the performances obtained from elaborations of AIS data and maritime network can regard:

- a macro level by using the aggregated AIS data, relative to the entire network; for instance Liu et al. [9] adopt a data-driven approach for individuating ship patterns, grouping different ship paths in relation to similar travel characteristics such as origin and destination areas;
- a micro level by using disaggregated AIS data, relative to a specific element of the network (e.g. port performances or route congestion); for instance, Russo et al. [26] study the ports' performances respecting to the seaside with the support of AIS data for calibrating calculating port's performance indicators at country level.

From the reviewed literature, it emerges that there are different approaches to building maritime transport networks from AIS data. These networks are used in some scientific fields for performing different applications. However, there is a limited quantity of works that combine AIS data with TSM approaches. The following section proposes a possible TSM approach empowered by the use of AIS data.

3 Modeling Maritime Transport Networks with a TSM Approach

AIS data can be used for building a maritime transport network adapting existing TSM approaches. This paper focuses on the transport supply modeling.

According to Russo [27] a transport supply model can be classified in:

- analytic, in which transport system is represented in aggregate form;
- topologic, in which the infrastructures and services are represented in a similar way as the services are in the real situation with an expansion in time; topologic model is composed by two macro models:
  - network model that comprehends two elements: models of connections among points (graph approach); cost functions for links and nodes;
  - system relationships (models of relationships in transport system).

In this paper we refer to the network approach used widely in literature to simulate a transportation system. Section 3.1 describes the main elements of a maritime transport graph. Section 3.2 illustrates the maritime transport network topology, recalling the main issues related to the simulation of maritime transport services.

3.1 Maritime Transport Topology

A great part of the methods available in the literature is based on the graph concept. A generic graph G comprehends two related sets: the set of nodes, named N and the set of links or a couple of nodes belonging to N, named L:

$$G = (N, L) \tag{1}$$

In the context of TSM the graph representing a transport network is oriented, then the links have a direction the couple of nodes are ordered. A generic link that connects a couple of nodes can be identified with the indexes used for the initial and final nodes (i, j) or with a unique index where:

$$(i, j) \neq (j, i) \tag{2}$$

In the case of the maritime transport network:

- the nodes represent the specific points in the maritime space of the vessel's maritime routes (ports or maritime crossroads); in the set of nodes, ports (or port systems) are considered centroids, where the trips vessel start or end;
- the oriented links connect two generic nodes representing a movement of the ships along the predefined maritime routes, sometimes called "maritime roads".

The methods proposed in the literature and recalled in Sect. 2 can be adapted to build a topology (nodes, links and routes) according to the TSM approach. The obtained graph represents the maritime links and paths that connect two generic ports. The generic port can be represented in an aggregate way, with a single node. For analysis aimed at measuring the port performances, it is necessary to represent the port in a disaggregate way, to consider all phases that characterize the outflows and inflow operations from and to a specific port.

Adopting the TSM approach, the topology can be represented with the following analytical elements [6, 28]:

$\boldsymbol{\Delta}$ the link–path incidence matrix that has a number of rows equal to the number of links and a number of columns equal to the number of paths; the generic element assumes value 1 if the link belongs to the path, 0 otherwise;

$\mathbf{c_A}$ the vector of additive link generalized costs (e.g. travel times), with dimension equal to the number of present links in the maritime network;

$\mathbf{g_{NA}}$ the vector of no additive path generalized costs (e.g. equipment costs), with dimension equal to the number of available paths in the maritime network;

$\mathbf{g_A}$ the vector of additive path generalized costs (e.g. naviagation times between two ports), with dimension equal to the number of available paths in the maritime network;

$\mathbf{f}$ the vector of link flows (e.g. number of ships/day), with dimension equal to the number of available links in the maritime network;

$\mathbf{h}$ the vector of path flows (e.g. number of ships/day), with a dimension equal to the number of available paths in the maritime network.

With these elements, it is possible to express analytically the topology of a maritime transport network, with the two following relationships.

The relationships between link and path generalized costs:

$$\mathbf{g} = \mathbf{g_A} + \mathbf{g_{NA}} = \mathbf{\Delta}^{\mathrm{T}} \Delta \mathbf{c_A} + \mathbf{g_{NA}} \tag{3}$$

The relationships between link and path flows:

$$\mathbf{f} = \Delta \mathbf{h} \tag{4}$$

The maritime transport network is completed by associating a cost function to each link:

$$\mathbf{c} = \gamma(\mathbf{f}) \tag{5}$$

where

$\gamma(\cdot)$ is the vector of the link–cost flow functions.

Note that the level of aggregation of the network depends on the aims of the analysis. Moreover, in most cases, it is necessary to disaggregate the nodes representing a port with specific nodes, links and cost functions for taking into account all the phases connected to the entry and exit manoeuvres (see [27]).

3.2 Maritime Transport Services

The graph approach, generally applied to simulate services for passenger terrestrial transport, comprehends two different approaches (see [6, 29, 30]):

- the frequency-based approach usually represents high frequency; the characteristic element of the system is the line, defined as a path used by transport means with fixed frequency; the service is simulated by nodes and links representing the stops and the line segments;
- the schedule-based approach usually represents low frequency and high regularity services; the characteristic element of the system is the run, defined as a path used by vehicles with explicit representation of time (diachronic network); for every stop a temporal axis is made on which the nodes represent the arrival and departure time of the run at the stop.

A great part of the works available in the literature represent maritime transport services by means of supply models that usually apply the frequency-based approach.

In the supply model, there is a network of infrastructures consisting of ports (nodes) and routes (links). Each port can be represented by a set of nodes and links with cost functions relative to times, costs. Each route is represented by a sequence of links for each service. This representation doesn't allow the analysis in detail of different runs flows or variations in service times. There are some simulations of variations in maritime service times [27, 31–33].

The use of AIS data empowers the application of the schedule-based approach because it is possible to have information about each ship's travel in space and time. However, the literature presents a limited quantity of works that adopt the schedule-based approach for representing maritime transport networks.

4 A Pilot Study

The pilot study regards maritime transport in the Strait of Messina in the South of Italy. With a spatial extension of about three kilometres, the Strait divides the Sicily region with the continental Italian territories. The included maritime stretch serves the connections in two perpendicular directions:

- the Sicily – Calabria direction enables the connections of people and freights mobility between Sicily and continent territories; this is possible employing maritime transport services (e.g. ro-ro and high speed) that connect two ports in the Sicilian coast (Messina and Tremestieri) and two ports in Calabrian cost (Reggio Calabria and Villa San Giovanni);
- the Tyrrhenian – Ionian enabling the connections between the Tyrrhenian Sea and the Ionian Sea, within the central Mediterranean; in this direction, there is the navigation of different kinds of ships (bulk, container, ro-ro, …) that cross the Mediterranean Sea and relative ports; one of the main port near to the strait is the Gioia Tauro port that plays transhipment and gateway functions in container trades at global level.

This configuration generates relevant maritime traffic flows between high-frequency services performed by ships that enable the different functions along the above directions. The intersection between the routes of different kinds of ships produces potential impacts in terms of congestion and safety. For instance, in 2007, there was a collision between a passenger hydrofoil navigating between Reggio Calabria and Messina ports and a containership navigating between Tyrrhenian and Ionian seas. As a result of the incident, in 2007 the International Maritime Organization (IMO) Assembly adopted the "IMO with SN.1/Circ.279 on 12 June 2009" resolution. This implies the introduction of a "roundabout-type" Traffic Separation Scheme (TSS), graphically represented in Fig. 1. After the resolution, the navigation in Strait of Messina is constrained to follow specific regulations and maritime way, controlled by the Vessel Traffic Services (VTS) that is a monitoring system that control the strait providing information messages to ships, such as spatiotemporal positions of vessels.

The introduced elements demonstrate the relevance of the pilot study and the necessity to follow the movement of ships in the study area. Starting from the AIS data collected in relation to a sub set of ships navigating the Strait of Messina (Sect. 4.1), a schematic representation of the maritime network is obtained (Sect. 4.2).

4.1 The Collected AIS Data

The pilot study case starts from the individuation of the maritime area in the Strait of Messina. The area comprehends the four ports located in the coastal area of Calabria and Sicily regions. The area constitutes the input for selecting AIS data from the "marinetraffic" platform. A sub-set of ships that perform the two described functions are selected. A sample of spatiotemporal positions relative to the temporal period from 28 January 2024 to 4 February 2024 is selected. The monitored ships and relative services are reported in Table 1 where are indicated: the monitored day (date), the travel time measured as the difference between arrival and departure times in the ports and final and initial times

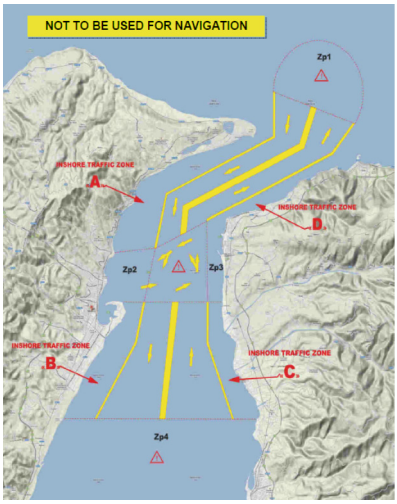

Fig. 1. Maritime traffic separation scheme (source [34]).

in the study area, the maximum and minimum speed, the main function and relative shipping services.

4.2 The Schematic Maritime Network

The collected data are mapped and ordered in a GIS by considering the spatiotemporal position of each monitored ship in the study area. The tracks of the ships were drawn by joining the points in space. It is possible to verify that the monitored ships follow the indications provided by the IMO resolution, navigating along the roundabout. It is necessary to consider the errors of GPS points in the space. By the intersections between the monitored routes, it is possible to individuate the main nodes in the maritime transport network including the ports and the maritime positions. After, it is possible to individuate the links that connect the nodes. The cost functions can be calibrated by observing the spatiotemporal profiles of each service.

Figure 2 represents the obtained schematic network in the strait of Messina. From this representation it is possible to define the analytical network topology of a transport subnetwork in relation to the prescriptive IMO regulation and relative "roundabout-type" TSS. Table 2 reports the links – paths incidence matrix ($\boldsymbol{\Delta}$) that represents the topology.

Table 1. Monitored ship services in the Strait of Messina

Direction	Ship Name	Date	Travel time in the area (minutes)	Speed (knots)		Service
				min	max	
Sicily–Calabria	Trinacria	28/01/2024	32	0.7	11.3	freigth Ro Ro
	Enotria	31/01/2024	53	0.6	12.7	freigth Ro Ro
	Giano	01/02/2024	44	0.1	11.3	freigth Ro Ro
	ALE M	03/02/2024	28	0.7	26.7	passenger High Speed
	Zancle	01/02/2024	28	0.8	11.8	mix Ro Ro
Tyrrenian–Ionian	Konet	01/02/2024	150	13.2	15.1	containership
	MSC Amanda	01/02/2024	160	10.8	15.1	containership

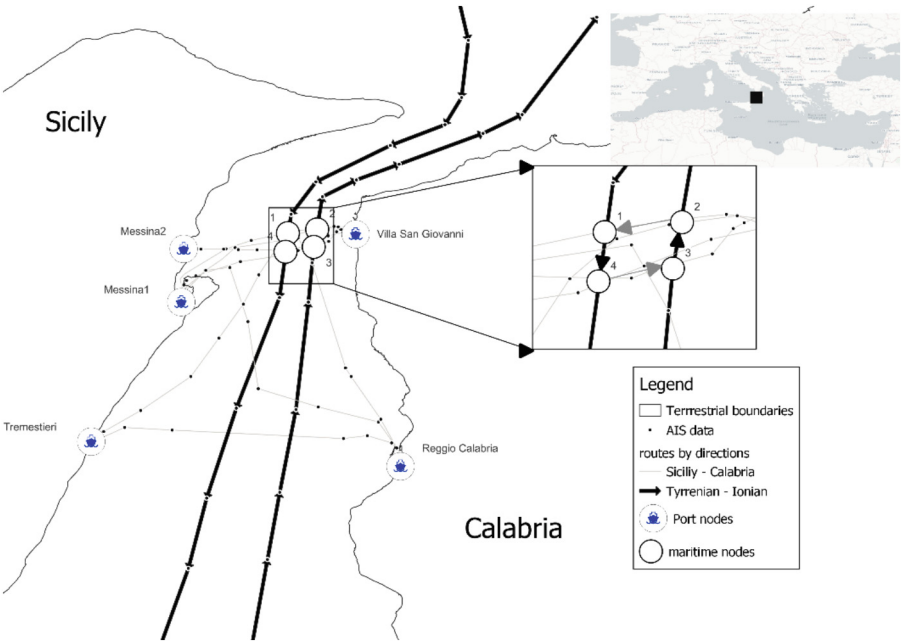

Fig. 2. Maritime transport network in the Strait of Messina.

Table 2. Links – paths incidence matrix of the roundabout in the strait of Messina ($\boldsymbol{\Delta}$)

Links	Paths			
	Calabria-Sicily	Sicily-Calabria	Tyrrenian-Ionian	Ionian-Tyrrenian
1–4	1	0	1	0
4–3	0	1	0	0
3–2	0	1	0	1
2–1	1	0	0	0

5 Discussion and Final Remarks

The maritime transport sector deserves particular attention as it allows the mobility of people and the exchange of goods at different territorial scales. Maritime navigation includes different infrastructures and services that allow the performance of different functions.

Recently, also thanks to the potential offered by emerging ICT technologies, the maritime phenomenon can be studied by using large data and information on the characteristics of ships, travel times and maritime itineraries followed. This information contributes to face the growing complexity of maritime transport networks. This paper focused on the potential of AIS data, now available in large quantities for different types of maritime traffic.

This paper presents some limitations regarding the literature and the experimentations. By considering these two limits, two research directions can be investigated in future developments.

The first development concerns the scientific literature. The main methodologies for extracting maritime transport networks from AIS data processing were analyzed. Several techniques based on statistical and geographical methods are available. However, based on the documents analyzed, there is a limited combined use of the TSM approach and existing techniques. The use of TSMs would allow for further applications especially connected to the development of implemented future scenarios and therefore to carry out a priori assessments of the effects produced by the plan actions. It is necessary to extend the research conduct, considering the growing interest in various disciplines regarding the maritime sector.

The second research direction concerns the development of a pilot study to build a maritime transport network in the area of the Strait of Messina. The area is particularly complex as it is crossed by various components of maritime traffic connected to different mobility components (people and goods). The study was carried out using a limited amount of AIS data referring to a limited sample of ships crossing the area. The obtained results are limited but at the same time encouraging. It is necessary to extend the findings in space and time to understand the further dynamics underlying the phenomenon. In particular, it is necessary to develop the potential of AIS data and the development of demand, supply and interaction models in transport systems.

Acknowledgement. This study is carried out within the research project "National and local factors affecting times of ships in container ports", Piano Nazionale di Ripresa e Resilienza (PNRR), Next Generation EU. Progetti di Rilevante Interesse Nazionale PRIN_2022_PNRR_P202292YFW. CUP: C53D2300878001. This presentation reflects only the authors' views and opinions, neither the European Union nor the European Commission can be considered responsible for them.

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Improving Sustainability of Freight Transport in the Port-City Interface Through the Use of Integrated Approaches

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Abstract. The ports represent the land-sea interface and the maritime-land transports junction point and are fundamental links of the global logistics chain. Thus, attention must be paid to a complex system, also made up of retro-ports, inter-ports and intermodal logistics platforms, because the port-city interactions, and between the decision-making actors involved in them, are multiple. Maritime transport and port operations generate externalities on the reference contexts in a direct and indirect way, above all from an environmental point of view. Logistics activities also exert further environmental pressure in the port-city interface and retro-port areas where the transported goods are carried at the end of the supply chain. In fact, the traffic of goods entering/leaving ports by road can influence the dynamics of the urban traffic flow. This paper aims to analyses the sustainability of freight transport in the port-city shared areas through the use of integrated approaches. In order to identify the main critical issues and possible solutions, promoting actions and measures that guarantee the efficiency of the transport of goods (and the relative priority of intervention), the research is articulated into different phases. The first concerns the analysis of the main criticalities in the port-city interface and inland port areas. In the second a literature review of state of the art was conducted. Then, common measures and best practices are examined. Finally, different scenarios have been implemented in order to predict the impact that these options will have on freight mobility. This methodology can allow to evaluate different options and to choose the best strategy.

Keywords: Port-city logistics · Sustainable maritime transport · Freight transport · Maritime transport policies

1 Introduction

The ports represent the land-sea interface and the maritime-land transports junction point and are fundamental links of the global logistics chain. However, maritime transport and port operations generate externalities on the reference contexts in a direct and indirect

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O. Gervasi et al. (Eds.): ICCSA 2024 Workshops, LNCS 14823, pp. 227–240, 2024.
https://doi.org/10.1007/978-3-031-65329-2_15

way, above all from an environmental point of view. For years, the policies of the European Union aim at sustainable development, encouraging a competitive, sustainable and safe transport policy. In accordance with the Sustainable Development Goals promoted by the United Nations, in particular with objectives 11 to reduce the per capita pollution produced by cities and 13 for the fight against climate change, the EU targets for sustainable include: to reduce CO2 emissions from the maritime sector at a rate compatible with the Paris Agreement (−40% by 2030 and −70% by 2050 compared to 2008 levels); to protect citizens from harmful exposure to air-borne pollutants; to reduce the pressure on port-city area roads unable to absorb increasing traffic; to promote the sustainable multimodal freight mobility and to mitigate relevant adaptation measures. Also, the intent of the International Maritime Organization (IMO) measures is to reduce emissions (carbon intensity), probably destined to grow if not counteracted quickly, avoiding as much as possible negative effects on trade and economic growth driven by maritime transport.

The port-city shared areas are of crucial importance for the environmental sustainability of mobility, as it is an area where vehicular traffic is particularly intense and can have a significant impact on air quality and greenhouse gas emissions [1]. The transport and logistics activities are not always included in urban and transport plans, but very often they are also carried out by private companies [2].

Thus, sustainable management of the port-city interface and retro-port areas can help reduce the environmental impact of freight transport, thanks to the adoption of more efficient and sustainable mobility solutions. Therefore, from what has been said so far, it follows that sustainable mobility solutions, for these areas, are important for the health and well-being of citizens who may be exposed to high levels of air contamination and noise disturbance.

In order to alleviate the external impacts previously mentioned, it is necessary a comprehensive approach that integrates territorial and mobility planning, port operation management and eco-friendly technologies integration.

In the European context, various measures, which will be described in paragraph 3, have adopted in order to mitigate the environmental impacts of the port-city shared areas.

Sustainability is a very important topic discussed at the level of States, institutions and companies. It is also an important issue for many seaports, port companies and municipal authorities. According to [3] the main sustainable issues for cities are associated with the evolution of more sustainable transport systems but also with architecture and spatial development as well as with energy use and others.

The already mentioned Goals 11 and 13 of Agenda 2030 focuses on the development of sustainable cities and communities and climate change [4]. Starting from this concept it is necessary to highlight how port cities must pay particular attention to sustainability problems due to pollution and noise caused by ships moved in the port and other port activities.

In fact, different factors that affect air quality coexist more than in inland cities, the most important of which are the emissions from ship engines. Port systems are in general the fulcrum of activities related to the sea economy of different contexts such as the Italian one and are scenarios characterized by national and international trade and the transit of goods and the movement of people [5].

Maritime transport also represents an important and growing share of green-house gas emissions produced in our country and ports, often inserted in densely populated contexts, have to face critical issues in terms of acceptance by the citizens who live in the areas where they insist [6, 7].

Fundamental is not only the evolution of strategies to develop and make ports more sustainable and accessible but also the surrounding urban areas [8–11].

The recent pandemic from COVID-19 has also produced, among the many critical issues, the sharp drop in GDP and trade and this has inevitably had a negative effect on Italian ports [12, 13].

This effect was strongly perceived in Italy considering that around 40% of all Italian commercial exchange takes place by ship, a value that rises to 90% for Italian import-export to Asia and America [14].

All Italian ports have experienced significant contractions, even if the ports of the South are more devoted to the energy sector and the agri-food chain and therefore have suffered less from these critical issues [15, 16].

These data are in line with the contraction that has been recorded globally in maritime traffic and containers, the result not only of Covid-19 but also of the growing international trade tensions, especially between China and the United States. The Pacific route had already experienced a significant decline in 2019 after a decade of uninterrupted growth but as of 2022 it has recorded a real collapse with -10%.

Even Suez, taken as a reference port related to the Silk Roads and the traffics that feed the commercial relations between Europe and China, confirms this trend: -15% of passages of large container ships on the route to and from Asia [17, 18].

At the same time, the big carriers, the shipping companies that govern the world market of freight transport by ship, have tried to face the crisis with “blank sailing” operations (cancellation of already scheduled routes) and at the same time with the search for routes and strategies for drastically reduce costs.

For example, the drop in the price of oil, particularly significant in the first few months of the year, saw the return of the Cape of Good Hope route, the circum-navigation of Africa. Certainly, much longer route but which nevertheless be-comes convenient with the low price of fuel compared to the cost of the passage from Suez.

Various signs connected both to the type and frequency of maritime routes underline a phase of acceleration of the process of regionalization of world trade which probably also affects value chains and supply chains. A tangible sign of this is the passages of ships within regional routes (America, Europe-Mediterranean, Asia) and the decrease in passages on global routes [19].

Several studies from 2012 to date have shown that the more ships depart from far away (Asia) and have a port in Northern Europe or the Atlantic coast as their final destinations, the more the center of gravity is shifted towards Gibraltar [20]. Conversely, less distant departure ports or destination ports closer to the Mediterranean area bring the center of gravity more to the centre. A shift of the point of maximum concentration of passages closer to the heart of the Mediterranean and to our country has therefore been observed [21].

The main objective of the paper is to analyze the sustainability of freight transport in the port-city shared areas through the use of integrated approaches.

Identified the main critical issues, the research is articulated into different phases: a literature review of state of the art; an examination of main common actions taken for mitigating environmental impacts and of some best practices to identify the solutions adopted; the implementation of different scenarios in three case studies, in order to predict the impact that these options will have on freight mobility.

2 Literature Review

The port-city interface is of crucial importance because the 90% of European ports are located in urban areas and the integrated management of air quality, water, waste, noise and energy consumption must be at the top of the agenda of port authorities and administrations.

The decarbonisation of ports is a fundamental step in strengthening the innovation and competitiveness capacity of the Mediterranean maritime industry. In fact, the port system plays a key role in international trade, in the transport of goods and people and is a vital element for the development of an efficient and sustainable intermodal transport network. The decarbonisation of ports therefore represents a very important environmental and industrial opportunity that the country must be able to seize [22].

Shipping accounts for a large and growing share of greenhouse gas emissions. Emissions associated with port sector are estimated at 940 million tonnes of CO 2 per year, equivalent to approximately 2.5% of global greenhouse gas emissions [23, 24]. These emissions are likely to increase significantly if mitigation measures are not implemented quickly.

In particular, the Mediterranean coast, with its hundreds of densely populated port cities, is heavily affected by pollution from the maritime sector. And, as air pollutants are transported up to 400km, inland areas are also affected [25, 26].

The evolution of port systems and the city-port combination must consider a range of strategies and actions aimed at decreasing emissions and increasing the ‘accessibility of these areas. As regards the strategies to be applied to port activities, various studies in the literature focus on issues related to infrastructure and means, namely:

- The evolution of cold ironing, related to the evolution and application of technologies by means of which it is possible to supply energy to boats while parked in port, through an electrical connection with the mainland, allowing the elimination of pollution and emissions by vessels in port [27].
- The decarbonisation of maritime transport as an intervention aimed at improving the environment and industry, taking into account not only the geo-morphological aspects but also the systems characterizing the European and Italian port system. This aspect is also correlated with the opportunity to achieve the objectives in the fight against the cli-mate crisis [28].
- The connection of ports with the railway network, to build “green” corridors: an opportunity of great interest for the development of sustainable intermodal logistics [29, 30].
- The electrification of short-distance maritime transport, the subject of numerous experiments to improve the sustainability of connections with the smaller Italian islands, is based on the use of renewable sources [31].

The concept of smart port [32] smart port based on the ability of new technologies to transform port services into interactive and dynamic, more efficient and transparent businesses has been spreading for several years.

This aims to meet the needs of customers and users without forgetting its responsibility towards the city and citizens.

Often the complexity of maritime transport and the lack of a unified system of indicators to evaluate smart ports slows down the implementation of more sustainable and participatory planning.

A limited number of research studies to date define a set of useful indicators to facilitate these actions.

In particular, the study conducted by [33] introduced 25 evaluation indicators and evaluated the key indicators of the quality of the smart port service and their causal relationships, revealing that the main success factors of smart ports are: the accurate and safe delivery of the load together with the accurate transfer of electronic documents. The factors associated with a rapid supply of port berths are also fundamental in order to shorten the rotation times of the ships; convenient and complete logistics and customs practices; transparent integration of in-formation on a single platform; and finally, the use of big data to organize container transport.

A study conducted by [34] points out that a spread of digitization combined with careful planning and management of port operations allows to find intelligent solutions to optimize logistics and environmental impacts, promote efficiency and improve the security of both seaports and the coastal regions involved.

Some studies have developed methodological approaches and have promoted some design applications, in terms of urban regeneration.

With reference to the Italian context, the study conducted by [35] started from the definition of urban regeneration to arrive at the identification of a circular approach and key issues applicable to the case study of Genova Pra'-Palmaro.

Still in the Genoese context, a study conducted by [36] proposed an optimal management strategy for a Smart Port equipped with renewable generation and composed of an electrified quay, operating Cold-Ironing, and a hydrogen quay, supplying ships with zero emissions.

Another study conducted by [37] defined the steps for the activation and co-ordination of a locally integrated partnership towards the development of a multi-term Smart Port Management Strategy to support innovation processes in the sustainable and safe management of the port of Ravenna.

The main methodologies for the mitigation of environmental impacts and best practices were analysed to identify the actions, processes or strategies that have led to positive results in other contexts.

3 Main Methodologies for the Mitigation of Environmental Impacts

The port-city shared areas are critical for the environmental sustainability of mobility, because the vehicular traffics are particularly intense and can have a significant impact on air quality and greenhouse gas emissions. Therefore, sustainable management of

these areas can help reduce the environmental impact of vehicular traffic by promoting the adoption of more efficient and sustainable mobility solutions. In addition, these externalities can be, due to the high levels of air and noise pollution, a risk for the health and welfare of citizens and, above all, of residents.

Logistics activities also exert further environmental pressure in these areas where the transported goods are carried at the end of the supply chain. In fact, the traffic of goods entering/leaving ports by road can influence the dynamics of the urban traffic flow. These emissions are likely to increase significantly if mitigation measures are not implemented as soon as possible and effectively. Thus, also thanks to a reconnaissance in the international sphere, some main common actions taken for mitigating environmental impacts were identified and reported in the following Table 1:

Table 1. The common practices for mitigating environmental impacts

IMPACTS	METHODOLOGY	ACTIONS
Noise generated by ships and port and logistics activities affecting quality of life of people living near the port	Use of noise emission control systems	Use of noise mitigation techniques (construction of noise barriers)
		Relocation of heavy port activities
Emission of exhaust gases and other pollutants to air and water generated by ships and port and logistics activities	Implementation of environmental emission control, management and monitoring systems	Integration of filtration systems for ship
		Management of port-generated waste
		Implementation of strategies for managing wastewater and preventing pollution
		Use of sustainable energy sources for port operations
	Development of low-emission zones	Introduction of speed limits, access restrictions and the adoption of low-emission technologies
	Promotion of alternative modes of transportation	Promotion of walking and cycling, the use of public transport and electric vehicles
	Digitization of port processes	Adoption of automation processes, process cargo at a higher speed with less error and increase their effectiveness

(*continued*)

Table 1. (*continued*)

IMPACTS	METHODOLOGY	ACTIONS
	Improving efficiency and safety	Use of innovative technologies such as Internet of Things, robotics and artificial intelligence
	Optimizing logistics processes	Use of port activity planning and management techniques to reduce waiting times
	Use of energy sources with low environmental impact	Use of environmentally friendly vehicles and fuels
Overlapping. Flows between network with local functions and goods distribution networks	Adoption of solutions to improve the efficiency of port and logistics traffic	Analysis of traffic flows through the use of mathematical models to identify critical points in the port system and interface area
	Involvement of the local community in decisions regarding port activities and environmental impact assessment	Inclusion of public consultation and participation in the planning of port activities

From what has been said above, it would be useful to identify some phases necessary to develop sustainable development strategies.

- Conduct a thorough examination of the port-city shared area in order to identify main critical issues and development opportunities.
- Engagement of different internal and external stakeholders, to foster shared and inclusive planning. In fact, given the consolidated importance of freight transport in urban areas, it is necessary to foster the cooperation among all stakeholders implicated at different levels. This further highlights the need to adopt an integrated approach as it demands the harmonized coordination and implementation of long-term policies and initiatives among the involved parties.
- Establish a coherent vision and objectives for the port-city connection area based on the assessment of the current situation.
- Plan appropriate infrastructure and related services to ensure the safe and efficient flow of traffic, support for commercial activities, and accessibility for residents.
- Adequately ensure cooperation and coordination among the various authorities involved in the planning and management of the port-to-city interface area. This may include establishing coordination mechanisms between local authorities, the port, businesses, and other stakeholders.
- Regularly monitor and evaluate the effectiveness of planning and implemented actions to ensure that objectives are being met and to identify any areas for improvement.

This means that port cities should work with stakeholders to ensure the necessary infrastructure for the development of the port and the city [38] city. They must have a clear and creative vision of the goals they want to achieve.

In the European context, several ports have adopted an integrated approach to mitigate the environmental impacts of the port-city interface. Therefore, some best practices have been reported briefly:

- In Rotterdam was developed a strategic plan for sustainability that aims to reduce CO2 emissions, increase energy efficiency, and promote inter-modality. The port has created a "Low Emission Zone" in the port-city interface areas to reduce air pollution caused by vehicle emissions. It partnered with municipal and provincial administrations to outline the criteria for authorized vehicles and entry zones, thus curbing private vehicle circulation. Consequently, the Rotterdam Harbor has witnessed a notable decrease in particle and nitrogen dioxide discharges within the harbor-urban interface.
- In Hamburg was adopted a strategy diminishing private vehicle circulation and advocating for interconnectivity. Has been formulated a traffic supervision system to enhance transportation effectiveness.
- In Valencia have been implemented various initiatives to enhance the ecological balance of the harbor-city shared areas, including harnessing renewable energy sources, fostering intermodal transportation, and instituting a traffic regulation mechanism.
- In Copenhagen has been implemented a sustainability blueprint geared towards diminishing CO2 discharges, advancing interconnectivity, and refining energy productivity. Thus, it has incentivized the utilization of eco-friendly technologies and instituted a shoreside power network for vessels to curtail the utilization of diesel generators while docked. Furthermore, the port has collaborated with municipal administrations to refine the harbor's accessibility and reduce individual vehicle circulation.

Among the various initiatives aimed at reducing greenhouse gas emissions, it is worth mentioning those promoted by the Port of Valencia through the application of renewable energy sources, the installation of shore-based electricity for ships and the promotion of intermodal transport and implementation of a traffic control system.

Furthermore, it is also necessary to remember the actions to promote alternative transport systems such as electric vehicles and bicycles. Finally, the port has introduced recycling and waste reduction programs and is promoting the use of recyclable materials in the port area.

4 Case Studies

All of the above strategies have produced a significant reduction in greenhouse gas emissions and an improvement in air quality in the port-city interface areas.

From this it is possible to draw inspiration to consolidate in other contexts a series of synergistic actions that can be achieved by local authorities and port authorities through the development of the following factors:

1. Integrated infrastructure planning:
   - Develop a comprehensive and integrated infrastructure plan focusing on the port-city area and including the different types of infrastructure and transport services that connect both areas and beyond.
   - Ensure the development of port structures in line with the overall urban development plan of the city. In this sense, it is necessary to apply an integrated approach to increase the sustainability of freight transport in the port-city areas.
2. Economic diversification:
   - Promotion of the development of industries and businesses near the port. These could, for example, be logistics companies, manufacturing plants and distribution centers.
   - Create special economic zones or industrial parks near the port attracting more businesses that can benefit from the port's services.
3. Urban redevelopment:
   - Use port development as a catalyst for urban regeneration through the enhancement and revitalization of port areas and public spaces and parks to improve the overall quality of life of citizens
   - Combine residential, commercial and recreational areas to create an integrated and sustainable environment.
4. Environmental sustainability:
   - Define and apply actions to combat environmental pollution through, for example, the reduction of emissions, the introduction of green infrastructures and the promotion of sustainable transport options.
   - Increase the number of green spaces and improve the seafront to improve the aesthetic appearance of the city while contributing to environmental sustainability.
5. Cooperative management:
   - Encourage collaboration between port authorities, local government and community stakeholders to make resolutions of critical issues, mitigation of impacts and participation of all stakeholders more effective
   - Establish joint committees or working groups to oversee the coordinated development of the port and the city.
6. Promote tourism and culture:
   - Starting from the historical and cultural significance, promote a series of actions to increase the tourist influx. In particular, to promote the development of cultural sites and promotion of heritage near the port and create attractions that attract visitors and contribute to the city's economy.
   - Promote events and festivals that celebrate the port's maritime heritage and attract both residents and tourists.
7. Education and innovation:
   - Foster the creation of educational and research bodies and institutes focused on maritime studies, logistics and related sectors. This action can encourage the increase in the qualified workforce and can promote technological evolution in the port and logistics sector

- Encourage collaboration between universities, research institutes and businesses, promoting innovation and technological progress applied to port operations.

In this way the port-city combination can be characterized by a dynamic and sustainable environment in which both entities thrive, to develop and support each other [39].

After having analyzed critical issues and some common practices adopted in the international sphere, different scenarios have been implemented in order to predict the impact that these options will have on freight mobility in three case studies analyzed: Catania (Italy), Trieste (Italy) and Koper (Slovenia). These are three medium-sized cities, which enjoy a strategic location and whose ports are important drivers of their regional economies. When comparing the city-port connections various factors such as transportation infrastructure, logistics, urban planning and overall integration are taken into account. In the Table 2 is a comparison for selected cities.

Table 2. The city-port connections

	Catania	Trieste	Koper
Geographical proximity	Port is close to the city, making it easily accessible for businesses and residents	Located close to the city center and is easily accessible for residents and businesses	Well-integrated port near the city center that is easily accessible to both residents and businesses
Transportation infrastructure	Port is connected to the city via the road and rail network, which facilitates the transportation of goods Catania's location in Sicily makes the city a strategic gateway for trade between Europe and North Africa	Port is well connected to the road and rail network and serves as an important transportation hub for goods moving through Central and Eastern Europe. Trieste has excellent connections to the most important European markets	A well-developed road and rail network connects the port with the city and the surrounding area, enabling efficient transportation of goods Koper is part of the Trans-European Transport Network (TEN-T), which ensures connectivity at European level
Logistics and trade	Port of Catania handles a variety of goods, including containers, bulk and general cargo, the logistics services contribute to the efficiency of trade operations in the region	Trieste is an important hub for container traffic, ro-ro services (roll-on/roll-off) and logistics activities The free port of Trieste enables efficient customs procedures and thus contributes to its role as a strategic trade gateway	Koper is an important logistics center offering services such as warehousing, distribution and customs clearance Various types of goods are handled in the port, including containers, cars and bulk goods

(*continued*)

Table 2. (*continued*)

	Catania	Trieste	Koper
Urban planning	Urban planning in Catania is likely to focus on harmonizing port activities with the overall development of the city, taking into account factors such as land use and traffic	The city and the port are integrated into the urban fabric, and urban planning takes into account the coexistence of port activities with other urban functions	Urban planning in Koper emphasizes the integration of port activities with the development of the city to ensure a symbiotic relationship

This overview provides a starting point for a detailed comparison. It's important to delve deeper into specific aspects based on your focus areas or criteria for evaluation. Additionally, considering the most recent developments or changes in each location will provide a more accurate picture.

5 Discussion and Conclusions

This paper aims to highlight some solutions to accelerate the decarbonization of maritime transport and the reduction of pollution in port systems not only be-cause a reduction in the use of fossil fuels is imperative in the fight against cli-mate change, but also because the containment of the environmental impact of port activity as a whole is crucial for the sustainability and public perception of these areas.

It also pays special attention to the challenges by the port-city interface, as outlined in the preceding sections, because it is evident that sustainable freight transport requires a multifaceted approach that integrates environmental, economic, and social considerations. The policy frameworks set forth by the European Union and other global entities provide important guidance for addressing these challenges, with an emphasis on reducing emissions, promoting inter-modality, and protecting public health. However, effective implementation of these policies necessitates collaboration among various stakeholders, including port authorities, local governments, businesses, and community representatives.

Therefore, the methodological comparison, previously described, allows us to define some impact mitigation actions, i.e. they offer a basis for the selection of practical solutions which may concern, for example, emission control systems and/or the digitalisation of port services.

These strategies not only make it possible to mitigate environmental impacts but bring benefits in terms of increasing operational efficiency and safety.

The case studies presented, namely the ports of Rotterdam, Hamburg, Valencia and Copenhagen, highlight the need for proactive measures such as the creation of low-emission zones and the integration of renewable energy in order to improve and make the port-city commubio more sustainable.

Among the actions to be promoted are:

1) increase in synergies between ports and port cities (for example through integrated infrastructure planning and economic diversification) which offer valuable ideas for holistic development strategies.
2) promotion of innovation in order to create dynamic and sustainable urban and port environments.
3) highlight specific actions and challenges as understood from the case study of Catania, Trieste and Koper.

In conclusion, improving the sustainability of freight transport at the port-city interface requires integrated approaches, aimed at mitigating environmental impacts and therefore at greater sustainability and improving competitiveness.

This could also bring medium and long terms benefits to residents living in the immediate vicinity of the port areas.

Acknowledgements. This work has been partially supported by the project "ARS01_00333 TETI - Tecnologie innovative per il controllo, il monitoraggio e la sicurezza in mare" (unique project codes CUP B45F21000050005) under the programme "PON Ricerca e Innovazione 2014–2020".

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Enhancing Climate Resilience in Maritime Ports: A Decision Support System Approach

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Abstract. Maritime ports, as critical nodes in global trade and transportation, face increasing challenges due to the impacts of climate change. Rising sea levels, extreme weather events, and shifting environmental patterns pose significant threats to port infrastructure and operations. This paper explores the intersection of resilience, maritime ports, and climate change, presenting a comprehensive framework that leverages a Decision Support System (DSS) to fortify port resilience in the face of evolving climate-related challenges. The study begins by examining the specific vulnerabilities of Greek maritime ports to climate change using the collected data from a questionnaire-based survey. Recognizing the complex and interconnected nature of these challenges, the research advocates adaptive strategies centered around the development of a Decision Support System (DSS). The proposed DSS provides decision-makers with actionable insights for long-term infrastructure development as well as actions for minimizing the potential disruptions caused by climate-induced events. The findings contribute to the growing body of knowledge on climate resilience in maritime infrastructure and offer valuable insights for policymakers, port authorities, and researchers seeking to address the complex challenges posed by climate change. By integrating climate considerations into decision support systems, this research provides a forward-looking approach to ensuring the sustainability and adaptability of maritime ports in an era of environmental uncertainty.

Keywords: Resilience · maritime ports · Decision Support System · Climate change

1 Introduction

With climate change, maritime ports—which are essential nodes in the world's transportation and commercial network—face ever-greater difficulties. These crucial nodes' operating efficiency and infrastructure are seriously threatened by the effects of increasing sea levels, more intense weather events, and climatic changes [1–4].

The study using data collected through a questionnaire-based survey addressed to over 150 Greek port authorities, identifies their vulnerabilities related to climate change

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O. Gervasi et al. (Eds.): ICCSA 2024 Workshops, LNCS 14823, pp. 241–252, 2024.
https://doi.org/10.1007/978-3-031-65329-2_16

and examines the development of a DSS that can support mid- and long-term decision and not day to day operations [5–9]. This approach provides the decision-makers insights for long-term infrastructure development and a roadmap for mitigating potential disruptions caused by climate-induced events.

By integrating climate considerations into decision support systems, sustainability and adaptability of maritime ports can be achieved in an era of environmental uncertainty. As the global community grapples with the imperatives of climate change, this paper emerges as a valuable asset, guiding stakeholders towards a resilient and climate-ready future for maritime ports worldwide.

2 Literature Review

Maritime ports are complex and dynamic infrastructures, facing a multitude of challenges, including cargo throughput, optimizing operations, and adapting to changing environmental and regulatory landscapes. To effectively address these challenges, maritime ports, as well as transportation systems in general [10, 11], are increasingly adopting Decision Support Systems (DSSs) as a valuable tool for enhancing decision-making and improving their operational efficiency [12] and develop corresponding risk management strategies [13–15].

These systems are information systems that provide decision-makers with the necessary data, models, and analytical tools to support informed decision-making [16]. They are designed to assist users in solving problems, which are characterized by uncertainty, incomplete information, and in some cases multiple conflicting objectives. The DSSs for maritime ports encompass a wide range of functionalities, including a) data integration by collecting and consolidating data from various sources, such as cargo manifests, vessel schedules, weather forecasts, economic indicators, etc.; b) modeling and simulation by developing and using mathematical models to simulate port operations, assessing the impacts of different scenarios and ultimately optimizing resource allocation [17–19]; c) visualization and reporting by generating interactive dashboards, charts, figures and reports to present complex information in a clear and concise manner [20–23]; d) decision guidance and supports by providing decision-makers with recommendations, alerts and insights to assist them make informed choices [24].

Based on what DSSs offer as functionalities, maritime ports' possible benefits are the following: a) improved efficiency and productivity, b) enhanced-decision making, c) risk mitigation and d) compliance and regulatory adherence. The DSSs for maritime ports are in most cases developed to address specific-decision needs. There are three (3) major types of DSSs: a) operational, focusing on real-time optimization of port operations, such as berth allocation, crane scheduling, and yard management; b) tactical, addressing medium-term planning and resource allocation decision, such as staff levels, equipment utilization, and pricing strategies; c) strategic, assisting port managers and authorities to make long-term strategic decisions related to infrastructure planning, capacity expansion, and market positioning [25, 26]. Despite the numerous benefits of DSSs, there are challenges that need to be addressed when implementing and using them effectively: a) ensuring the accuracy, completeness, and timeliness of data is crucial for the reliability of DSS outputs, b) DSS users need to be trained on how to effectively

utilizes the system and interpret its outputs, c) DSSs should integrate seamlessly with existing port management systems to avoid data silos and duplication of effort, and d) DSSs should be designed to accommodate the growth and complexity of maritime operation over time. It must be noted that the future of DSSs for maritime ports is promising, with advancements in Artificial Intelligence (AI), Machine Learning (ML), and big data analytics enhancing further their capabilities.

In addition to the above, DSSs that are specifically designed to assist maritime ports strengthen their resilience against the impacts of climate change are gaining increasing prominence. These systems utilize advanced data analytics, modeling, and simulation tools to assess the vulnerability of port infrastructure and operations to various climate-related hazards, such as sea level rise, extreme weather events, and changes in precipitation patterns. By integrating real-time data from weather stations, tide gauges, and other sources, DSSs can provide port operators with predictive insights into potential disruptions and risks. This information can then be used to implement proactive measures to mitigate the impacts of climate changes such as: a) enhancing the resilience of port facilities, such as raising quay walls, building seawalls, and installing flood barriers, b) optimizing port operations to minimize the impact of weather disruptions, such as shifting berthing schedules and rerouting vessels, c) developing contingency plans and risks mitigation strategies to address potential disruptions, such as developing alternative supply chains and securing backup power sources, and d) integrating climate-resilient design principles into new port developments and implementing energy-efficient operations.

The implementation of DSSs focusing on climate resilience is essential for maritime ports to adapt to the charging climate and ensure the continued safe and efficient movement of goods and people. These systems can help ports make informed decisions, optimize operations, and minimize the impact of climate change-related disruptions. For example:

- DSSs can help port operators assess the potential inundation of port areas due to sea level rise, this information can be used to plan for the relocation of critical infrastructure, such as terminals and warehouses.
- DSSs can simulate the impact of hurricanes, typhoons, and other extreme weather events on port operations. This information can be used to develop contingency plans for evacuations, cargo protection, and equipment repair.
- DSSs can analyze historical precipitation data and climate models to predict potential changes in water availability for ports operation. This information can be used to develop strategies for water conservation and drought mitigation.

3 Methodology

As above mentioned, the objective if the research is to develop a DSS to enhance the resilience of maritime ports against the impacts of climate change. The first step in achieving this goal is to determine and evaluate how vulnerable maritime ports are to risks associated with climate change. Therefore, a Resilience Index (RI) is under development taking into consideration the international experience, such as the Climate Vulnerability Index (CVI) developed by the United Nations Development Programme (UNDP) to assess the resilience of ports in the Caribbean [27], and the Ports Resilience

Index (PRI) which is a self-assessment tool developed by the United States Resilience Toolkit [28].

Second, gathering pertinent data on port operations, infrastructure, and climate change is crucial as well as involving all stakeholders [29]. Lastly, the Analytical Hierarchy Process (AHP) is the foundation upon which our method to building the DSS rests when determining the weights of indicators (see Fig. 1) pertaining to the following areas:

- Infrastructure resilience (4 indicators);
- Operational and supply chain resilience (8 indicators);
- Digital resilience (6 indicators);
- Socioeconomic and Environmental resilience (9 indicators);
- Governance and Compliance resilience (6 indicators).

The selection of the aforementioned criteria was predicated on the creation of an efficient DSS that addresses the long-term strategic requirements of the maritime ports rather than their daily operations. In addition, the DSS needs to accurately evaluate the five areas of interest pertaining to the indicators that are vulnerable to climate change, take into account all pertinent factors that may have an impact on their resilience, offer guidance on strategic decision-making, be simple for port operators and administrators to use and comprehend, and be reasonably priced to implement and update.

It should be highlighted that not all of the 33 indicators are based on quantitative data, despite the fact that their total number might be considered as noticeably high. Ninety percent (90%) of the indicators use qualitative data, which reduces the amount of data required and streamlines the AH Process. The choice was made to avoid giving the experts a very large comparison matrix, which would have complicated their decision-making and, consequently, the process of calculating the weights [30].

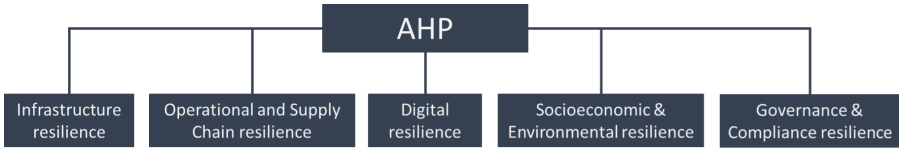

Fig. 1. Proposed areas of interest for examining the vulnerability of maritime ports related to the impacts of climate change

4 Analysis and Results

The under development DSS, is effectively related to a questionnaire-based survey addressed to maritime authorities and operators as well as to Living Labs implemented with the participation of stakeholders involved to ports' operation (see Fig. 2).

Regarding port resilience, the questionnaire-based survey offers insightful information about the viewpoints and experiences of authorities and maritime operators. The survey aids in obtaining a comprehensive picture of the resilience landscape of the port by requesting respondents to rate their opinions of the port's existing resilience levels,

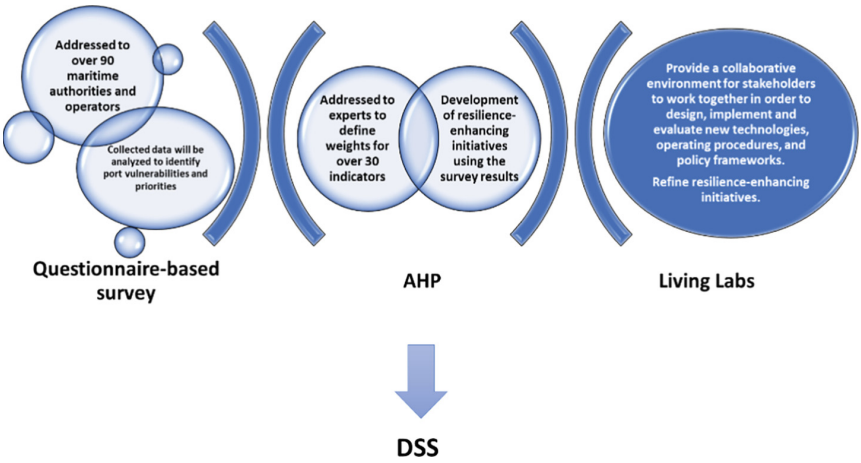

Fig. 2. Integrated approach for developing a Decision Support System to enhance maritime ports' climate resilience

identify potential risks and vulnerabilities, and prioritize areas for development. In order to help design specific resilience-enhancing strategies, the survey collects specific data on port infrastructure, operating procedures, and stakeholder engagement. The questionnaire is addressed to over 90 port operators and authorities, and the response rate at the moment is almost 15%.

As mentioned on the above, an AHP will be used to define the weights (addressing the indicators to multidisciplinary experts covering different scientific and research areas) of multiple indicators which will be then used to calculate the Ports Resilience Index (PRI) identifying the ports' level of vulnerability against the impacts of climate change. The AHP as a multi-criteria decision-making (MCDM) method will be used to prioritize and evaluate potential resilience-enhancing initiatives and also identify the most impactful and feasible interventions for improving ports' resilience.

In parallel with the so far described process, Living Labs (LLs) are organized and implemented, as they can be an invaluable resource for creating and executing creative resilience-boosting solutions. The objective of these LLs is to verify the efficacy and acceptability of new technologies, operating processes, and regulatory frameworks by working with stakeholders, such as marine operators, port authorities, and local populations. The under development DSS will be updated with the insights gained from the LLs as well as the collected data by the questionnaire-based survey, resulting in ongoing enhancements to ports' resilience. In particular, the core actions of the and to be implemented LLs can be summarized as following:

- Engaging Collaborative Stakeholders.
- Evaluation of the risks of climate change.
- Co-creation of innovative solutions.
- Proposing potential pilot projects.
- Constant monitoring and adaptation.
- Information exchange and capacity building.

It must be mentioned that LLs are used worldwide to address the mitigation of climate change impacts, focused however mainly on urban areas, such as the Climax [31], the Urban Living Lab for Climate Resilience [32], the Climate-KIC Living Lab [33] and the Nordic Urban Living Lab [34].

Through the combination of the best features of AHP-based DSS, questionnaire-based surveys, and LLs implementations, ports will be assisted and guided to develop a holistic resilience management strategy. The LLs will test and improve resilience-enhancing activities in real-world settings, the AHP will prioritize and assess resilience-enhancing projects, and the questionnaire survey will supply the first baseline data. By using an integrated strategy, ports will be able to make well-informed decisions regarding resilience investments and achieve long-term enhancements to their infrastructure and operations.

According to Lind et al. [35] four factors were identified as essential for ports to be successful:

- Efficient handling of cargo: This includes having the necessary equipment and facilities to load and unload cargo quickly and efficiently.
- Effective connectivity: Ports must be well-connected to other modes of transport, such as roads, railways, and waterways. This ensures that cargo can be easily transported to its final destination.
- A competitive cost base: Ports must be able to provide services at competitive prices in order to attract customers.
- A safe and secure environment: Ports must be safe and secure for workers, cargo, and the environment.

Based on the data from the questionnaires collected so far by 12 maritime operators and administrators, it was made clear that although the majority of Port Authorities (PAs) collect and analyze data on climate parameters, their measurements mainly concern wind speed/direction, waves (height, length, period, direction) and water quality, for specific areas. When PAs were asked about what additional information would be useful for the development of a Climate Adaptation Plan (CAP), the answers were divided between the assessment of vulnerability of port infrastructure, economic impact assessments and stakeholder engagement data (see Fig. 3).

Specifically, the following additional information was requested:

- Vulnerability assessment of port infrastructure to climate change impacts. This includes assessing the potential impacts of climate change on port infrastructure, such as sea level rise, storms, and extreme weather events.
- Economic impact assessments of climate change on ports. This includes assessing the potential economic impacts of climate change on ports, such as the cost of damage to infrastructure, the loss of trade, and the disruption of supply chains.
- Stakeholder engagement data. This includes data on the views and concerns of stakeholders, such as port users, residents, and environmental organizations.

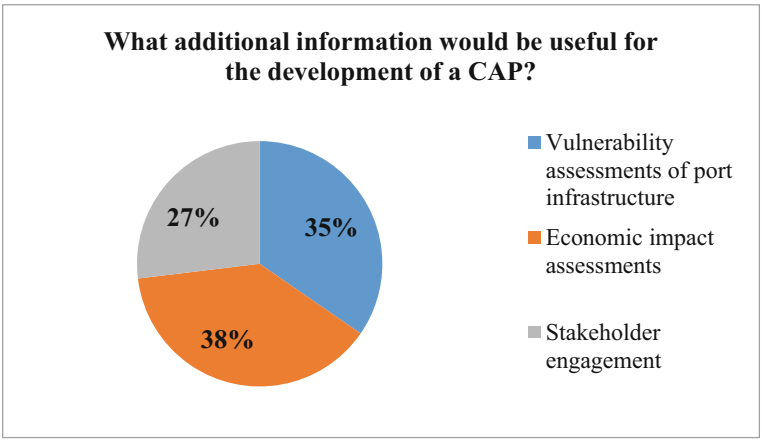

Fig. 3. Assessment of additional information for the development of a DSS

In a subsequent question, the opinions of the PAs were explored on whether and to what extent data sharing, collaborative planning, scenario analysis, and stakeholder engagement can contribute to a DSS to assist them to coordinate with other stakeholders (shipping companies, port clusters, local communities) as well as to address the impacts of climate change. Focusing on the answers that consider that these measures can offer 'a lot' and 'very much', it is concluded that 50% of the PAs believe that collaborative planning can contribute in this direction, while 60% believe that this can be achieved through scenario analysis and stakeholder engagement. 60% also believe that data sharing can contribute from 'moderately' to 'not at all'.

According to Cortes Arbues et al. [36] who "*estimated the relative changes in value added (factor measuring the contribution of each individual sector to GDP) for nine sectors*", Greece's GDP will be affected mostly in a negative way by the seal level rise. The worst scenario regarding Greece's inland regions concerns the Region of Thessaly, which is estimated to be heavily affected losing up to 10% of its GDP. For Greek islands, the above-mentioned research estimated that they all be negatively affected, losing from 0.5% (Crete) to over 10.0% of their GDP (North Aegean). Through the survey, Pas were asked about their opinion on how feasible is to reinforce existing or/ and building new infrastructure as well as implement adaptation measures to address possible future extreme events related to climate change. Figure 4 presents the distribution of the (so far) 12 PAs returning the questionnaires, among the possible choices (Not at all, Somewhat, Neutral, Very, Absolutely) given to them as answers for the respective question.

Although 33% of PAs are neutral on this issue, 50% of them think that it is quite necessary and feasible for them to interfere with their ports' infrastructure (with either reinforcing the existing and/ or building new) in order to address possible future extreme events related to climate change. A recent report analyzed data from several countries and case studies and came to the following (among other) conclusions [37]:

- Without further emissions reduction measures, the shipping industry could face an additional cost of $25 billion per year by 2100.

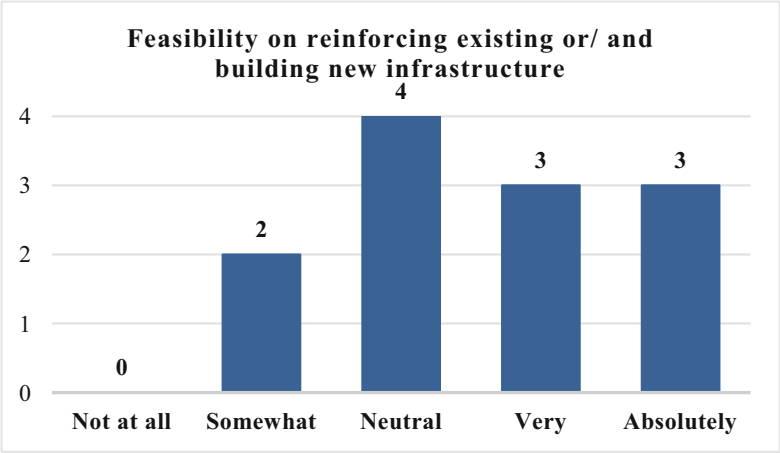

Fig. 4. PAs opinion on how feasible is to reinforce existing or/ and building new infrastructure as well as implement adaptation measures to address possible future extreme events related to climate change {own elaboration)

- An analysis of extreme weather events related to storms in 74 ports in 12 countries found that an additional 1 m in wave height or 10 m per second in wind speed are associated with an increase of 2 days in the average duration of port closures.
- Most studies on the costs of port adaptation have focused on raising the elevation of port facilities, with costs ranging from $30 million to over $200 million per km^2 of port area.
- Global annual storm damage to ports is estimated to be around $3 billion.
- By 2100, the additional annual damage and port closure costs are projected to reach $25.3 billion.
- The cost of raising the elevation of port facilities to protect them from sea level rise and storm surges is likely to be significant.

Combining the above mentioned, it is quite evident that PAs, inevitably, will have to invest to innovative technologies, infrastructures and measures in order to address the impacts of climate change. A DSS developed to support based on real data, PAs' decision for med- and long-term periods is essential. Figure 5 presents the framework for the under development DSS based on the above mentioned.

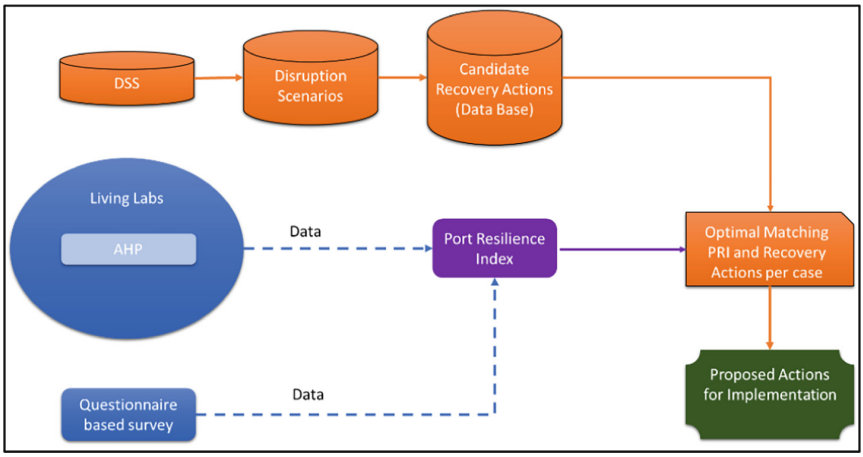

Fig. 5. Basic architecture of the under development DSS

5 Conclusions

Our research has demonstrated the pressing need for maritime ports to enhance their resilience against the impacts of climate change. A Decision Support System (DSS) is proposed as a promising tool to address this challenge. The DSS will be developed by integrating data from a questionnaire-based survey, an Analytical Hierarchy Process (AHP) analysis, and Living Labs (LLs). The questionnaire-based survey was used to gather information from port authorities and operators about their vulnerabilities to climate change, while the AHP analysis will prioritize resilience-enhancing initiatives. The LLs provide a platform for stakeholders to collaborate on developing new resilience-enhancing strategies using real-world settings.

The research findings have also highlighted the importance of data sharing, collaborative planning, scenario analysis, and stakeholder engagement in developing a successful DSS for maritime ports. By incorporating these elements, the DSS can provide port authorities with the information and tools they need to make informed decisions about resilience investments.

The research has several limitations. The questionnaire-based survey has only been completed by a small number of port authorities; however, it is expected the response rate to be increased on the following time period through direct communication between PAs and the authoring team. Additionally, the DSS is still under development, so its effectiveness has not yet been fully evaluated. Furthermore, the proposed methodology has to be tested during the scheduled Living Labs, mostly to verify whether the AHP (Analytic Hierarchy Process) as estimated by the authors or the ANP (Analytic Network Process) will be the more suitable, as the DSS is directly related to the Port Resilience Index that will be calculated for all ports.

Despite these limitations, the research has provided valuable insights into the challenges and opportunities associated with developing a DSS for maritime ports. The findings will be used to refine the DSS and make it a more effective tool for supporting ports' resilience.

Acknowledgments. The research project titled "Enhancing resilience for Greek ports - ResPorts" is being implemented within the framework of the "Natural Environment & Innovative Actions 2022/Priority Axis 3: Research and Application" program, with a total budget of €199,647 Euros. It is funded by the Green Fund and beneficiary is the Department of Shipping Trade and Transport of the University of the Aegean.

Disclosure of Interests. The authors have no competing interests to declare that are relevant to the content of this article.

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Times of Ships in Container Ports: AIS Data for Maritime Transport and Ports Applications

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Abstract. In the context of a global trade, ports are critical nodes in the supply chain. For such reason, monitoring operations have a relevant role for both shipping companies and authorities. In particular, the time of ships in ports affects not only the performance of the ship but also the supply chain as a whole. So, it can be considered as an indicator of competition in the international trade challenge. Disaggregated and aggregated data related to different maritime activities can be used to evaluate this time. Thus, this study focuses on the innovation enabled by the introduction of automatic identification systems (AIS) and the use of data delivered by on board devices. AIS data provide information on the position of a ship allowing to analyze the activities of the ship within a port (e.g., the stop times). This paper aims to provide some general examples, taken from the literature, on the use of this type of data. From the analysis emerged that AIS data, since their introduction, have used for several scopes. Those can be broadly resumed into five different categories, referring to safety and security, environmental issues, route planning and shipping operations, data fusion and economical performances for both ports and vessels company strategies.

Keywords: automatic identification system · AIS · safety and security · route estimation · data fusion · port performance · literature review

1 Introduction

The volume of international seaborne trade reached 12,027 million tons in 2022, with a decrease of 0.4% compared to 2021 (UNCTAD, [1]). The rate of goods transported by sea is approximately 80% [2] of the total. In descending order, this volume is made up of dry bulk, oil shipments, and containerized trade. Therefore, the transport of goods is crucial in international trade [3], representing a pillar of the global economy. In fact, it has been seen (for example, the block of the Suez Canal, geopolitical tensions, wars) that obstacles to the maritime trade have repercussions throughout the world. Research on this topic covers different aspects: port management [4–6]; optimization of shipping operations [7–9], cost/time assessment [3, 10, 11]; the environmental impacts [12–14], the shipping services [15–17] and the use of new technologies [18–21]. In addition to this line of research, we can consider the cases of medium/short-range maritime transport (e.g., [22–27]), which in some cases support international seaborne trade (e.g., feeder

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O. Gervasi et al. (Eds.): ICCSA 2024 Workshops, LNCS 14823, pp. 253–268, 2024.
https://doi.org/10.1007/978-3-031-65329-2_17

services). Several research studies used data collected automatically from devices on board ships (e.g., [28–32]). In December 2000, the International Maritime Organization (IMO) updated the requirements imposed by the Safety of Life At Sea (SOLAS) international agreement [33] by introducing the use of an automatic identification system (AIS). This regulation (effective at 31 December 2004) is mandatory for all passenger and cargo ships in relation to the gross tonnage[1].

The AIS is a device capable of sending (receiving) information on the position of a ship, and the collected data can be used for different purposes (e.g., safety and security, emission estimation and other [35–41]). The rules established that AIS sends information (ship identity, type, position, speed, status, and safety-related information) to seaside stations, other ships, airplanes, satellites, and receives information from other ships. The mandatory use of such a device has made available data on naval activities that can be used in the field of research with multiple purposes [42–45]. The data provided by AIS (and the importance of international trade by sea) pushed the research on this topic; consequently, methods and models have been developed by using such data. Research ranges from safety and security and emission assessment to route evaluation and design. Figure 1 shows a possible classification of the AIS data to be used in the research. It differentiates between historical and real time and also considering the possibility to gather data from multiple sources. Thus, it is possible to identify some topics frequently treated in the literature.

1. Risk assessment;
2. Emissions assessment;
3. Route estimation and planning;
4. Data fusion;
5. Ports and ships performances.

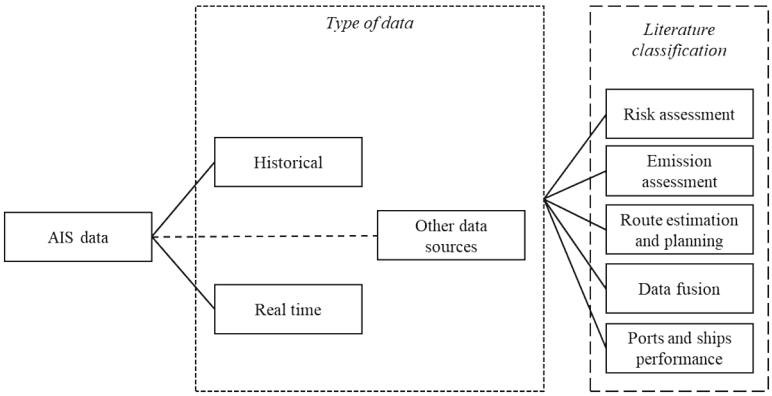

Fig. 1. AIS data and applications.

[1] *Ships fitted with AIS shall maintain AIS in operation at all times except where international agreements, rules or standards provide for the protection of navigational information* [34].

The rest of the paper follows the previous classification, dedicating a paragraph to each of the previous points. Section 2 contains papers on the topic of risk assessment, Sect. 3 summarizes papers on environmental emission assessment, Sect. 4 is on ship route estimation and planning, Sect. 5 contains some studies on the use of AIS integrated with other databases, while Sect. 6 contains some studies on ports and ship performance. Finally, the conclusions.

2 Risk Assessment

An element in defining the risk of collision between ships is the domain of the ship, intended to be the domain around a ship where other ships avoid entering. Therefore, the definition of the domain may be useful in risk assessment. As an example, Kundakçı et al. [46] proposed a domain model based on the type of ship and on different safety criteria. The relative positions between the ships were analyzed, and changes in the domain size of the ship based on ship type and size were highlighted. Bye and Almklov [47] used historical AIS data to provide some normalized statistics on maritime accidents, focusing the study on two events (groundings and allisions) and for two categories of ships (cargo and passengers). The paper focuses on strategies to monitor the level of risk and develops some strategies to mitigate it. Altan and Otay [48] focused their study on collisions between ships on congested waterways by using a collision model (from molecular theory) that takes historical AIS data and gives as output a probability of encounter. The results of the model are compared with the observed data. Oruc and Altan [49] analyzed risk patterns due to the encounter of ships on narrow waterways. The interactions between ships are explored starting from AIS data and using an unsupervised learning algorithm to determine the risk value. Similarly, Zhang et al. [50] proposed a convolutional neural network to classify the risk of collisions. The proposed framework consists of two levels: at the first level the potential collision events are extracted from the AIS data, this information represents the input for the second level that provides a risk rating for collisions. Liu et al. [51] proposed a multi-step analysis for assessing collision risk based on game theory. The first step consists of identifying the collision risk of each ship in a cluster by pairwise analysis. Then, the analysis is extended considering the contribution of each group to the risk value.

Zaman et al. [52] analyzed traffic conditions in the Singapore strait over the time classified by ship type. The aim consisted in monitoring the flow along the waterway and provide support in improving ship risk in the strait. Similarly, Wu et al. [53] studied the behavior of ships approaching a hotspot in narrow and busy waterways considering different types of trips and linking speed with density. The goal is to estimate the risk of ship collisions at hotspots. Mou et al. [54] proposed a statistical model based on historical AIS data to simulate collision among ships in a port. The predictors used in the regression model include ship characteristics, course characteristics and speed. Liu et al. [55] introduced an analysis method to assess the risk of ship collisions based on static and dynamic AIS data. The approach is non-linear and the collision risk is obtained by integrating the position vector and the speed of the ships.

Considering the case of ships sailing in open water, Zhang et al. [56] proposed a method to evaluate in real time the probability of a ship collision using AIS data. The

approach focuses on autonomous maritime surface ships and uses a distance indicator to classify risk in different situations. Similarly, van Iperen [57] developed methods based on distance and time to classify ship encounters (distinguished into head-on, crossing, and overtaking encounters, also considering the routes structure) and monitor ship safety. Feng et al. [58] proposed a method for assessing collision risk based on AIS data within a port. The approach is based on the calculation of the entropy and clustering. The conclusion is that the method could be used to improve the safety level. Rong et al. [59] studied the behavior of ships in avoiding an accident, the procedure is based on AIS data used to recognize those cases where the accident was avoided. A sliding window algorithm is applied to identify the moment in which the ship performed an evasive maneuver to avoid colliding with another ship. Zhu et al. [31] have proposed a framework to classify ship encounters and some predictors are selected in order to estimate a model. A sensitivity analysis approach is applied in the phase of predictors selection. Zhao and Fu [60] proposed an index for the assessment of real-time collision risk based on AIS data. Such an index aims to establish if two ships can collide while maintaining the current state of motion, so the obstacle's speed is considered a fundamental element in the index definition. An improvement of the previous approach has been proposed by Chen et al. [61]: the proposed method considers that the obstacle travels with non-linear variable speed. Note that, in this method, the encounter between two ships is considered as a process that takes into account the spatio-temporal relationship between them. Chen et al. [62] propose an extension of this work, taking into account the encounter of multiple ships, is proposed by Chen et al. [62].

AIS data are also useful for analyzing the risk faced in collisions between ships and fixed structures (e.g., bridges). As an example, Zhao et al. [63] consider the risk connected to the collision between a ship and a bridge, and the AIS data are used to obtain the attributes (such as speed, position, etc.) to be putted in the model. The model is based on the finite element approach. Xiao et al. [36] investigated the risk of collision between ships and bridges on some waterways in China. AIS data are used to individuate traffic conditions, and the interaction among different ships is simulated through a multi-agent model. To understand ship behavior, two different cases studies are simulated and compared. Cai et al. [64] proposed a model to assess the risk when a ship crosses a river considering different elements, such as the distance to the closest point of approach and the time to the closest point of approach. In a similar study, Wang et al. [65] proposed a method (based on real-time AIS data) to model ship flow characteristics and estimate the correlation between speed and flow. The aim is to obtain an estimated value of the speed to compare it with the limitation imposed by the traffic regulation. Horteborn and Ringsberg [66] studied possible ship allision against a bridge, considering three possible scenarios: drifting ship, sharp turning ship and miss of turning point. The scenarios are simulated using the Monte Carlo approach.

3 Emissions Assessment

Ship emissions attract attention worldwide, and several methods (e.g., [67]) are used to quantify them. AIS data can support this task by providing ship and route data (e.g., engine load factors). Indeed, AIS data allow for separating the ship's activities (ship

at anchor, ship docked for load/unload operations, port arrival/departure) and linking them with the estimation of ship emissions [68]. Procedures based on such data are often indicated as bottom-up approaches. Tian et al. [69] demonstrated the impact of AIS data thinning in the emissions, namely, how the amount of data used in emission estimation of emissions affects the quality of the results. The conclusion is that the data must be thinned differently depending on the position of the ship (e.g., in port, coastal navigation, etc.). Ng et al. [37] exploited data from AIS (and, in particular, ship movement and speed information) to estimate the engine load factor used, together with data from other sources, to assess ship emissions. The procedure is also aimed at supporting decision makers in policy planning. In Tichavska and Tovar [70] the AIS data are used to geographically locate the emissions in a port. The procedure identifies the activities of a ship (in berth, in maneuver) and puts them in the procedure for emissions inventory. The aim is to classify the emissions in a port according to their location to assess the policies (environmental, operational, or political) aimed at minimizing the environmental impacts. Furthermore, the procedure supports monitoring of the effects of such policies. In Bojic et al. [71] a model to estimate ship emissions in a port has been proposed; the AIS data are crossed with ship technical details. Huang et al. [72] extended the previous approach by proposing a spatio-temporal approach to estimate emissions. The proposed model differentiates among ship classes and navigation states. The model has been tested using a port as a case study. Chen et al. [73] focused their study on the contribution of ships on the particulate matter concentration in the city near the analyzed port (about the 13% in summer). A classification of emissions based on the type of ship is also provided, highlighting that container ships are the main contributor to emissions in the study area. Peng et al. [74] applied the power-based emission inventory calculation using AIS data to obtain the emissions in the urban area near the port. The model is updated by introducing a correction coefficient for the engine propeller to optimize the results. Toscano et al. [75] investigated the activities and emissions in the Naples port through AIS data, obtaining a temporal trend of the emissions. In addition, they used a dispersion model to assess the impact on the nearby urban area. Li et al. [76] estimated the emissions considering different types of ships, taking also into account the influence of speed on emissions (and, consequently, the influence of the different ship operational activities). A spatio-temporal analysis of emissions is provided. Similarly, Chen et al. [77] developed a spatio-temporal emission inventory and analyzed the emission variation within a month using the uncertainty estimation procedure. Variation in emissions over time is attributed to variation in the quantity of freight transported. Huang et al. [78] introduced a method to develop AIS data in real time to obtain the ship emissions from the ship route. The approach provides results in the spatio-temporal domain. Goldsworthy and Goldsworthy [79] used terrestrial AIS data to develop a model to estimate emissions and to allocate them spatially (in port and in coastal waters). Emissions are calculated by ship characteristics (type and size), operating mode, and engine type. This analysis has been extended in [80], where a method based on the search for the shortest path has been used to improve the estimation of the spatial distribution of pollutant elements. Woo and Im [81] proposed a bottom-up approach based on AIS data to assess emissions in a port over time. The authors correlated the emissions with the speed of the ships in the port, demonstrating that a speed regulation would reduce emissions. In a similar work,

Woo and Im [82] used AIS data to estimate the spatial distribution of emissions in real time. The goal is to verify the efficiency of the ship speed reduction policy in reducing emissions (in the real-world application, the spatial analysis showed the reduction of emissions with the reduction of the speed). Kim et al. [83] calculated the volume of emissions from ships in a port considering separately activities (cruising, maneuvering, hoteling) in order to estimate the engine load factor of the engines. The activities of the ship in the port are determined by analyzing the AIS data. Jiang et al. [84] proposed a model to calculate the emission from ships in the inland areas. As in other similar models, the emissions are calculated for the different activities of the ship in port. Cheng et al. [85] used AIS data to assess the emissions in a port and verify the results of a policy aimed at reducing the emissions of ships in the port. The conclusion is that the contribution of the ship in emissions was reduced (mainly in terms of SO_2 and PM) by applying this policy. Kao et al. [86] estimated the emission over time considering different scenarios (e.g., speed reduction). The aim is to improve environmental conditions, at the port, allowing us to identify the elements on which to intervene to reduce emissions. To estimate ship emissions in port, Chen et al. [87] proposed a model based on ship activities. In particular, AIS data are used to identify the operation in port (dock, undock, maneuver), and the emissions are estimated separately for each activity.

4 Route Estimation and Planning

Today, maritime transport is becoming an essential stream in global trade. Several scholars focused their work on AIS to exploit the information contained therein and propose data-driven predictions on arrival and operating times.

Yin et al. [38] developed a model to forecast the destination of the ship by combining historical and real-time AIS data. Ma et al. [88], proposed a neural network approach in which the trajectories were first extracted with a clustering method and then developed a forecast procedure based on neural networks. Similarly, Wen et al. [89] used AIS data for the design of ship routes, applying cluster analysis to individualize waypoints and the neural network to generate routes (also considering different dimensions of the ship). Chen et al. [90] proposed a deep learning approach by crossing speed and position information as a training input for the neural network. The aim consisted in improving fitting accuracy of the observed routes. In addition, the missing points of a route are correlated with the known points near routes, if available. Mehri et al. [91] proposed a model based on deep neural networks to individuate the trajectory of the ship and to foresee ship position (using as input the type of ship and geographic information). Wang et al. [92] developed a cluster analysis to extract routes from AIS data taking into account the density of ships. In addition, an approach to determinate the optimal number of clusters is provided. To consider the ship behavior in trajectory estimation, Wei et al. [93] proposed a procedure based on an algorithm to simplify the trajectory of the ship (related to the data on the position of the ship) and on a sliding windows algorithm (related to the variation of the course and the ship characteristics). Yan et al. [94] proposed a method (based on a semantic model) to individuate ship routes based on historical AIS data and used graph theory to provide a simplified representation of such routes. The aim is to forecast the traffic of the ship and analyze the activities of the ship.

Guo et al. [95] proposed a kinematic interpolation method (KI, [96]) to reconstruct the trajectory of the ship using AIS data. The approach starts from the search and elimination of incorrect data, and it individuates the trajectory by using an improved version of KI. Such a version of the interpolation procedure also provides for the reconstruction of missing parts of the trajectory. A multistep prediction model has been proposed by Gao et al. [97] to estimate the trajectory of a ship. The historical data are used to identify a support trajectory, starting from a point of them the next point is calculated by cubic spline interpolation. Another aspect that can be considered is the distance between similar routes collected with AIS, with this in mind, Luo and Zeng [98] proposed a framework to measure the distance of the ship trajectory based on a neural network. The procedure has been tested on a real trajectory dataset. Filipiak et al. [99] presented a method to obtain a maritime graph (consisting of nodes and links) based on historical AIS data. The approach starts from the detection of maneuvering points and waypoints (intersection between different routes) and builds the links. The maneuvering points are individuated by using a cumulative sum approach, while the waypoints are the output obtained by applying a genetic algorithm to the set of maneuvering points. Lee et al. [100] proposed a method to obtain routes and waypoints based on cluster analysis and kernel density estimation. In their work, the authors individuated, for each route, the vertices among which the waypoints will be identified.

5 Data Fusion

Sometimes, AIS data are integrated with other data sources to obtain more accurate results. As an example, Liu et al. [101] combined AIS with data from SAR (Synthetic Aperture Radar) to identify oil spill pollution. For tracing oil discharge from ships, a framework is proposed in which the SAR is used to identify suspected oil slicks (time, location, range). Then, the suspect ships are individuated by combining oil-sick trajectory simulation and data from AIS (in a time slice after the identification of the oil). Similarly, Pelich et al. [102] proposed a procedure for ship monitoring based on SAR data and used AIS data to validate the results (in fact, the objective is to evaluate the accuracy of satellite observation in relation to the dimension of the ship). Asborno and Hernandez [103] used historical AIS data and aggregated port throughput data to estimate the quantity of freight transported by ships for each travel. The study focuses on inland waterways with the aim of reducing freight flows and (eventually) supporting decisions about investments in transportation infrastructures. Huang et al. [104] integrated AIS data with ocean environment information (such as winds, waves, and currents) to estimate ship emissions. This approach allows to consider how the environment affects the activities of the ship, increasing the performance of ship activity-based method used to estimate the emissions. Abebe et al. [105] integrated AIS and marine weather data with the aim of forecasting ship speed, the approach used is based on machine learning. Different techniques of machine learning are used, in order to compare the accuracy of each of them. Wang et al. [65] combined AIS data with waterway data to simulate the flow of the ship and correlate them with speed. The main goal is to compare the forecasted speed with that required by maritime regulation. To predict the ship trajectory, Borkowski [106] proposed an algorithm that takes advantage of current ship position collected by

several devices, and AIS is among them. The data fusion is based on Kalman filter, and the procedure works using a generalized regression neural network. Kaklis et al. [107] presented a method for the design of the route of ships using historical AIS data. An algorithm for the route search is implemented to find the optimal one to compare with the observed one. AIS data are integrated with real-time weather condition data; the goal is to optimize the route and also considering environmental conditions. Li et al. [108] crossed AIS data with VIIRS boat detection (VBD) to monitor the activities of fishing boats; the aim is to identify the fishing by zone over time. Thoya et al. [109] proposed a method to estimate fishing activities by combining AIS data and the vessel monitoring system (VMS). The aim is to identify discrepancies between the two databases and integrate them to have a more accurate analysis of the studied area. The correlation between fishing activities and oceanographic elements is investigated by Li et al. [110]. The AIS data are integrated with satellite-derived sea surface temperature (SST) and chlorophyll a concentration.

6 Ports and Ships Performance

AbuAlhaol [111] proposed a data mining framework to obtain three indicators (spatial complexity, spatial density, and time of service) to quantify port congestion. Historical and real-time AIS data are as an input; the approach combines these two data sets and gives the indicators as output. Chen et al. [112] defined some port performance indicators (port productivity, ship traffic, berth utilization) and proposed an approach (based on AIS data) to evaluate them. The study focuses on container ports to identify infrastructure weaknesses and intervene with appropriate policies and procedures to improve productivity and optimize liner scheduling. Chen et al. [113] have proposed an approach based on the sliding window algorithm to evaluate the congestion index of a port. In it, the AIS data are used to explore the ship's trajectory in the port: from this, the time in port and the related monetary costs are evaluated. De Langen et al. [114] proposed an index to measure the connectivity of roll-on roll-off ports by using, among others, AIS data to individuate the ship route and the related travel time. Similarly, Jia et al. [115] proposed a connectivity index considering different ship types; such an index depends on the number of port calls, the rate of international traffic, and the characteristics An approach able to estimate the port locations and related operational zones has been proposed by Millefiori et al. [116] by using historical AIS data and a distributed machine learning method. The approach is tested in an existing port. Peng et al. [117] proposed an evaluation model to assess the competitiveness of a port, using geographic data and AIS data. The method is based on the concept of entropy and considers ship trajectories, infrastructural facilities of the port, and socio-economic data. Feng et al. [118] proposed a framework for estimating the time a ship spends in a port that exploited the ship trajectories provided by AIS data. The time estimation is provided for different port zones and vessel categories, and performance indicators are defined to assess the payload productivity. Jia et al. [119] proposed a methodology based on the ship draught information (collected from AIS) and ship and travel-specific information to estimate the ship's payload. Lee et al. [120] studied the ship trajectories in a port exploiting AIS data, distinguishing ship arrival and departure. A clustering method is

applied to search for possible patterns in the analyzed trajectories. Liu et al. [121] combined principal components analysis, a clustering approach, and a soft dynamic time wrapping method to identify ship trajectories, separating in-port and out-port ship routes. The input data comes from historical AIS data.

7 Conclusions

This paper reviews the current use of the AIS data in maritime analyses. From this literature emerged how versatile result AIS data are. It emerged that one of the primary uses consisted of collision risk assessment analyses whose approaches range from statistical analysis to neural networks to microsimulation. Another highly-covered topic concerns environmental analyses and carbon emissions. Some approaches were thought to find the emission inventory for vessels in navigation and others for vessels in port (in this case, the emissions are estimated for each type of activity of the ship into the port). Data collected from AISs are often used in planning operations to evaluate effective policies to reduce air and noise pollution. Therefore, the data from AIS are used to estimate/optimize the route, for example, to reduce the ship's travel (and related impacts). The approaches used contain neural networks, cluster analysis, and heuristic approaches. Often, AIS data are integrated with other data to increase the database and improve the quality of the results obtained.

The emerging availability of real-time data offered by AIS devices enabled the possibility of enriching analyzes to estimate the time of ships in port. For example, the AIS data allow the analysts to infer the various activities carried out by the ship and the identification of possible predictors to use in the models (for example, type of ship, size of the ship, period of the year). Even if AIS data till today are not fully explanatory to assist the analyst in such a compelling domain, and other data, as well as information on terminal equipment and facilities, are necessary to unveil different segments of activities that took place in container ports; the introduction for AIS data offered the opportunity to deliver a valuable tool to overcome the limitations imposed by direct surveys and the restrictions related to the use of data provided through VTS systems whose nature is confidential and for exclusive use by the authorities.

Acknowledgments. This study is carried out within the research project "National and local factors affecting times of ships in container ports", Piano Nazionale di Ripresa e Resilienza (PNRR), Next Generation EU. Progetti di Rilevante Interesse Nazionale PRIN_2022_PNRR_P202292YFW. CUP: C53D2300878001. This presentation reflects only the authors' views and opinions, "neither the European Union nor the European Commission can be considered responsible for them".

Disclosure of Interests. The authors have no competing interests to declare that are relevant to the content of this article.

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The Importance of the Centrality of Ports for Passenger Transport in the Adriatic-Ionian Basin

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Abstract. The European port system must continue to play a strategic role considering three different aspects: economic, geopolitical and logistical.

Several parameters can be considered in order to improve the definition of these transport nodes and among these the study of centrality is of fundamental importance. This study focuses on the analysis of the network of passenger transport services within the Adriatic-Ionian basin that are part of the TEN-T network. To these ports (both core and comprehensive) was added Durres, which has the characteristics of a major port in the Adriatic basin, as well as being the main port in the Southern Adriatic, although not belonging to the EU context. The study was conducted by monitoring the systemic passenger transhipment services and initially evaluating the Origin-Destination matrix and for each pair of values the average weekly number of connecting services in the year 2023, extrapolating some considerations in the most critical months.

Through the calculation of the centrality parameters (Ci degree and Si force centrality), a partial correlation with seasonality emerged.

Specifically for 2023, it emerged that the value of Ci defines Igoumenitsa as the most central port in the basin for all months considered. The Croatian and Albanian ports are less significant on a basin scale.

Furthermore, the assessment of Si places Igoumenitsa, Bari and Ancona as the ports with the most connections. In the Croatian ports, a more marked seasonality emerges. In particular, it emerges that Croatian ports are more interested in tourism, which could mean that the Italy-Greece and Italy-Albania connections are also connections made for reasons unrelated to summer tourism.

These results lay the foundations for actions and strategies to improve maritime transport services and optimise passenger services at certain times of the year.

Keywords: Ports networks · Sea passenger transports · Degree and strength centrality · Sustainable mobility

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O. Gervasi et al. (Eds.): ICCSA 2024 Workshops, LNCS 14823, pp. 269–282, 2024.
https://doi.org/10.1007/978-3-031-65329-2_18

1 Introduction

Sustainable Development Goals are the main topic that guide the development of countries in terms of sustainability. The main document, "Transforming our world: the 2030 Agenda for Sustainable Development" [1] contains the main elements to be followed to pursue a sustainable development. Even if all the topics are of public interest, in this context it is useful to recall two specific goals: "Goal 9. Build resilient infrastructure, promote inclusive and sustainable industrialization and foster innovation" and "Goal 13. Take urgent action to combat climate change and its impacts". In a context of improve quality of life for people, reduce pollution and carbon footprint and reduce inequalities between people, a great attention has to be paid to modal shift towards more sustainable transportation means. Considering the environmental impact of several transportation mode [2] it is important to consider the importance of sea passenger transport [3].

In the context of European union, White paper 2011 on transportation [4] has severely recalled the importance of sustainable transportation and of an integrated space. Several maritime basins are included in the EU geographical area; most of them links different countries. So, sea transportation is also an opportunity to enforce links between European countries, in the context of the Trans-European Network on Transportation (TEN-T) [5]. Several European corridors consider ports as main node, and several ports are included in the Core network. TEN-T is meant to improve connections between European countries, with the possibility, for non-EU countries in the area, to cooperate. In this context, a primary role may be assumed by Adriatic Sea. Adriatic Sea is an open basin that links seven different EU and non-EU countries; Adriatic is linked to another basin, Ionian Sea, that separate Southern Italy from Greece. Adriatic Sea and Ionian Seas, together, form the sea that separate two of the three main southern European peninsulas: Italian peninsula and Balkan peninsula. The region considered is crossed by several trans-European corridors: Scandinavian-Mediterranean, in eastern Italy; Mediterranean, in north-eastern Italy and western Balkan; Baltic Sea-Adriatic Sea in Adriatic coast of Italy; Western Balkans, in Greece, Croatia and Slovenia. The latter one, also, includes several non-EU countries.

The importance of maritime transportation, and the key role of Adriatic-Ionian area in European development has been recalled. The aim of this work is to better understand the opportunities given by these basins in terms of passenger transportation. The topic is the study of centrality in network of services in the area, highlighting gaps and evaluating if there are point of strength and weaknesses.

Section 2 of this work discusses the evolution of ports and the role of passenger ports today. Section 3 shows the methodology used. For this analysis, tools from network analysis are considered, evidencing several indicators that can show different aspects of centrality in a network. Section 4 illustrates the results of methodology applied to the case study. Finally, in Sect. 5 results are discussed, and the most relevant conclusions are provided.

2 Ports Evolution

The United Nations Conference on Trade and Development (UNCTAD) classifies ports in four categories, starting from their functions [6, 7]:

- First generation ports are those directly connected to the city; the port is born even before the city itself. Genova, Trieste, and Venice are example of first generation ports;
- Second generation ports are large industrial agglomeration, often placed where they need to serve large industrial area. Taranto is an example of second generation port;
- Third generation ports are specialized in containers management and transportation. Gioia Tauro in as example of third generation port;
- Fourth generation ports are linked to the possibility to create multiple port-cities aggregation under the same authority. The creation of Port System Authority in Italy defines the desire to pursue fourth generation port models.

The availability of computing resources, 5G networks and clouds makes it possible to deliver port services in a way that can be as 'standard' as possible. In this sense, the pursuit of the re-appropriation of data allows the port system to configure itself as a fifth generation "Digital Hub". Therefore, the "new" port is no longer just a system that provides a portal of services, like a first-generation system, but is able to offer the possibility of accessing data to build a series of services, capitalizing on its use and versatility [8, 9].

Consider how the definition of generation k port does not imply an improved condition to a generation k-1 port; the idea of port generation is connected to the main functions performed by it.

It is important to establish the role of first-generation ports in the context of passenger transport. Second- and third-generation ports, serving industrial and commercial ports, are less concerned with passenger transport; fourth-generation ports, by definition, can fulfil several functions. First-generation ports have traditionally been those most concerned with passenger transport.

In particular, in open sea basins, the role of first-generation ports has been to be hubs for the exchange of people, as well as goods, between different countries. Several works in the literature refer to the connectivity and accessibility of sea-side ports, with reference to both port-city, peripheries and inner harbors interaction [10–13].

The effects of poor port connectivity have been studied by [14] emphasizing the limitation of competition between carriers, high freight rates and higher inventory costs for shippers, i.e. the main factors that jeopardize a port's international competitiveness.

Good connectivity is crucial for port and neighboring areas' growth.

As defined by [15] there is a relationship between connectivity-centrality taking into account the degree of difficulty of a port to connect to other ports in a global context.

The present research work is within the framework of the analysis of sea-side port connectivity, considering a basin-wide service system. In this sense, it is intended to recall how the tools that will be discussed in Sect. 3, network analysis, are used in the literature to describe seashore port connectivity problems but are also widespread for other transport systems [16–19]. The present work intends to develop an example of a study of port connectivity and centrality in an open basin.

3 Methodology

The methodology under consideration is described in Fig. 1.

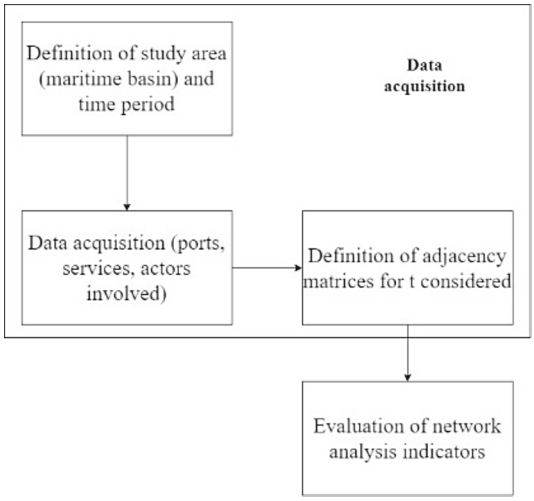

Fig. 1. Methodological framework

3.1 Data Collection

The elements to be defined for the construction of the network are:

- A maritime sea basin of reference;
- A time interval *t*;
- A criterion the identification of ports network. Ports are the nodes of the network;
- A quantitative parameter for the definition of a link

The central element of the analysis is the existence of one or more services connecting two ports. Once the reference basin is defined, *i, j* are defined as the generic pair of nodes. It is possible to define the ordered set $p_t = [i,\ldots,j]$ as the generic route *p* having origin in *i* and destination in *j* at time *t*, in which *i* and *j* are ports belonging to the identified basin. Since it is possible that the generic nodes *i, j* are not, respectively, the origin and destination of a route, it is necessary to generalize by introducing the nodes *z* and *s*. The generic route is defined as $p_t = [s,\ldots,i,\ldots,j,\ldots,z]$ as the generic route that includes a direct connection between *i* and *j*. Consider, in particular, how *s* and *z* do not need to belong to the reference basin; however, the existence of a connection between i and j makes their consideration essential.

Consider the existence of a route $p_t = [i,g,j]$, an ordered set that involves stopping at an intermediate node. The service considered, expressed by the route p_t, connects *i* to *g* and *g* to *j*. However, despite the existence of an intermediate stop, the service also connects *i* to *j*. To highlight this element, it is necessary to break down each route $p_t = [s,\ldots,i,\ldots,j,\ldots z]$ into the individual pairs of relations that compose it.

It is possible to define $k_t(i,j) = 1,2,\ldots,Kt(i,j)$ the generic connection between nodes *i* and *j* at time *t* on the network considered, being $K_t(i,j)$ also the total number of services between *i* and *j* at time *t*. In this way, it is possible to define also the adjacency matrix

of the network as

$$A_{ij}(t) = [a_{ij}(t)] \tag{1}$$

where

$$a_{ij}(t) = \begin{cases} 1, \exists k_t(i,j) \vee k_t(j,i) \neq 0, i/j \\ 0, \nexists k_t(i,j) \vee k_t(j,i) \neq 0, i/j \end{cases} \tag{2}$$

It is possible to define the adjacency matrix, therefore, starting from the condition of existence of at least one link connecting i and j regardless of the order in which they are considered. The service graph $G = (N, E)$ is defined, where $N = \{1,2,3,\ldots,i,j,\ldots,N\}$, $E = \{(i,j)|i,j \in N, i \neq j\}$.

3.2 Data Preparation

Network analysis allows the study of the characteristics of the network. The elements are the main indicators of the centrality of a network. Since each indicator is defined starting from different quantitative elements, it is essential to define different indicators. The purpose of this operation is linked to the need to show different aspects related to the centrality of networks. The first indicator considered is the Degree centrality c_i. It is defined as

$$c_i(t) = \frac{\sum_i a_{ij}(t)}{N-1} \tag{3}$$

where the variables have known meaning.

The degree centrality refers to the maximum centrality obtainable from a node. It is evaluated starting from the sum of the rows on the adjacency matrix and is related to the maximum number of connections that a node i could have $(N-1)$. This indicator, therefore, measures the centrality of a node by considering only the existence of connections with other nodes. In the specific case, considering the data proposed in Sect. 3.1, the degree centrality quantifies the number of ports with which the port in question is connected, at time t. A value of $c_i(t) = 1$ indicates that the port, at time t, has at least one connection to every other port in the network. The degree centrality indicates the possibilities offered by the system, but sometimes it is necessary to introduce a further quantitative term, associated with the arc, to further define the centrality of the network. Consider a case where node i is connected to node j and node z at time t. However, in the example considered, it should be noted that node i has three connections with node j, and only one with node z. The Degree centrality, in this case, returns the same value to both connections: it gives topological information on the network.

To partially solve this problem, it is possible to introduce a quantitative measure associated with the generic edge (i,j). In the case in the measure proposed is the number of services that connect i and j at time t. The indicated term, $w_{ij}(t)$, is defined as

$$w_{ij}(t) = K_t(i,j) + K_t(j,i) \tag{4}$$

It is possible to define the second indicator, strength centrality, as

$$s_i(t) = \sum_j a_{ij}(t) w_{ij}(t) \tag{5}$$

The indicator quantifies for each node i the number of services with the nodes j with which it is connected. In this way, the resulting value can define characteristics in terms of the frequency of connections in the interval t, as well as the nodes j with which i is connected. The two indicators considered show complementary information. Finally, the application to the port system can be carried out by considering different periods t on the same network, verifying the existence of modifications. The possibility of existence of predominantly tourist destinations determines the need to consider seasonality in the system, and to evaluate the centrality as it changes.

4 Results

The study is focused on the network analysis of the service routes between TEN-T ports on Adriatic-Ionian basin.

4.1 Study Area

The case study considered is the Adriatic-Ionian basin. As mentioned in Sect. 2, it is an open basin, in which the western coast is entirely Italian, while the eastern coast is divided between six states: Slovenia, Croatia, Bosnia, Montenegro, Albania and Greece. Of these, Greece is the only country on the eastern shore of the Ionian coast. The five Adriatic countries have a very different coastline in terms of extension; Croatia and Albania are predominant; Montenegro and Slovenia have a smaller extension; the Bosnian coastal strip has a small extension. The ports chosen are those that:

- Belong to the TEN-T, Core or Comprehensive network, or its extension to neighboring countries;
- Are totally or partially passenger ports, and are included in at least one national or international passenger service route;
- Have at least one link with another port of the network.

The first of the two criteria considered allows the scope of application to be narrowed, limiting the study to a basin level, and therefore removing local connections; connections with smaller islands, for example, are often linked to specific constraints due to territorial continuity. Furthermore, the extension to neighboring countries extend the study to important realities at the basin level but outside of EU planning.

The second of the two criteria allows the study to be limited to ports that have an interest in passenger traffic with systematic characteristics. Finally, third criteria the third criterion allows to create a network that is entirely connected in at least one month of the year. Within the basin considered, and once the criteria for choosing services have been identified, the operators who manage sea transport services are defined in Table 1.

The network evaluation carried out identifies $N = 11$ ports. The ports are identified in Fig. 2.

Table 1. Operators considered in Adriatic-Ionian basin

Operator	Reference
TP Line	[20]
Krilo kapetan Luka	[21]
Liberty Lines	[22]
SNAV	[23]
Gomo viaggi	[24]
Jadrolinija	[25]
Venezia Lines	[26]
Adria Ferries	[27]

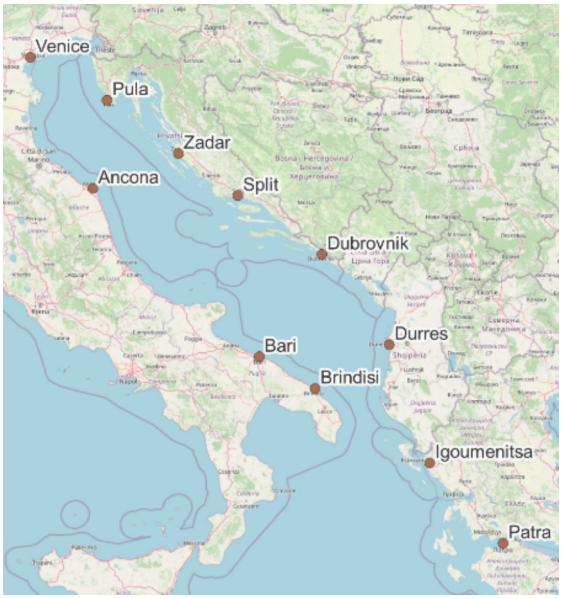

Fig. 2. Port network considered (Source: authors' elaboration based on QGIS [28] and OpenStreetMap [29])

Table 2 shows the main characteristics of the ports considering country and Core/Comprehensive network.

The ports considered are part of 4 countries of the 7 considered. The ports are all in EU countries, except for the port of Durres, indicated as a port of the Comprehensive network extended to neighboring countries. Once the basin, the operators, the services, and the nodes of the network have been identified, it is possible to define the number of services that connect nodes i and j for each t. Consider how the services identified present a considerable seasonality, with notable variations between months and minor fluctuations between weeks of the same month.

Table 2. Ports considered and their geographic characteristics

Port	Country	Core/Comprehensive
Ancona	Italy	Core
Bari	Italy	Core
Brindisi	Italy	Comprehensive
Dubrovnik	Croatia	Comprehensive
Durres	Albania	Comprehensive
Igoumenitsa	Greece	Core
Patra	Greece	Core
Pula	Croatia	Comprehensive
Split	Croatia	Comprehensive
Venice	Italy	Core
Zadar	Croatia	Comprehensive

Therefore, the reference time unit is the week of the month, and the value of services studied is the average number of services per week of the month. In this way, it is possible to reconstruct the average number of weekly services that, for each month, connect nodes *i* and *j*. This value is shown in Fig. 3.

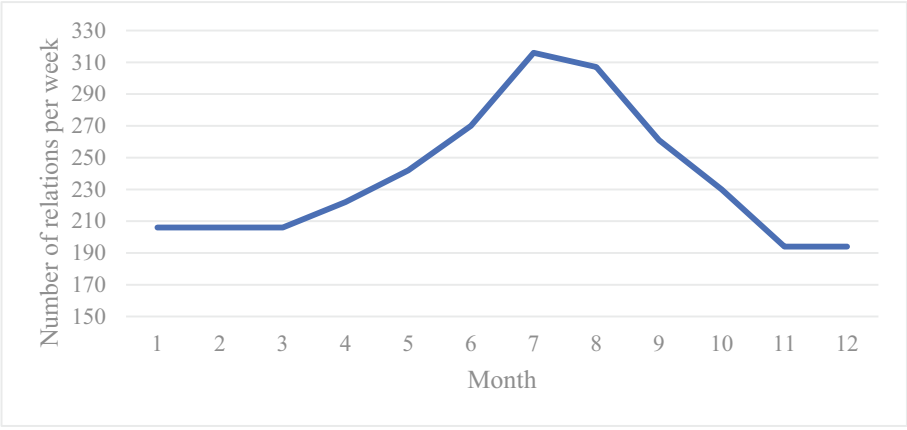

Fig. 3. Trend in the number of weekly reports over the different months.

In this way, it emerges that there is a rather marked seasonality, with a considerable peak in the month of July and high values also in the months of June, August, and September. This allows us to define the need to study the characteristics of the network in several periods, to evaluate whether there are any changes in centrality.

4.2 Network Analysis Indicators

Two months are proposed for the next results exposition: $t = 7$ (July) and $t = 11$ (November). They are, respectively, the month with the highest and lowest average number of services per week. Below is the representation of the network for $t = 11$ and for $t = 7$. Consider how the structure of the graph changes considerably between the two periods (Figs. 4 and 5).

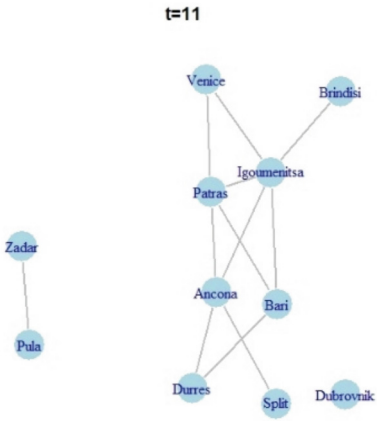

Fig. 4. Network considered, $t = 11$ (Source: authors' elaboration using R software [30])

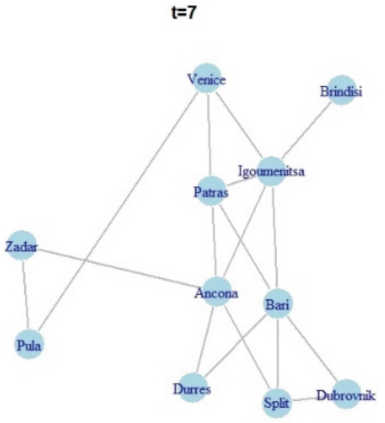

Fig. 5. Network considered, $t = 7$ (Source: authors' elaboration using R software [30])

Similarly, the summary of the results for the three indicators c_i and s_i for each of the nodes i of the network for $t = 7$ and $t = 11$ is proposed in Table 3. A considerable difference emerges between the values between the months considered, for both indicators. Although some nodes emerge with greater centrality (Igoumenitsa, Patras, Ancona), none of these have values greater than $c_i = 0{,}5$; this indicates that the network is not

very interconnected and there are no nodes of main importance at the basin level. The network is instead characterized by many one-to-one connections. Considering values of s_i, related to number of services per week, it is interesting to consider how several nodes see a strong reduction in number of services (especially the Croatian ones), while other see only a relatively small variation (Brindisi, Durres).

Table 3. Ports considered and relative Network Analysis Indicators

Port	c_i		s_i	
	$t = 7$	$t = 11$	$t = 7$	$t = 11$
Ancona	0,5	0,4	84	46
Bari	0,5	0,3	98	78
Brindisi	0,1	0,1	28	22
Dubrovnik	0,2	0	46	0
Durres	0,2	0,2	64	56
Igoumenitsa	0,5	0,5	132	98
Patras	0,4	0,4	70	64
Pula	0,2	0,1	20	4
Split	0,3	0,1	60	4
Venezia	0,3	0,2	18	12
Zadar	0,2	0,1	12	4

5 Discussion and Conclusion

Different considerations are necessary. The system considered has a strong seasonality; this is connected to the nature of some locations in the area considered, characterized by considerable tourist flows, especially in the summer season. Furthermore, only some of these locations are continuously connected to the rest of the system in any month.

The network had considerable variations between the two months analyzed. In the month of July, the formal representation of the port system considered returns a connected graph; in November, some nodes are disconnected from the system. Specifically, Dubrovnik has no connections with other nodes of the network, while Split and Zadar form an autonomous system. Consider how the three ports indicated are Croatian; they are involved mainly in passenger transport connecting main coastal citiese with the numerous smaller islands of Croatia. The port with the largest values of s_i and c_i is Igoumenitsa, Greece's gateway to the Ionian Sea and the main connection hub with other mediterranean countries. Igoumenitsa shows connections with the four Italian ports considered and with the port of Patra, in the northern Peloponnese, which shows considerable values of both c_i and s_i. Relative to Italian ports, the most significant values are associated with Ancona and Bari. The two nodes share the same connections in

the month of July (the two Greek ports, Split, and Durres), but have connections with Zadar and Dubrovnik respectively. Even the evaluations on eigenvector centrality tend to reward Igoumenitsa, Patras, Ancona, and Bari. It is appropriate to recall the absence of Italy-Italy connections in this context; vice versa, there are Greece-Greece connections. Services connecting Igoumenitsa to Patras are very widespread, often including several Ionian islands (mainly Corfu) in their routes. Similarly, there are several Croatia-Croatia services, also serving the smaller islands. The results generally show that:

- The centrality of Greek ports shows high values. This is probably linked both to the geographical proximity to various Italian ports, and to the presence of various tourist-oriented destinations in western Greece; this may also be related to the Greek geographical conformation and the lack of "direct" territorial continuity between Epirus and Peloponnese;
- The centrality values of Italian ports reflect, however, a less interconnected reality. There are no connections between Italian ports; this is probably linked to the greater competitiveness of the other modes on the Adriatic coast, entirely connected by high-speed rail services. An opposite situation occurs to that of the Tyrrhenian Sea, where there is a dense network of services that connects the main ports, thanks to the presence of two large islands [31];
- The low centrality values of Croatian ports instead reflect an even less dense situation. Croatia has coastal development and numerous smaller islands; there are several ports of global and local importance, but many of them are mainly linked to the service of the smaller islands;
- Finally, the importance of the port of Durres in the maritime connections between Italy and Albania is underlined. Although the port is relatively little central at a system level, it assumes considerable importance in the relations between the two countries indicated.

The services at the core and comprehensive network level in the Adriatic were studied. The focus was on the passenger and Ro-pax transport service, aimed at identifying the most central nodes and being able to define the weight characteristics of each node. The research has shown how in the Adriatic Sea, an open basin, different sub-systems interact between each other: in some of them, elements that refer to both transport on long routes and short trips are present at the same time. However, it was clear that the network is alive and vibrant and must be considered as a crucial element in a logic of decarbonization of transportation, supporting a modal shift towards the maritime in relations between the countries overlooking the Adriatic. Furthermore, it is intended to underline how the work carried out supports the logic of integration within the Corridors of the TEN-T network.

The research limited the analysis of services involving Core, Comprehensive or Extension ports, interested by passenger transportation services. This limit is linked to the desire to provide a preliminary analysis at basin level of the entire system; future developments may include a centrality analysis that also considers sub-systems, such as the Ionian islands and the smaller Croatian islands. Croatia has several archipelagos that form sub-systems whose centrality and connectivity certainly need to be investigated.

Another line of research concerns the possibility of quantitatively combining the results of port connectivity and centrality with those referring to other modes of transport.

As stated previously, the Adriatic coast is not connected by maritime services, but is equipped with a widespread HSR network; similarly, services seem to connect more with ports where there is no solid modal alternative, as in the case of Greek ports. This hypothesis should be tested by verifying whether port connectivity is complementary, or alternative, to rail connectivity.

Furthermore, the possibility of developing connectivity work for maritime services that considers the entire transport of goods on the same basin is highlighted; as mentioned in Sect. 2, the Balkan peninsula could become a reference point for the international transport of goods passing through the Suez Canal.

The research carried out is of interest to three categories of stakeholders: researchers, shipping companies and public administrators. The scientific interest of this work has been recalled in several passages; shipping companies can define, starting from the results, elements to improve investments in connections; finally, public administrators can start from the node centrality results to improve port-city interactions (such as improved transport infrastructure and services such as complementary services like demand responsive transport (DRT) or increased deployment of mobility as a service (MaaS) and relative digital platforms digital platforms)) and to push for sustainable solutions for both users and companies.

Acknowledgement. Activities supported by the MIUR (Ministry of Education, Universities and Research [Italy]) through a project entitled WEAKI TRANSIT: WEAK-demand areas Innovative TRANsport Shared services for Italian Towns (Project code: 20174ARRHT/CUP Code: J74I19000320008), financed with the PRIN 2017 (Research Projects of National Relevance) program. Activities also supported by the MUR (Italian Ministry of University and Research) through SMART3R-FLITS: SMART Transport for Travellers and Freight Logistics Integration Towards Sustainability (Project protocol: 2022J38SR9_03, CUP: J53D23009330008), financed by the PRIN 2022 (Research Projects of National Relevance) program. This manuscript reflects only the authors' views and opinions, neither the European Union nor the European Commission can be considered responsible for them.

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State of the Art of Factors Affecting Times of Ships in Container Ports: Characteristics Identification of Port Generations

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Abstract. Several classifications of ports were proposed in the literature, but there is no single established or accepted framework or taxonomy due to the complexity and diversity of the port entities. UNCTAD introduced a classification based on the definition of port-generation, according to which a prevalent port's characteristics could be associated to each port, the so-called generation. UNCTAD fully defined the characteristics of three generations of ports, while the fourth-generation of ports was less specified. Later, several researchers criticized the definition of port-generation and proposed new elements of classification, mainly of qualitative nature. Today five generations of ports may be identified. The paper proposes a set of characteristics to identify each port-generation. Several ports were object, in the time, of a process of hybridization. They were born with specific characteristics and, later, they evolved in acquiring new ones. The paper de-build the hybridization offering the possibility to identify the operative single generation. The paper introduces a set of material and immaterial characteristics to identify the port generation and then the correct tools to support planning and evaluation activities.

Keywords: commercial ports · port-generation approach · time of ships in port · port classification

1 Introduction

There have been different attempts to establish categorizations for ports in various scientific and technical works. The challenge in identifying universally accepted classifications arises from the complex and diverse nature of port systems. In 1994, UNCTAD [1] introduced the notion of "generation" and outlined the distinctive characteristics of three generations of ports. The characteristics of the three generations are summarized below; it should be noted that these have had, and have, a wide sharing in international literature.

First generation ports are those located just near cities and are an integral part of urban areas. These ports essentially give rise to cities, with urban centres evolving alongside port development [2–4]. Cities rely on their ports to receive supplies of goods consumed within them; the goods produced are transported to other cities via maritime

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O. Gervasi et al. (Eds.): ICCSA 2024 Workshops, LNCS 14823, pp. 283–295, 2024.
https://doi.org/10.1007/978-3-031-65329-2_19

routes. Initially, ships arriving in these ports handled both freight and passenger traffic indiscriminately. Today the two traffics are mainly segmented with ships specifically destined for each type of traffic.

Second generation ports developed in line with the significant industrial advances of the 20th century. Key industries of economic development, such as steel, petrochemicals and energy, have played a fundamental role in the creation of these ports. The physical and technological infrastructures differ significantly from those of first-generation ports. Second generation ports are characterized by large yards adjacent to the docks, or oil terminals, or more generally energy terminals, equipped with advanced security measures and directly integrated with oil pipelines and electricity networks [5–7]. In territorial development, priorities are reversed: industrial plants are built first, and then ports are built, to support large energy and metallurgical plants. The ships that call at these ports are always specialized, in particular oil and gas tankers.

Third generation ports emerged with the advent of containerized shipping during the second half of the 20th century. Since then, container shipping has increasingly become the most efficient way of transporting goods [8, 9], using a structure of service defined hub and spoke. The importance of the generic port as a hub of a system depends on its degree of centrality [2, 10–12]. These ports are equipped with well-defined technical and operational characteristics, including long quays, deep drafts, large container yards. Furthermore, these ports are equipped with a specific fleet of machines linked to their main functions: rail-mounted quay cranes over 50 m high; straddle carriers for distribution in yards; wheeled convoys serving the cranes; reach stackers for stacking empty containers. Unlike other, third generation ports not only serve as hubs for containerized transport, but they are often vital nodes within the global supply chain; that is, in these ports a significant added value is generated on freight in transit. The ability to generate added value distinguishes them from first- and second-generation ports, which functioned primarily as cost centers, even if costs are highly optimized. Third generation ports have required the development of significant research which has focused on two key territorial elements [12]: the areas internal to the port, which are important for the efficiency of handling, loading and unloading, and transportation [13, 14]; the port hinterland, where activities related to the handling of freight develop and where the increase in added value of the freight passing through is therefore obtained [15–17].

UNCTAD subsequently [18] introduced the concept of fourth generation ports [19, 20], further proposals have been made to define the characteristics of fifth generation ports [21–23], but the technical and scientific debate is still ongoing, on these last two generations [24, 25], and there is no single shared definition. The evolution of port-generation is depicted in Fig. 1, where it is possible to identify a historical period in which each generation of ports was born.

The paper presents a state of the art on the port-generation approach and proposes a set of characteristics to identify each port-generation. The work is part of an ongoing research project titled “National and local factors affecting times of ships in container ports” composed of different research lines. Among them, it is worth recalling the Automatic Identification System (AIS) data for maritime transport and ports applications [26] and for building a transport supply network [27].

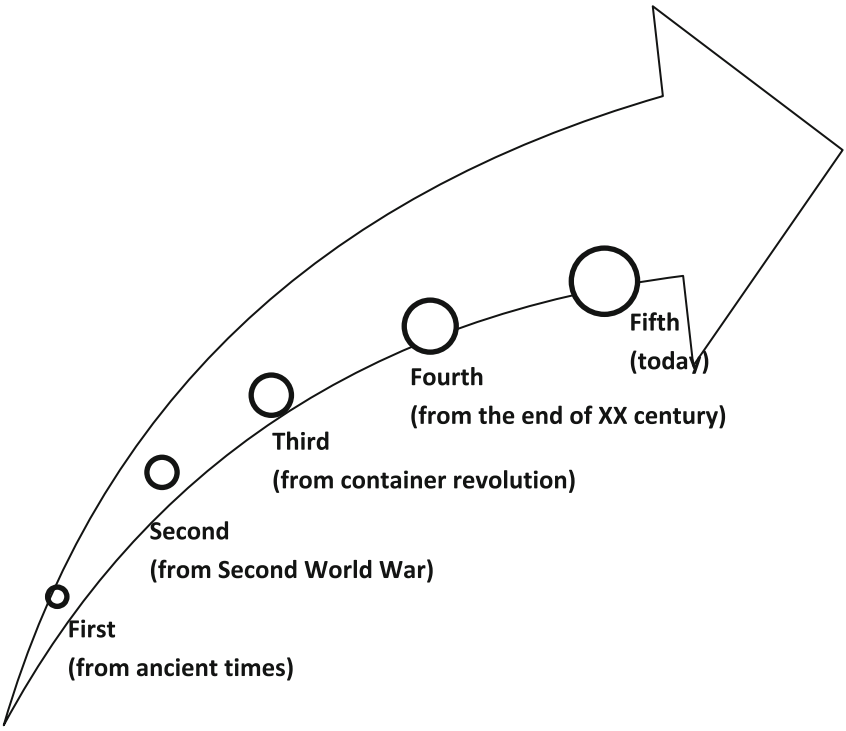

Fig. 1. Evolution of port generations

The paper consists of four sections. After the introduction, Sect. 2 examines the state of the art related to the classification of ports by generation, as initially proposed by UNCTAD and then developed in the international literature. In Sect. 3, a systematization of the different generations of ports is proposed, introducing the physical infrastructures, ships and equipment connected with each generation of ports. In the conclusion, the main results are summarized, outlining what are the guidelines for the development of ports that can now be evidenced from some paradigmatic elements.

The work is useful for both technicians and planners of the port authorities and relevant ministries. It is useful for researchers because it allows them to develop adequate forecasting models by clearly identifying the type of ports of reference.

2 Port-Generations: State of the Art

Although several classifications of ports have been proposed, there is no single established or accepted framework or taxonomy. The major obstacle against this is due to the complexity and diversity of the port entities. The study in [28] pointed out the main four differences among ports: organizational, issues of ownership (public versus private), institutional status (landlord/tool versus service), social arrangements (labour and manpower); operational, types of cargo handled, ships serviced, terminals operated; physical and spatial, location, access, connectivity, available capacity; legal and regulatory,

trade and transport policy, administrative procedures, safety and security regulations, environment.

In 1994 UNCTAD [1] introduced the definition of port generations and coined the term "third generation ports", as the product of the unitization of sea-trade and multimodal cargo packaging, mainly in the form of containers [29]. They led to the development of ports as logistics and intermodal centres offering value-added services, with technology and know-how being the major determining factors. In 1999, UNCTAD [18] suggested the arrival of the "fourth generation ports" as a result of vertical and horizontal integration strategies, and they are identified as being separated geographically but with common operators or administration.

The idea of a fourth generation port was introduced in an earlier work [30], which documented functions and roles of ports from the first to the fourth generation under the category of external environment, functional organization, spatial organization and port organization and strategy.

In the later years a number of papers have criticized the port generation approach defined by UNCTAD, and they have attempted to introduce further elements in order to capture the complexity and diversity of ports. The study presented in [31] argued that the idea of a third generation port could be sufficient if the world economic growth pattern could be forecasted with any certainty; but, this is not the case. The authors claimed that to cope with this uncertainty ports should adopt a new logistics approach based on agility and proposed a methodology for implementing the concept of agile ports. The work in [32] critically examined the UNCTAD generation ports classification and concluded that, rather than developing in discrete steps, ports evolve continuously, adapting to new technologies, evolving legislation, adapting working practices and other influences. They showed that several streams of evolution can be observed simultaneously; the speed of change within each stream can vary substantially. Ports often have several terminals, some operating along traditional lines while others may be leading edge in terms of technology, working practices or other aspects. According to the authors, the UNCTAD model, implying ports development in discrete steps, or generations, is shown to be fundamentally flawed. The study in [33] added on existing models on the spatial and functional evolution of ports and port systems, the paradigm of port regionalization. They showed that the regionalization phase, together with hinterland concepts, demands new approaches to port governance and a functional focus that goes beyond the traditional port perimeter. According to [28], the huge corpus of literature on ports' assets, functions and institutional organizations lie along an ideal line between two extremes. At the one extreme, ports have been defined through a macro-analytical approach as being geographical, physical and corporate assets. This approach is typically illustrated in the study of port aggregate impacts which has proven to be a controversial subject; but also with different methods of assessment and analysis (e.g. added-value, input-output analysis, statistical analysis). The other extreme is to look at ports from a micro-perspective approach in terms of sets of activities and operations shaping a ports' roles and functional dimensions, even this approach has specific methods. An intermediate approach between the two extremes tries to combine both the macro- and

micro-elements through providing a mixed definition of port roles and functions. One of these is the widely cited port generations of UNCTAD.

Port roles and functions, but also institutional structuring, operational and management practices vary significantly from generation to generation. According to [28], the flaws of the generation-type taxonomy outweigh its merits for some aspects. Firstly, it identifies port generations through sea/shore interface developments with little interest in port potential for shore/land-side expansion, as in the case of dry ports and distriparks. Secondly, it applies a rigid categorization far from reflecting the composite reality of ports. Many ports still perform first or second generation-type functions, and even within a single port, there may be a variety of operational and management systems intersecting across different generation categories. Thirdly, it hypothetically equates all cargo/ship type operations and functions under the same generation. In practice, many ports that declared to be fourth generation still carry out activities of first or second generation-types through, for instance, handling first generation-type cargo and ships. The study [34] highlighted the way in which ports and the services they provide develop in an evolutionary rather than a revolutionary way, as defined by the port generation approach by UNCTAD. The political dimension plays a lead role in ports' evolution, as ports are often seen both as a vital part of the supply chain and as a natural focus for regional development and employment. But, where they have been made more responsive is in tailoring services to individual customers' needs, thus becoming more agile.

Table 1 synthesizes the core elements of the main studies present in the literature concerning the port-generation approach, described in this section.

The authors examine the different forms and development process that ports have taken within the supply chain. In the last years some researchers attempted to overcome lacks of the 'fourth-generation ports' definition [35–37]. According to [35], the fourth-generation ports definition proposed in [18] focused on internal efficiency, but it was not sufficient to reflect the port functions required by community stakeholders' requirements and the needs of port users in the rapidly evolving globalised economic system.

They proposed the conceptual framework of the "fifth-generation ports", or Customer-Centric and Community (CCC) port. Key elements of the framework are networking and capacity management between: (1) "customer and port system: customer needs to enlisted as a partner to change certain behaviours in order to optimize work and capacity management"; (2) "commercial and production teams"; (3) "port and intermodal connections: reach a commercial, strategic positioning of the port and national economy, as well as offer an integrated solution".

The works presented in [36] and [37]) examined the competition of four major Asian ports (Shanghai, Singapore, Hong Kong and Busan) based on a revised version of the fifth generation ports framework, previously defined in [35]. They referred to the same factors of fourth generation ports and fifth generation ports, as defined by UNCTAD: service quality, information technology, community environmental impact, port cluster, maritime cluster, logistics hub, inland connection, and waterside connection. They did not explicitly consider in their analysis the vertical and horizontal integration process involving ports.

Recently, an operative basis for the quantitative specification of ports' characteristics according to the port-generation approach was defined [9]. The definition of a specific

Table 1. Main scientific publications about the port-generation approach

Author	*Main elements*
UNCTAD (1994; 1999) [1, 18]	• "port-generation" concept under the category of external environment, functional organization, spatial organization and port organization and strategy • "third-generation port "as the product of the unitization of cargo in the form of containers • "fourth generation port" as a result of vertical and horizontal integration strategies
Van Klink (1995) [30]	• Role of ports from first-generation to fourth-generation • Not all ports pass through all stages. Some remain at one stage, others skip one or more steps in their development
Paixao and Marlow (2003) [31]	• Third generation port not sufficient due to uncertainty of world economic growth pattern • New logistics approach based on agility • Methodology for implementing the concept of agile ports
Beresford et al. (2004) [32]	• Ports evolve continuously, rather than in discrete steps • Several streams of evolution can be observed simultaneously; the speed of change within each stream can vary substantially • Additional operational and development issues than UNCTAD
Bichou and Gray (2005) [28]	Limits of port-generation approach: • Focus on sea/shore interface developments with no interest on shore/land-side expansion (dry ports, distriparks); • rigid categorization not reflecting the composite reality of ports • all cargo/ship type operations and functions under the same generation
Notteboom and Rodrigue (2005) [33]	• Paradigm of port regionalization • New approaches to port governance and to functional concern beyond the traditional port perimeter
Flynn et al. (2011) [35]	• Fourth-generation ports focused on internal efficiency, not sufficient to reflect the port functions required by community stakeholders' requirements and the needs of port users • Conceptual framework of fifth generation ports with world-class Customer-Centric and Community (CCC) ports

(*continued*)

Table 1. (*continued*)

Author	*Main elements*
Lee and Lam (2015, 2016) [36, 37]	• Revised concept of fifth-generation port • Empirical comparison of four Asian ports: Shanghai, Singapore, Hong Kong and Busan • Qualitative analysis with sharper demarcation borders of factors
Russo and Musolino (2020) [9]	• Operative basis for quantitative specification of ports' characteristics according to the port-generation approach • Application to Italian ports
Russo and Musolino (2021) [20]	• Description of theoretical approaches to support the evaluation of fourth-generation ports • Case studies of cooperation among ports
Russo and Musolino (2021) [21]	• Benefits and challenges connected with the introduction of shared emerging ICT among stakeholders inside fifth-generation ports

generation for a port highlights its main characteristics, as several ports were object, in the time, of a process of hybridization. The paper proposed some indicators to identify each of the three generations defined by UNCTAD, which were calculated to a set of Italian ports. The paper [20] presents the main theoretical approaches to support the evaluation of fourth-generation ports, which could respond to the new requirements imposed by gigantism, carriers' alliances and land-sea integration. Furthermore, some representative case studies of cooperation among ports are reported and classified, in order to aggregate the observed processes in some macro-classes. The study in [21] presented a framework to evaluate the new benefits and challenges connected with the introduction of shared emerging ICT among decision-makers inside fifth-generation ports. The paper sketched and compared some scenarios with the presence of different level of emerging ICT inside a port (e.g. the presence of a Port Community System). The aim was to estimate the gain in port performance generated by the solution of shared port stakeholders' decisions by means of the emerging ICT.

In relation to the examined literature, it is possible to identify the main characteristic of each port generation. The result of this process is synthetized in Table 2, where a keyword and a main characteristic is reported. It is worth noting that the definition of a specific generation for a port is not an element of ranking; but, expresses its main role in the worldwide transport network. Several ports were object, in the time, of a process of hybridization. They were born with specific characteristics and, later, they evolved in acquiring new ones.

Table 2. Main characteristics port-generations (elaboration from [1, 4, 9].

Port-generation	*Keyword*	*Main characteristic*
First	City	High port-city interactions
Second	Industrial	Heavy industrial plants closer to the port
Third	Container	Container traffic
Fourth	Cooperative	Common public governance with other ports
Fifth	Digital	Emerging ICT (e.g. port community system) with horizontal integration

3 Port-Generations: Identifying Criteria

The section introduces a set of criteria for identifying each generation of port. The issue that arises is to be able to identify a set of characteristics that allows, in a homogeneous way, to identify the generation of a port.

It is necessary to first define two components that identify a port both among those involved in maritime trade, throughout the vertical chain, and among the technicians and researchers who work in this field.

Governance Component. Generally, the ports are managed by a port authority. This authority can have different economic, financial, legal and administrative nature: from completely or predominantly private entities, as in the USA to completely public entities, as in Spain. At the governance level there are therefore a multiplicity of governance structures.

Spatial Component. Inside a harbor space without solution of continuity can be present, more or less contiguous, deeply different commercial functions. From the analysis of the two above elements in the ports of international importance emerge different situations:

- governance and spatial component coincide, that is all the harbor space, continuous, is managed from a single port authority
- governance and spatial components do not coincide, in this case there are two possibilities, the governance entity is unique but the spaces are not continuous, or the space is unique but there are different governance entities.

A *port* could therefore be defined as the intersection of governance and spatial components, i.e. a continuous space managed by a single port authority. Even in the presence of this definition, it appears that the two components, spatial and governance, do not allow us to univocally identify the generation of the port, because over time, radically different port operations have been defined in the same space. The diversity of port operations has led to the hybridizations mentioned above.

The different port operations can be aggregated in relation to the characteristics of:

- *static physical infrastructures* necessary for carrying out port operations;
- *dynamic mechanical infrastructures* that allow the movement of goods;
- *type of ship* that requires the port operations.

In general, a defined combination of these characteristics makes it possible to unequivocally identify the membership to one of the first three generations. Considering that the ships/infrastructures/equipments are internally integrated and therefore fixed, it may be sufficient to know only one of the three characteristics to identify the generation of a port.

Given the components and characteristics, a port is defined as: *the intersection of governance and spatial components in which port operations are carried out with a homogeneous trio of characteristics*, i.e. a continuous space managed by a single port authority in which port operations are carried out with a single homogeneous trio of ships/infrastructures/equipments characteristics.

A highly homogeneous trio, and therefore a strong specialization of the port, implies the handling of very specific loading units.

If this position is necessary, it is also sufficient, i.e. given a type of unitization of the goods, it is possible to know the trio of characteristics necessary for its handling in a port.

A further defining feature of the port is the *territorial scale* at which the goods handled in the ports are distributed. The scale to be considered may be different by considering incoming and/or outgoing goods. In this note, we consider ports that have an intercontinental scale in one or both of the two in/out directions.

Other types of ports, i.e. with in/out directions on a local scale, can have a considerable promiscuity in the use of equipment and therefore the same infrastructures can be destined to significantly different port operations. Obviously, promiscuity does not allow a full identification of generation, which is not necessary because these ports operate on the margins, if not outside, of the global market.

While the first three generations, as mentioned in the introduction, are defined in their components, the fourth and fifth generations are less defined. The fourth generation ports were born because of the significant increase of international trade, that imposed to ports to move from competitive attitudes towards a cooperative one. Fourth-generation ports allow the reduction of the time of ships in transit because they offer greater capacity of both infrastructure and equipment. The fifth generation ports were born with the massive introduction of Information and Communication Technologies (ICT) in port operations. The main characteristics concerns the sharing of ICT among all port operators (i.e. horizontal integration). The systems developed are called Port Community Systems (PCS), which makes it possible to reduce port operations times with a decisive intervention on the information flows connected to the freight handling.

4 Conclusions

The paper reports a state of the art concerning the scientific literature about the port-generation approach and proposes a set of characteristics to identify each port-generation. The different generations are identified and characterized by introducing the physical infrastructures, the ships and the equipment connected with each generation of ports, considered as structural factors of the internal production process of the "port fabric".

From what have been proposed, a first important result emerges: the transition from the first generation to the subsequent, second and third, reduces the time in port for specialized ships, mainly oil tankers and container ships, but requires longer time journeys for the ships compared to first generation ports, because the first generation ports are more present in the regional areas, and are the final destination in the hub and spoke system.

Considering each generation, the relevance of the factors presented in the paper will be validated in the next step of the research by putting them in correlation with the ship times in the ports. With the increase in the size of ships, each hour of stop has a considerable cost, of different types: ship costs due to crews and depreciation of the ship; costs for goods to be loaded/unloaded and for those that remain on board waiting for the next ports. This significant amount of costs can be reduced by optimizing the process of port operations. The type of optimization that can be pursued, depends on the generation of the port in question and therefore with a range of actions ranging from increasing infrastructure capacity to speeding up information flows.

The prospects for sustainable development of ports consider different directions that can contribute to improving the times. These include: lean development, i.e. the elimination of parts of tangible or intangible procedures that weigh down port operations; agile development, i.e. capable of adapting to demand dynamics, both predictable due to seasonal fluctuations, trend fluctuations, and those due to unpredictable random events; resilient development, i.e. the ability to recover after serious unforeseeable events; green development, which is identified as one of the most important frontiers for the development of ports.

The scope defined in this note makes it possible to identify the key factors for the reduction of ship times in port, in relation to the generation of belonging to the port itself. The work can be useful to the technicians and planners of the port authorities and state structures responsible for the financing of ports because it allows them to identify for each port the most important factors on which to act by financing appropriate interventions. The work can be useful to researchers and analysts because it allows to organize statistical-descriptive models that allow to identify in a disaggregated way the major deficiencies of the single port and in aggregate the deficiencies of the set of ports of a country.

Acknowledgments. This study is carried out within the research project "National and local factors affecting times of ships in container ports", Piano Nazionale di Ripresa e Resilienza (PNRR), Next Generation EU. Progetti di Rilevante Interesse Nazionale PRIN_2022_PNRR_P202292YFW. CUP: C53D2300878001. This piece of work reflects only the authors' views and opinions, neither the European Union nor the European Commission can be considered responsible for them.

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Smart Transport and Logistics - Smart Supply Chains (SmarTransLog 2024)

Cold Ironing: An Analysis of Policies and Its Implementation in Europe with a Focus on the Italian Context and the Future Prospects in Sardinia

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Abstract. This article studies the policies and current state of Cold Ironing. The research reveals that on the one hand this policy was successfully implemented in Alaska twenty years ago, while its development in Europe is recent and not widespread. The Port of Gothenburg is one of the leading ports in Europe, which has developed several sustainable maritime policies such as shore power and methanol propulsion. In Italy, several challenges, such as different electricity supply requirements and high electricity supply costs, hinder the implementation of Cold Ironing. However, the proximity of Italian ports to urban centers offers opportunities to promote cold ironing technology and mitigate port emissions. The implementation of cold ironing in Europe, Italy and particularly Sardinia, offers significant potential to reduce greenhouse gas emissions and promote further sustainable maritime practices.

Keywords: Cold Ironing · Sustainable Maritime Policies · Port of Gothenburg · Italian Ports · Sardinia's Ports

1 Key Environmental Policies for Ports

The European Union's "Strategy for Sustainable and Intelligent Mobility: Putting European Transport on the Right Path for the Future" [1] attributes 5% of EU GDP to the transport sector, employing 10 million people. The importance represented by the growth and structuring of mobility over time is, however, increasingly burdened by the costs arising from it, social, environmental and therefore also economic, which contribute to the expression of increasingly stringent policies in favor of sustainability, circularity and environmental protection. The strategy is a useful tool in pursuing the goals of the European Green Deal (11.12.2019), which aims "…to transform the EU into a just and prosperous society with a modern, resource-efficient and competitive economy that generates no net greenhouse gas emissions in 2050 and in which economic growth is decoupled from resource use" [2]. The pollution factor caused by emissions from various human activities, the weight of which in the EU accounts for 75%, inevitably leads to the decarbonization of the energy sector, which is essential to face climate change and global warming that the Paris Agreement (2015) set at 1.50.

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O. Gervasi et al. (Eds.): ICCSA 2024 Workshops, LNCS 14823, pp. 299–310, 2024.
https://doi.org/10.1007/978-3-031-65329-2_20

The intent of the agreement was to reduce CO2 emissions by 40% by 2030, compared to 1990 levels, while it is in 2021 that the EU climate law passed by the Parliament sets climate neutrality by 2050 as legally binding in the Green Deal program [3]. The dynamism of policies related to these issues is also evident in this law, which proposes a new threshold, the reduction of emissions by at least 55% below 1990 levels by 2030, and formulates a regulatory package called "Fit for 55," a set of proposals to revise and update EU regulations, which aims to make Europe a zero-emissions continent by 2050 [4].

It is in this context that the mobility strategy with its 10 flagship initiatives, the second of which, creating zero-emission airports and ports, directs these facilities toward multimodality and the transformation of mobility into more sustainable forms of connectivity. Ports can play the role of new hubs in which alternative and low-carbon energies and techniques related to the circular economy serve as inputs for the improvement of entire areas. Globally, major ports of call are investing in sustainability through the energy transition, setting themselves up as a complex system of systems where multiple independent systems interact creating a network [5]. An example of this is the bunkering of new propellants such as LNG that finds space in as many as 178 ports, usable by ships for connections to the shore power grid, cold ironing. Ports with multiple prerogatives and services that are considered instruments of geopolitical influence as they connect and create synergies with those countries considered strategic [6]. Growing global awareness of the dictates of environmental sustainability has changed many of the rules of behavior of society as a whole, and according to the transposition of the policies that each country has adopted, the practices chosen in the various sectors of the economy have evolved in order to abate the sources of pollutants derived from it. The efficiency provided by new technologies, however, still fails to abate greenhouse gas emissions from transport, the European Environment Agency in fact states that these emissions have been increasing over the past 30 years, contrary to the European Union's goal of reducing emissions from transport by 90% by 2050, compared to 1990 levels. While, therefore, transportation has undoubtedly become more efficient, this progress still fails to balance its growing volume [7].

The Report on the Environmental Impact of European Maritime Transport (2021), prepared by the European Environment Agency reports that 77% of European foreign trade and 35% of trade between EU member states is by sea, representing the main international supply chain. Among the various types of transport, at the level of greenhouse gas emissions, maritime transport ranks third (13.5), after road transport (71%), the most polluting by far, and air transport (14.4). The introduction of increasingly stringent measures at European ports in the coming years should further cut emissions. Future challenges envisioned by the report include sea rise in ports, further reduction of emissions that can be abated by reducing the speed of vessels docking, use of nontraditional energy sources and fuels, and shore power supply (which involves turning off engines when ships are docked in port).

The aforementioned "Fit for 55" package calls for an 80% reduction in emissions from ships by 2050 compared to 2020, and mandatory, by 2030, for container ships and passenger vessels to be connected to the power supply of the docks in the port where they will stall.

The current geopolitical moment may have important repercussions on the Mediterranean and Italian logistics and port system, and long-range international trade will be relevant as well as necessary to connect distant and internationalization-oriented production systems translating into increased demand for port services and onshore cargo traffic.

The Ministry of Sustainable Infrastructure and Mobility's (MIMS) "Climate Change, Infrastructure and Mobility" [7], highlights that the Mediterranean Sea is still an important route in terms of container traffic but highlights a concern about the impacts of climate change that in ports translates into planning more resilient infrastructure in terms of both greenfield and brownfield investments.

Italy's port logistics network has 58 ports and 24 interports, and the country is the second largest in Europe (second only to the Netherlands) for the movement of goods by sea, thus the importance that has been given to the sector by the National Plan for Recovery and Resilience (PNRR) is clear. The NRP has dedicated as much as 750 billion euros to the Next Generation EU (NGEU) program to combat the crisis which raised by the Pandemic from Covid 19. The program, which supports various activities, is divided into strategic axes and missions and devotes specific objectives to mobility and ports whose sustainability, intermodality, climate change resilience and energy efficiency it is concerned with. At its core, the Green Ports project "aims to make port activities sustainable and compatible with urban port contexts through the financing of interventions aimed at the efficiency and reduction of energy consumption of port facilities and activities" [9]. Additional goals are the preservation of natural heritage and biodiversity, all through interventions such as:

- energy production from renewable sources;
- energy efficiency of port buildings;
- energy efficiency of lighting systems;
- use of electric means of transportation;
- interventions on inefficient port energy infrastructure;
- construction of infrastructure for the use of electricity;
- reduction of pollutant emissions from ships at the docks.

The map in Fig. 1 shows the 47 Italian ports dedicated to electrification.

Given the complexity of the cold ironing infrastructure, a strategy has been defined that is based on six pillars, factors, and objectives, the details of which are provided in the PNRR, and only the six pillars are named here, which are subject to further declination: port identification, availability of electric power capacity, reform of the authorization process, electric tariff, type of ships, and supply chain management [9].

Among the Urgent Measures for the Implementation of the National Recovery and Resilience Plan (NRP) D.L.36/2022, Article 33, "in implementation of a reform envisaged by the NRP for the simplification of authorization procedures for cold ironing facilities, considers projects intended for the construction of works and facilities for the electrification of ports to be of public utility and characterized by indifference and urgency…" [10].

Fig. 1. Italian ports dedicated to electrification. Source: own processing with ESRI and MIMS data.

2 Methodology

In this article has been carried out a review of the academic literature, an analysis of the legislation and a survey of local newspapers. The literature review was conducted in order to gain a theoretical understanding of the policy of Cold Ironing and its implications. This involved studying scientific articles relating to the environmental impact of Cold Ironing and its implementation in Europe and Italy. The literature review helped to understand the historical context, current status and future prospects of this policy.

A review of the rules and regulations of this policy was carried out which covered national and international regulations on Cold Ironing, environmental standards and maritime laws. The regulatory analysis provided insights into the legal and regulatory framework relating to Cold Ironing, its implementation and the funding provided for this policy.

Local newspapers were examined to understand the practical aspects of cold ironing implementation, in particular for the analysis relating to the Sardinia region. Local newspapers provided information on ongoing projects and progress made in implementing Cold Ironing.

3 Cold Ironing in Europe

The first successful implementations of cold ironing can be traced back to about twenty years ago in Alaska, where energy costs were lower than in Europe, a continent where the development of cold ironing occurred only in recent years and only in some ports [11].

The application of Cold Ironing policies in Europe is mainly observed in the port of Gothenburg. Other policies have also been combined which have made it possible to further mitigate port emissions. Port Collaborative Decision Making (PortCDM) was implemented, a practice that powers docked ships, which allows for the reduction of greenhouse gas emissions [12].

The map in Fig. 2 shows the five ports, with red icons, along the city of Gothenburg, which have adopted cold ironing policies.

In the process of electrification of the docks where tankers moor in Energihamnen, Göteborgs Hamn AB has initiated a project called "Green Cable" which, in collaboration with different stakeholders, including shipping companies in Donsö, national ports and European ports, companies Port Oil and the Swedish Transport Agency, aims to establish a new global standard for shore power for tankers berthed in national ports [13]. The environmental benefit following the electrification of the Energihamnen docks can be quantified as a reduction of 1,800 tons of carbon dioxide per year, compared to when tankers use their diesel-powered engines while at berth [13].

The Port of Gothenburg, a pioneer in offering coastal energy in Europe [14], is also involving shipping companies such as Furutank, Donsötank, Tärtank, Ektank, Veritas Tanker based in Donsö and Tarbit Tanker on the island of Tjörn and aims to create a new structure at the Energy Terminal, aimed at ensuring safety in the spaces that house the electrical equipment [13]. These are plants that guarantee a reduction of 1,800 tonnes of CO2 every year thanks to the use of green energy and as announced by the port of Gothenburg, the first tanker will be connected to this network in the first quarter of 2024 [14]. This project was partially financed by the Swedish government through the Climate Investment Support Program with approximately 1 million euros. It is also part of the Gothenburg Port Authority projects in which approximately 60 million euros were financed by Sweden to be able to implement emissions mitigation measures by 2030 [13, 15].

The Gothenburg Port Authority can be seen as a driving force for the sustainability of the city's port. It plays an important role in achieving the global sustainable development

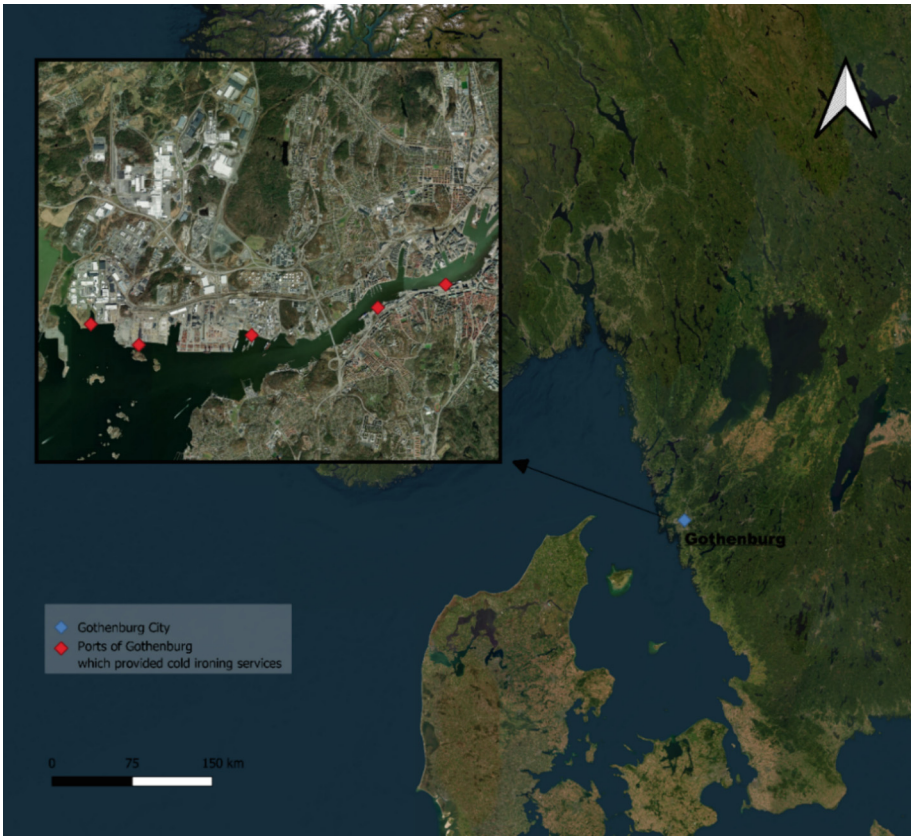

Fig. 2. Cold Ironing in Gothenburg. Source: own processing with ESRI data.

goals dictated by the European Union. Furthermore, its commitment extends to 15 of the 17 objectives of the 2030 Agenda in its industrial plan [13].

The port of Gothenburg thus paves the way for the environmental sustainability of ports through innovative solutions, reported in this paper, which should lead to substantial CO2 reductions in the port area.

4 Cold Ironing in Italy

The implementation of cold ironing has been developed in the main Italian ports and in this context it is possible to mention the port of Ancona and the port of Venice [16; 17].

4.1 Venice

The Venice cruise terminal is one of the main ports in the Mediterranean [18] and welcomes a large part of the national maritime traffic and is mainly made up of cruise ships [17].

Fig. 3. Cruise terminal of Venice, Italy. Source: own processing with Google Satellite data.

The map in Fig. 3 shows the Cruise terminal of Venice dedicated to electrification.

In recent case study [19] the analysis focuses on the technical and economic aspects of the port of Venice, pays particular attention to the reduction of emissions and attributes the high energy consumption of cruise ships to on-board equipment. This research proposes different scenarios to deal with this type of emissions, one of which requires the reassignment of ships to the docks, moving the mooring of the most polluting ships in the Isonzo and Tagliamento basins, a condition that requires an overall reconfiguration of ship mooring.

In the case study of the port of Venice by Pasetto and Giacomello [20], was performed a multi-criteria analysis (MCA) using the Analytic Hierarchy Process (AHP). The results suggest that the optimal solution, in order to reduce the maritime pollution in Venice, would be to connected the Port of Venice to both the Montesyndial terminal and the port of Padua via a rail shut-tle train service.

Furthermore, their study shows that the implementation of cold ironing in the port of Venice also requires constant review by port authorities and could improve maritime trade for both the city of Venice and nearby cities, particularly Padua, Treviso and Rovigo and this is in line with the improvement and development of the ports outlined by the PNRR, which also provides funding for the construction of new maritime infrastructures [20].

Regarding the concrete implementation of cold ironing policies, the Northern Adriatic Sea Port System Authority (AdSPMAS), responsible for promoting sustainable investment programs, has submitted a request for an agreement with SOGESID S.p.A. of the Ministry of Infrastructure and Sustainable Mobility, which is granted on 21 February 2022. Consequently, on 3 March 2022 an agreement was signed between AdSPMAS and SOGESID S.p.A., to regulate the provision of services aimed at implementing the interventions by AdSPMAS. Based on the agreement obtained, SOGESID S.p.A. will be provide technical support for the Cold Ironing project of the port areas of Marghera and Venice whose total amount is 1,181,429.11 euros [21].

4.2 Ancona

The port of Ancona, shown in Fig. 4, is located along the Italian Adriatic coast and serves as the main logistics hub of the central Adriatic region [22, 23].

In the study by Esposito et al. [16] three different Cold Ironing application scenarios were tested within the port of Ancona. Through an environmental analysis, emissions within the port were then analyzed and compared. The results of this study show a reduction in emissions in all three scenarios. The first one involves the implementation of a cogeneration plant which will start the electrification of the docks serving mooring in this port.

In such manner, a more significant reduction in emissions was achieved compared to the other two scenarios. The reduction counted is in fact equal to 98.58% for nitrogen oxides, 79.06% for PM10 and 100% for sulfur oxides.

Therefore, the implementation of a cogeneration plant in this port, as demonstrated in the research by Esposito et al. [20] mitigates the environmental impact and reduces emissions in the port area of Ancona.

5 Current State of Cold Ironing in Sardinia

The ports of Sardinia have recently enrolled a process of sustainable conversion of port systems, through the publication of the “technical-economic feasibility design for the construction and commissioning of a shore power system for the electrical supply of ships moored in the ports of Cagliari (Porto Storico and Porto Canale), Olbia – Isola Bianca, Golfo Aranci, Santa Teresa Gallura, Porto Torres and Portovesme” [24].

The importance of cold ironing in Sardinia is also underlined by the PNRR 2022 report, “Investments and reforms for the port”, which aims to improve port energy supply at a national level [8].

Fig. 4. Port of Ancona, Italy. Source: own processing with ESRI data.

5.1 Policies and Funding for Cold Ironing in Sardinia

The six ports of Sardinia, as reported in this paper, join the development of sustainable port systems in response to the examples of the Cold Ironing policies implemented in the various ports of the European Union [24, 25].

The main objective of the onshore energy project in Sardinia is to supply energy to moored ships through installations of shore-based electrical power systems which allow the ships' engines to be turned off, with a consequent reduction in emissions [26–28].

Figure 5 shows a cartographic representation of the main ports in Sardinia that are actively implementing cold ironing policies.

The following ports are maked in blue on the map: Cagliari (Porto Storico and Porto Canale), Olbia (Isola Bianca), Golfo Aranci, Santa Teresa di Gallura, Porto Torres and Portovesme, previously mentioned.

The technical-economic feasibility planning for the implementation of Cold-Ironing thus gave rise to Sardinia's Green Revolution, as defined by the Sardinia Port System

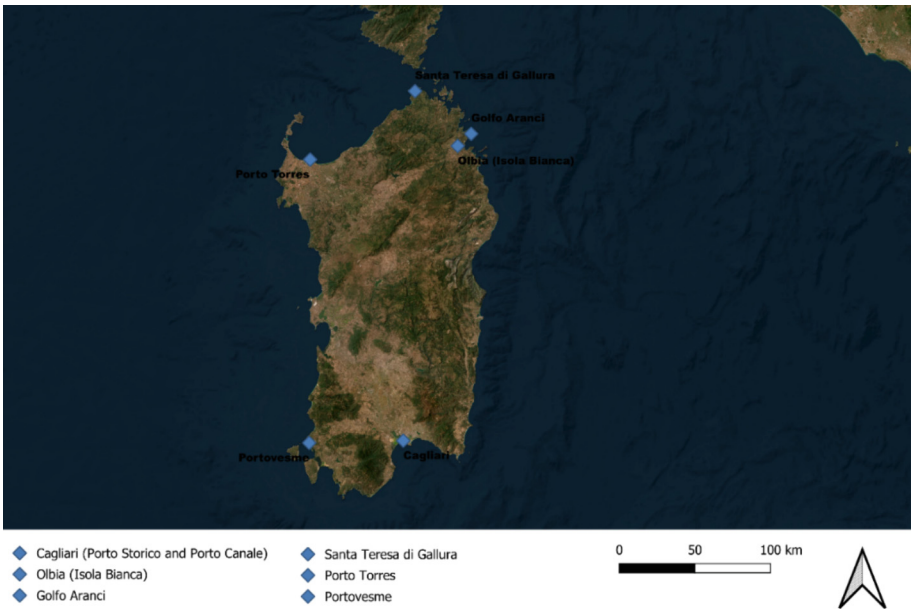

Fig. 5. Ports of Sardinia active in Cold Ironing policies. Source: Own processing, with ESRI data.

Authority [24]. This study verifies the electrification process of the docks at the commercial ports of Sardinia, for which the PNRR has allocated a total of 70,830,000 euros [26]. The objective of the feasibility program is to analyze the opportunities and possible critical issues of the implementation and adoption of cold ironing systems on the island [24]. Specialist technical reports, archaeological checks, sustainability checks and also environmental impact studies are part of this process [26].

The facilities envisaged by the project provide total financing of 21,560,000 euros for the port of Olbia, 2,400,000 euros for Golfo Aranci, 500,000 euros for Santa Teresa and Portovesme, 12,750,000 for Porto Torres, and as regards Cagliari, 20,900,000 for Cagliari Porto Storico and "ro-ro terminal" and 12,200,000 for Porto Canale [26]. Furthermore, in terms of electrical energy power, the plants envisaged by the project provide 22 megawatts of power for Olbia, 3 megawatts for Golfo Aranci, 0.6 MW for Santa Teresa and Portovesme, 15 MW for Porto Torres, 22 MW for the port of Cagliari (Porto Storico and ro-ro terminal) and 13 megawatts for Porto Canale [27].

6 Conclusions

Cold ironing is a practice that powers docked ships via land-based electricity. It has emerged as a promising solution to reduce greenhouse gas emissions in the maritime sector and its first implementations can be traced back to twenty years ago in Alaska.

However, Cold Ironing in Europe has only been promoted in recent years. The port of Gothenburg represents one of the main European ports to have embraced this sustainable policy. The commitment in the Italian context has been observed in the ports of Venice and

Ancona and is also starting to develop in other regions. Sardinia has recently started the assignment of the technical-economic feasibility design for the creation of a cold ironing system for the electrical supply of ships moored in six of its ports. The implementation of cold ironing on the Island thus represents an opportunity to contribute to the global effort in reducing greenhouse gas emissions and promoting sustainable port systems.

Acknowledgement. This research is part of the project "Regional observations and analyses of yachting and tourist ports in Sardinia" funded by the Autonomous Region of Sardinia (R.A.S.), Department of Tourism. Scientific Director Professor B. Brundu.

Author Contributions. This article is the result of the joint work of both authors. In particular: paragraphs 1, 2 and 3 were written by Brunella Brundu and paragraphs 4, 5 and 6 by Stefano Carboni

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Ports of the Future - Smartness and Sustainability (SmartPorts 2024)

Bibliometric Analysis and Knowledge Mapping of Greenhouse Gas Emissions in Ports: A Review

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Abstract. Globally, the freight transport sector is a significant contributor to greenhouse gas emissions. Within international supply chains, seaports play a crucial role. The aim of this research is to analyse how the scientific literature addresses the issue of greenhouse gas emissions in ports. With the application of the software VOSviewer, bibliometric analysis and knowledge mapping will be used to investigate the research sectors studying polluting emissions in ports. The aim is to identify and define clusters associated with the most frequently used keywords. Literature reviews typically begin with a limited set of keywords, which can constrain the scope and allow for personal bias. Several researchers have conducted literature reviews, but they have typically focused on only one specific aspect.

Data was collected from the Scopus database, focusing on English language publications that addressed the following topic: greenhouse gas emissions at seaports. Two categories of terms were selected. The first category was related to greenhouse gas emissions. It included terms such as "emission(s)", "GHG" and "greenhouse gas". The second category was referred to the localization area, i.e. seaports, and included terms such as "port(s)" and "seaport(s)". The search was conducted for the terms in the title, abstract, and keywords, restricted to only articles published in journals, resulting in 1,556 documents, between 2009 and March 2024. The documents were subjected to a preliminary evaluation by reading the title and the abstract and based on the co-occurrence of the most frequently used keywords, five clusters were identified using the VOSviewer software.

The work will be presented as follows. Section 2 will be dedicated to the literature review, which will address the literature on port emissions. Section 3 will provide information about the data collection. The Sect. 4 will focus on the methodology used, while Sect. 5 will illustrate the main results. Finally, the last chapter will summarise the work and present some proposals for further research.

Keywords: ghg emissions · bibliometric analysis and knowledge mapping · port

1 Introduction

Globally, the freight transport sector is a significant contributor to greenhouse gas emissions [1]. Within the international maritime transport sector, seaports play a crucial role and are significant contributors to pollutant emissions [2].

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O. Gervasi et al. (Eds.): ICCSA 2024 Workshops, LNCS 14823, pp. 313–325, 2024.
https://doi.org/10.1007/978-3-031-65329-2_21

Ports are under increasing pressure to reduce their negative impact on the climate and environment [3]. Their roles and functions in transport systems and the economy make them a key factor in promoting sustainability [4].

This study examines how the scientific literature addresses the issue of port greenhouse gas emissions. With the application of the software VOSviewer, bibliometric analysis and knowledge mapping will be used to investigate the research sectors studying polluting emissions in ports. The objective is to identify and define clusters associated with the most frequently used keywords. For instance, Guo et al. [5] used bibliometric analysis to review the progress of smart city research.

Literature reviews typically begin with a limited set of keywords, which can constrain the scope and allow for personal bias. To address this issue, for example, Guo et al. [5] reviewed the progress of smart city research using a bibliometric analysis. Nevertheless, most researchers conduct literature reviews typically focused on only one specific aspect.

In the following sections, the study will be described in more detail. Section 2 will be dedicated to the literature review, which will address the literature on port emissions. Section 3 will provide information about the data collection. The Sect. 4 will focus on the methodology used, while Sect. 5 will illustrate the main results. Finally, the last chapter will summarise the work and suggest some potential avenues for future research on the topic of pollutant emissions in ports.

2 Literature Review

Through a systematic review, Alamoush et al. [6] review and categorise ports' technical and operational measures to reduce greenhouse gas emission and improve energy efficiency. The authors have proposed dividing the measures into two groups: portside and ship-port interface. Within these groups, seven categories have been defined: information, equipment, energy, energy efficiency, operation, land transport, and ship-port interface measure. Alamoush et al. [7] investigate the role of ports in decarbonizing shipping, beginning with a bibliographic search. The main findings suggest that only a small number of incentive schemes are implemented by ports due to their burdensome nature. Azarkamand et al. [8] carry out a literature review based on initiatives and methodologies to reduce carbon emissions and climate change effects in ports. The results of their work indicate that although many ports have begun calculating and reporting their carbon footprint, this still varies between authorities and operators, making it challenging to compare results. Additionally, not all sources of GHG emissions occurring within ports are considered in some cases. Therefore, the authors suggest the development of a standardised tool for calculating carbon footprints in ports. In their opinion, this could enable the establishment of benchmarks and facilitate comparisons of results between ports. Bojić et al. [9] suggest that the development of a standardised system for quantifying shipping emissions would aid in predicting and mitigating ship-sourced emissions in the future. The study also proposes a method generated through a multi-layered analysis approach.

A comprehensive review of pollutant emissions in ports was conducted by Barberi et al. [2]. The authors demonstrate a correlation between emissions and port infrastructures. They also show that proper interventions can help reduce both pollutant emissions

and financial costs. Bjerkan and Seter [4] reviewed 70 scientific articles on tools and technologies for sustainable ports. They categorized them into four main groups: port management and policies, power and fuels, sea activities, and land activities.

Ports are struggling to reduce their energy consumption and, consequently, their pollutant and greenhouse gas emissions. In this regard, Iris and Lam [10] present a literature review on operational strategies, technologies, and energy management systems for achieving energy efficiency in green ports. The authors suggest that ports should start implementing several methods, technologies and management systems only after having carried out a careful economic, technical and environmental analysis. Serra et al. [11] carried out a survey based on a literature review of port key performance indexes (KPIs) considering the environment dimension of port sustainability.

Existing measures to reduce carbon emissions often focus on the control and management of fossil fuels. Vessel optimization and port operations are currently top priorities. Such measures have limited potential to optimise emissions reductions in ports in the future. Operational measures could reduce emissions by 20% to 55%, while energy-related measures have the potential to reduce emissions by more than 80%, excluding nuclear energy [12]. Therefore, the authors conclude that energy-related measures could be the answer for future decarbonisation of ports.

Issa Zadeh et al. [13], Serra and Fancello [14], and Song [15] conduct a literature review focused on seaport decarbonization, based on the options and the efforts that could be taken in order to meet net zero emissions. Wang and Li [16] attempted to find reduction strategies of port carbon emissions in literature.

3 Data Collection

Data was collected on April 10, 2024, from the Scopus database. Scopus database contains over 70 million bibliographic citations, abstracts, and bibliometric data for peer-reviewed scientific publications. It covers various subject areas, including social sciences and humanities, physical sciences, health sciences, and life sciences.

The collection focused on English language publications that addressed the following topic: greenhouse gas emissions at (sea)ports. Two categories of terms were selected. The first category was related to greenhouse gas emissions. It included terms such as, “emission(s)”, “GHG” and “greenhouse gas(es)”. The second category was referred to the localization area, i.e. seaports, and included terms such as “port(s)”, “seaport(s)”.

A search was conducted for the terms in the title, abstract, and keywords. Only studies meeting both categories were selected, resulting in a total of 17,059 documents. Then, the document type was restricted to “Article” while the source type was limited to “Journal”, resulting now in 11,203 articles. At this stage, a further restriction was added to refine the sample. Unrelated subjects, such as medicine, biochemistry, physics, planetary science, and others, have been excluded. At this point, 3,289 documents between 1964 and 2024 were obtained.

Finally, after a first manual screening to exclude papers that focused on irrelevant topics, a dataset of 1,556 articles was obtained. Only the articles published between 2009 and March 2024 will be considered. All documents were exported in ‘full record and reference’ text file format. Figure 1 shows the change in the number of publications from 2009 to March 2024, with a significant increase observed from 2017.

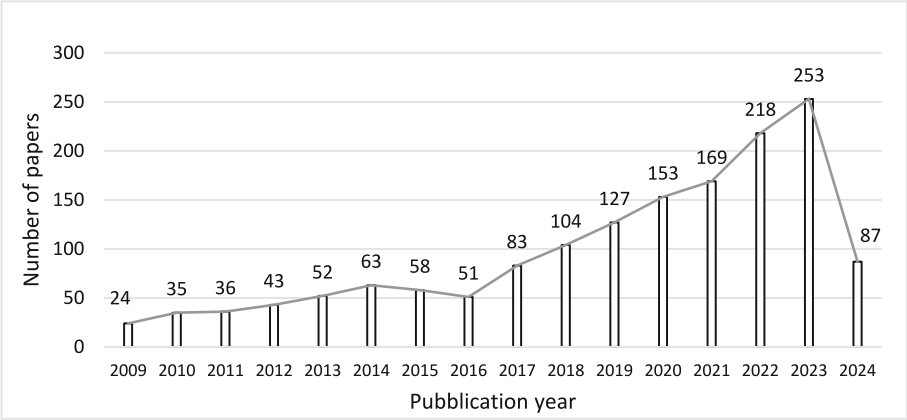

Fig. 1. Distribution of the number of published papers from 2009 to March 2024.

4 Methodology

This paper presents a detailed bibliometric analysis based on knowledge mapping. The combination of these two methods is increasingly recognized by researchers as a valid approach [17].

4.1 Bibliometric Analysis

Bibliometric analysis is a quantitative and objective method used to identify the state of the art of a research field and predict future development trends [18]. It analyses bibliographic information in academic literature, such as article titles, author names, and publication dates [19]. Bibliometric analysis visualises the distribution and relationships of literature attributes using statistical and mathematical theories [20].

For this purpose, the VOSviewer software, a computer program designed for viewing bibliometric maps, will be used. VOSviewer constructs maps using the VOS (visualization of similarities) mapping technique [20]. Maps can be created based on co-citation data for authors or journals or based on co-occurrence data for keywords. For example, Fan et al. [21] conducted a bibliometric analysis to review carbon emissions in transportation using CiteSpace and VOSviewer. A bibliometric knowledge mapping approach was also used by Moshiul et al. [22]. The authors reviewed the research progress and future trends in the use of alternative marine fuels to break down port emissions.

4.2 Knowledge Mapping

Knowledge maps are diagrams that represent ideas as node-link assemblies [23]. According to Balaid et al. [24], research on knowledge maps is still in its early stages, but progress is being made in areas such as network analysis, information visualization, and text mining. Few researchers highlight its importance for researchers to identify topics for conducting systematic reviews [17, 18, 25, 26].

Scientific literature is often analysed with two network-based methods: co-citation and keyword co-occurrence networks [27, 28]. Co-citation network analyses links between citations in the literature, while the co-occurrence network focuses on examining the links between keywords.

4.3 Co-occurrence Networks

In this study, the co-occurrence network method will be applied. Co-occurring keywords are identified to determine the most frequently appearing keywords in publications [22]. Keywords provide a brief summary of the significant content and essential points of a body of articles [29]. A weighted network is created by treating each keyword as a node and each co-occurrence of a pair of words as a link between those two words. The weight of the link connecting two keywords is determined by the number of times they co-occur [30].

5 Results

This study utilized VOSviewer software to analyse and generate a co-occurrence map of the most frequently used keywords. A fractional counting co-occurrence method was used. All keywords with a minimum of 10 occurrences were included in the analysis. The final total number of keywords was 468.

Figure 2 displays the mapped distribution of keywords, providing information on the hotspots of the topic under examination. The network comprises nodes and edges, with each node representing a keyword and its diameter being proportional to its frequency of occurrence.

Keywords within the same cluster share a high degree of similarity with the research themes and form subsets. Each cluster is assigned a tag based on its constituent keywords. Under each cluster, a table presents the top 25 keywords for each cluster, along with the number of occurrences, links, and total link weight for each keyword. Displaying co-occurrence clusters in a scientific knowledge map enables the analysis of the structure, rules, and distribution [31].

5.1 Cluster 1 (Red): Pollution

The largest cluster, colored in red, is characterised by the keywords “atmospheric pollution”, which appears 185 times, followed by “air pollution” (173) and “air quality” (158). Most of the terms are related to human activities or activities that are not strictly related to ports, given that ports are often located in urban areas with high human activity. This cluster can be defined as a cross-cutting one, as it includes mainly words linked to the concept of environmental sustainability and air quality. This cluster comprises 150 keywords. Table 1 lists the top 25 keywords.

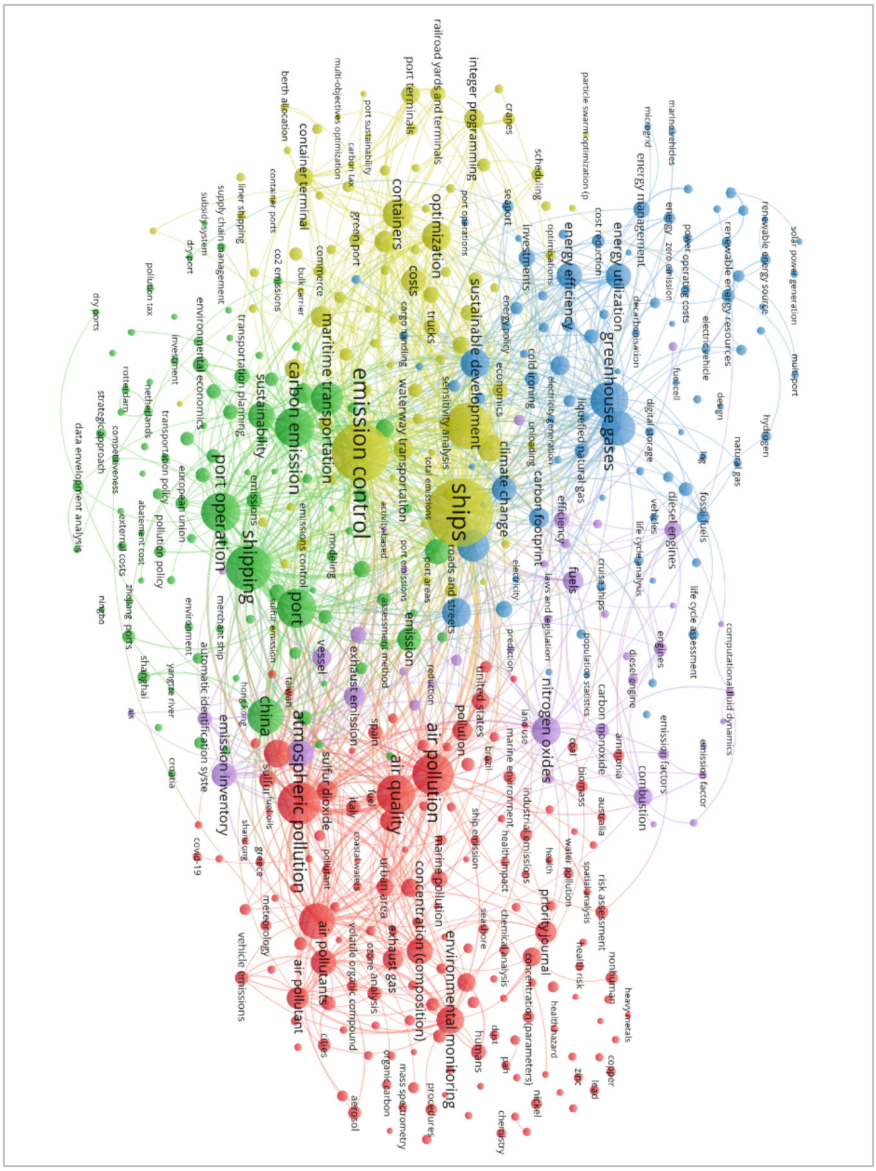

Fig. 2. Co-occurrence keyword map.

5.2 Cluster 2 (Green): Maritime Transport

The second cluster (green) pertains to the topic of shipping and sea transport. The most frequently occurring keyword is “shipping” with 205 occurrences. This cluster is associated with activities that occur near ports, specifically on the seaside. The topic of this cluster focus mainly on emissions caused by ships during port entry and exit operations,

Table 1. Cluster 1, Top 25 keywords.

Keyword	Occurrences	Links	Total link strength
atmospheric pollution	185	388	185
air pollution	173	388	166
air quality	158	366	157
particulate matter	141	344	141
environmental monitoring	92	310	91
traffic emission	92	345	92
concentration (composition)	86	285	86
air pollutants	81	312	81
air pollutant	66	289	66
priority journal	63	283	63
ship	63	309	62
sulfur dioxide	63	305	63
exhaust gas	59	278	59
pollution	56	298	55
controlled study	49	265	49
human	49	271	49
pollution monitoring	49	280	49
united states	47	261	47
urban area	45	273	45
marine pollution	41	211	41
sulfur	41	246	41
humans	36	222	36
Spain	35	258	35
city	34	231	34
analysis	33	209	32

as well as emissions resulting from maneuvering operations within the port. This category includes emissions associated with port berthing periods. According to literature, solutions such as cold ironing, battery usage, and alternative propulsion sources can be implemented to reduce these emissions. Table 2 lists the top 25 keywords.

5.3 Cluster 3 (Blue): Energy Efficiency

The third cluster, in blue, represents keywords linked to energy efficiency, which in some cases can lead to a reduction in the emission of greenhouse gases. The most frequently term within this cluster is “greenhouse gases”, which appears 153 times. Other keywords

Table 2. Cluster 2, Top 25 keywords.

Keyword	Occurrences	Links	Total link strength
shipping	205	422	204
port	163	413	162
carbon emission	160	378	158
port operation	160	389	160
China	139	385	139
maritime transportation	120	367	119
sustainability	87	259	84
greenhouse gas	80	303	80
emission	76	318	75
fuel consumption	57	217	57
maritime transport	46	194	43
numerical model	41	223	41
emissions	39	180	39
environmental economics	38	199	38
Europe	38	218	38
transportation planning	38	227	38
logistics	35	162	34
shipping emissions	35	219	35
simulation	35	194	33
freight transport	34	189	33
container ship	33	207	33
environmental protection	32	203	32
traffic congestion	32	181	32
cost analysis	31	195	31
environmental policy	31	211	31

are “energy efficiency”, “energy management”, “energy utilization”, as well as keywords related to alternative energy sources such as hydrogen, natural gas, fuel cells, and cold ironing. Table 3 lists the top 25 keywords.

5.4 Cluster 4 (Yellow): Port Terminals

The fourth cluster (yellow) shows a significant correlation with the second and third clusters. The most occurring keyword is “ship”, which appears 378 times, ranking first among all keywords. Its position suggests its centrality in relation to the sample under examination. Additionally, within the cluster we can find other terms that refer to a

Table 3. Cluster 3, Top 25 keywords.

Keyword	Occurrences	Links	Total link strength
greenhouse gases	153	356	152
gas emissions	131	364	131
ports and harbors	114	402	114
sustainable development	101	298	100
environmental impact	100	375	100
energy efficiency	81	248	80
energy utilization	80	234	79
climate change	78	294	76
carbon footprint	56	286	56
global warming	52	233	52
environmental management	42	223	41
investments	42	190	42
energy management	41	151	39
cold ironing	33	162	32
energy conservation	33	159	33
liquefied natural gas	33	185	33
renewable energy resources	32	116	32
life cycle	31	168	31
cost reduction	30	159	30
fossil fuels	30	174	29
greenhouse gas emissions	30	163	30
fleet operations	26	155	26
seaport	25	144	25
cost effectiveness	24	162	24
energy	24	98	24

specific zone of ports, namely port terminals. Port Terminals are areas of significant interest due to the various activities that take place within them. The key terms include "port terminals", "container terminals", "containers". Additionally, there are terms that refer to activities that take place in the landside port area, such as "tracks", "railroad yards". Furthermore, in relation to activities carried out within the port terminals, the keywords "optimization" and "costs" suggest topics related at improving port operations, which could result in a reduction of greenhouse gas emissions. Table 4 lists the top 25 keywords.

Table 4. Cluster 4, Top 25 keywords.

Keyword	Occurrences	Links	Total link strength
ships	378	456	377
emission control	297	435	296
carbon dioxide	207	397	206
containers	103	301	103
optimization	100	248	100
carbon	87	325	87
costs	75	291	75
carbon emissions	62	204	59
decision making	62	240	62
integer programming	56	171	56
waterway transportation	55	289	55
freight transportation	53	247	53
container terminal	52	185	52
port terminals	49	170	48
emission reduction	43	192	43
trucks	41	189	41
green ports	40	190	39
supply chains	38	192	38
economics	37	229	37
railroad yards and terminals	37	152	37
green port	35	149	33
economic and social effects	34	192	34
transportation	33	199	32
international trade	32	182	32
roads and streets	32	236	32

5.5 Cluster 5 (Purple): Engines

Cluster 5 (purple), the smallest cluster, is characterised by a high concentration of the term "engine" in various forms. The most frequently occurring term is "nitrogen oxides" with 99 occurrences. This cluster is related to the theme of engine efficiency, and it emphasizes the growing recognition of one of the principal sources of port-related pollution, namely ships at berth that require their engines to remain operational in order to power services on board. Table 5 lists the top 25 keywords.

Table 5. Cluster 5, Top 25 keywords.

Keyword	Occurrences	Links	Total link strength
nitrogen oxides	99	320	98
ship emissions	88	296	83
emission inventory	77	298	77
exhaust emission	61	262	61
fuels	58	272	58
vessel	53	272	53
combustion	50	218	48
automation	42	238	42
diesel engines	42	216	41
efficiency	36	167	36
automatic identification system	33	193	33
carbon monoxide	32	198	32
engines	30	125	27
environmental regulations	23	133	22
emission factors	22	137	22
emission inventories	22	151	22
pollution control	22	186	22
diesel engine	21	138	21
forecasting	18	117	17
nitric oxide	18	172	18
computational fluid dynamics	17	69	17
fuel economy	17	72	16
laws and legislation	16	140	16
machine learning	16	97	16
emission factor	15	55	14

6 Conclusions

The issue of emissions in ports is constantly evolving due to the global trend to reduce emissions. It is therefore important that scientific research develops all current issues.

The combined bibliometric analysis and knowledge mapping of greenhouse gas emissions in ports, presented in this paper, allows us to define some preliminary assessments. The construction and definition of co-occurrence keyword clusters could be the first step towards a more detailed literature review, that can include a subsequent subdivision of papers by thematic areas and sub-cluster categories. The five clusters provide some initial indications of potential future research areas, such as pollution, maritime

transport, energy efficiency, port terminals and engines. In particular, the emergence of energy-efficient technologies and alternative fuels could influence the policies of reduction of emissions in ports.

However, further investigations are necessary to investigate the individual clusters in a more specific way. Furthermore, as was discussed in the data collection section, the sample was extrapolated only from the Scopus database. Therefore, it is necessary to include other databases, such as Web of Science and others.

Acknowledgements. This study was carried out within the MOST – Sustainable Mobility National Research Center and received funding from the European Union Next-GenerationEU (PIANO NAZIONALE DI RIPRESA E RESILIENZA (PNRR) – MISSIONE 4 COMPONENTE 2, INVESTIMENTO 1.4 – D.D. 1033 17/06/2022, CN00000023). This manuscript reflects only the authors' views and opinions, neither the European Union nor the European Commission can be considered responsible for them.

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Port Cities Symbiosis. Port Network Authority of the Eastern Adriatic Sea and of Sardinia Sea (Italy)

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Abstract. Port cities have always been key hubs for the transport of goods and people. Ports meet global transportation needs, while being integrated into geographies subject to local policies. Maritime and logistical flows pass through ports and densely built-up areas, creating new environmental challenges. Political interests and strategies, technological development, migrations, trafficking of goods and flows of people are factors that influence spatial organization as well as land use to respond to the new challenges of the global market. This also involves changes in the morphology of port cities, which are by their nature dynamic, cosmopolitan and more open to change and the reorganization of the coastal space, from port cities to port regions. Ports are becoming increasingly hybrid, progressively changing shape and inserting new functions even beyond their administrative borders, renewing the relationships of Port Cities Symbiosis. In this paper we focus on the hybridization process of ports, to address new international challenges in particular. By analyzing some theoretical and real cases of Italian port system authorities - of the Sardinian Sea of the Eastern Adriatic Sea, Ports of Trieste and Monfalcone -, it is proposed to evaluate a synthetic hybridization matrix of ports, within the framework of the broader Port cities symbiosis phenomenon.

Keywords: Port-Cities · Port Cities Planning · Port Cities Symbiosis

1 Introduction

The ports have long been the foundation of socio-economic development in many coastal regions where they have played and continue to play multiple roles. In their historical evolution, the ports have chronicled the economic, technological and social transformations of the territories on which they gravitated.

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O. Gervasi et al. (Eds.): ICCSA 2024 Workshops, LNCS 14823, pp. 326–339, 2024.
https://doi.org/10.1007/978-3-031-65329-2_22

The European territorial context is configured in a network of over 1,200 seaports and the horizontal relationships established between 'land and sea' are manifested through - positive and negative - environmental, socio-economic and cultural impacts. The port areas see the transit of around 420 million passengers and a 74% handling of imported and exported goods. At the same time, it is necessary to consider that daily these coastal areas are traversed and experienced by some 1.5 million workers who are employed in the different port sectors - logistics and cargo handling, passenger services, infrastructure maintenance, etc. - and who contribute to strengthening the local economy by facilitating economic, cultural and tourism exchange.

Hence, different and multiple vertical and horizontal relationships are put in place between the port, neighboring cities and gravitation regions. Globalization and revolution in the transport sector, such as containerisation and intermodality, have in fact contributed to modifying and intensifying these connections and in achieving common interests such as economic development, these areas often find themselves competing for different spaces and goals [1, 2]. In this perspective is the process of 'hybridization' that sees ports striving to create more flexible and adaptable structures to meet the changing needs of the global market. This 'new' approach aimed at continuous and dynamic transformation takes several forms, including, for example, the adoption of digital technologies to optimize port operations, the diversification of functions - including commercial, cultural and/or residential -, and the implementation of sustainable policies to address environmental challenges. These transformations give rise to the concept of 'Port Cities Symbiosis' in which the 'reading' of the territory requires closer interconnection and synergic collaboration between port facilities and cities by investment in infrastructure and services that benefit both the port and the city [3, 4].

In this context the aim of the work is to deepen the issue related to the process of ports hybridization, to address new international challenges in particular. By analyzing some theoretical and real cases of Italian port system authorities - of the Sardinian Sea of the Eastern Adriatic Sea, Ports of Trieste and Monfalcone -, it is proposed to evaluate a synthetic hybridization matrix of ports, within the framework of the broader Port cities symbiosis phenomenon.

The paper is organized as follows: Sect. 2 Related works; Sect. 3 Method and Study Area: Sect. 3.1 Methodology; Sect. 3.2 Study Area; Sect. 4 Results and Discussion: Sect. 4.1 The port of Cagliari and Olbia; Sect. 4.2 The port of Trieste; Sect. 5 Conclusions and Future Developments.

2 Related Works

The port areas emerge as vital hubs for the blue economy. Since ancient times their versatility and the variety of activities involved (industrial, commercial and tourism) reflect a complex network of interconnections that stimulate economic growth, improve the quality of life and preserve the environmental balance of the regions involved [5, 6].

In the second half of the 20th century, an increased interest in understanding the functional structure and evolution of port cities was triggered by changes in the patterns of international maritime trade (delocalisation and re-functionalization of port-city activities) and technological innovations that accelerated transformations, particularly

in the 1980s and 1990s. In this context, at different territorial scales, public and private actors have financed and activated programs and projects aimed at improving the quality of life and relations in the port-city space [7]. These relations have been analyzed since the first decade of the 1900s when the 'American Association of Ports and Harbors' was established in the United States, and subsequently, there have been several studies by authors who have explored and described the development and the relational evolution between port and city from different perspectives: port-city interaction, growth and estrangement, isolation and separation, and port-city integration [8–13]. With reference to the dialogue between port and city, it is worth mentioning the work carried out by Bird J. in 1963 [14] in his 'Anyport Model' in which he emphasized the idea that any location along a coastline could potentially turn into a port, given the right conditions - geographical (sheltered harbor, access to deep water, proximity to transport networks), economic (market demand, industrial and commercial development), and political (regulations and investments that facilitate and/or hinder growth). Consequently, ports, in order to be able to respond to different conditions, must allow their dynamic and flexible nature to emerge and grow.

Historically, ports have always been seen as engines of economic growth and cities as hinterlands supplying labor and resources. However, this traditional dichotomy has often led to conflicts over space and significant impacts on the landscape.

Thus, in the context of growing environmental awareness, increased international competitiveness and new job opportunities, the world's major ports have taken substantial measures to elevate their functional, operational and integrative capabilities by changing perspective [4, 15–18]. The approach adopted is configured through the concept of 'Port Cities Symbiosis' that considers ports and cities no longer as competing entities, but as realities that coexist, thrive and influence each other through the exchange of goods, people and information. The economic success of a port can catalyze urban development, creating job opportunities, attracting investment and promoting a vibrant local economy, and at the same time a thriving city can provide the port with a qualified workforce, infrastructure support and a business-friendly environment [19]. The interdependence between ports and cities therefore offers an opportunity to address economic, environmental and social objectives in a cohesive way, creating a framework for resilient and adaptive urban development. Following these objectives, several working groups and associations are involved in broadening scientific-disciplinary comparisons to improve the port-city relationship in a territorial development perspective.

The first organization, the Association International Villes et Ports, was set up in 1988 to improve the relationship between cities and ports by establishing and developing dialogue and cooperation. In 2001, RETE, another international non-profit organization, was formally established in 2004 in Venice, thanks to a protocol of agreements between Italian, Portuguese and Spanish ports and cities, who strive 'to improve the relationship of reciprocal collaboration in order to achieve a balanced and qualified development of urban and port areas'. This approach finds a place in the Mediterranean cities and ports with their own 'constitutive specificity' in terms of the organization of the port infrastructure and its relationship with the urban public space. An integrated urban space in which the port becomes an 'urban living room' stimulating the development of a new city identity [20].

3 Method and Study Area

3.1 Methodology

Analyzing the relationships of Italian port cities is a complex issue. The multiple urban areas, ports, waterfronts, semi-peripheries and suburbs create a network of interconnections that requires the integration of different analyses. An essential first step is the analysis of strategic and urban planning tools - Approved (AP), Adopted (AD) or In Progress (IP) - (Fig. 1) [21]. The objective is to observe and assess their capacity to manage land uses (urban and peri-urban) and their consequent effects on urban and port centers in an integrated way. In addition, it is important to examine not only the coordination and interconnection level of urban and port planning tools, but also those related to 'ordinary' industry and transport planning, and special attention must be paid to the 'spontaneous' behavior of logistics operators. Their location in space may be unstructured and follow logistical logics different from the traditional ones, with significant logistical impacts on the territory.

The following methodological approach, complemented by concrete examples, literature research and policy proposals, is configured in Fig. 1 through an analysis matrix that aspires not only to measure the efficiency and effectiveness of policy actions, but also to promote a balanced integration between different strategic and planning tools [22].

The analysis required the review and systematization of the different available documents considered relevant for understanding the pressures and areas of symbiosis in the city-port areas. Planning documents, overview maps and field surveys represented important sources for setting up the matrix related to the different scenarios.

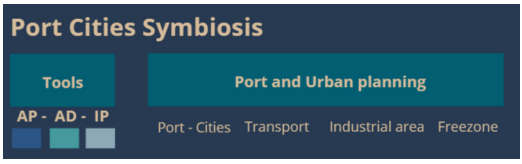

Fig. 1. Port Cities Symbiosis: Analysis matrix. Source: Authors' elaboration

3.2 The Study Area

The port-city relationship in Italy is historically rooted and has evolved over time taking on different forms and configurations. Just to mention a few, the urban structure of Venice, Pisa, Genoa, Naples and Ravenna was born and has been linked to the port infrastructure, creating a cohesive and distinctive urban fabric and an important center of trade and cultural exchange. The dynamic coexistence of these spaces has allowed ports, in their ordinary modernization and redevelopment processes, to integrate their infrastructures and activities more closely with the urban area, favoring new development models linked, for example, to green mobility and environmental sustainability.

The analysis includes the urban-port relations in the city of Trieste (Friuli-Venezia Giulia) whose port is managed by the Port System Authority of the Eastern Adriatic Sea and in the cities of Cagliari and Olbia (Sardinia) where both ports are managed by the Sardinian Sea Port System Authority - other ports managed on the island are Cagliari, Foxi-Sarroch, Olbia, Porto Torres, Golfo Aranci, Oristano, Portoscuso-Portovesme, Arbatax, and for Santa Teresa di Gallura - commercial dock only.

The three cities are characterized as 'central places' that insist on the surrounding territories with their supply of goods and services [22, 23]: a) the Province of Trieste, includes six municipalities, including the homonymous capital, is a compact and densely populated area, with a catchment area of about 240,000 inhabitants; b) the Metropolitan city of Cagliari involves an area of about 400,000 people spread over 17 municipalities; c) the city of Olbia, considered the main gateway to the island, insists on an area involving 26 municipalities - former Province of Olbia-Tempio, now the Eastern part of the Province of Sassari - for a total of 159,000 residents.

In the port sphere, all three areas play an important role as commercial hubs and are part of the cruise ship network, although with different purposes and specialized markets. The three ports welcome 652,300 cruise passengers to their urban waterfront for a total of 331 landings in 2022 [24]. In particular, Trieste is a predominantly international port, serving as a gateway to central Europe; Cagliari focuses on Ro-Ro and ferry traffic for the western Mediterranean; Olbia with about 3 million passengers (2022) is Sardinia's main passenger port - on a national scale it ranks eighth. The three ports are distinguished not only by their specialization but also by their size and different integration with the city.

Sardinian Sea Port System Authority. As mentioned above, the Sardinian Sea System Authority, instituted by Legislative Decree No. 169 of 4 August 2016, has complete management of the island's ports, including Cagliari and Olbia. The policy, planning and coordination actions of the ports under its jurisdiction are based on the three 'Three-Year Operational Plans' (2018–2020; 2021–2023; 2024–2026) in which the primary objective is to contribute to the socio-economic growth of port areas in synergy with urban areas. The projects activated and planned concern not only 'ordinary and extraordinary' activities related to port functions (e.g. quayside infrastructures, seabed maintenance), but also those dedicated to a greater synergy with the urban areas of reference - e.g. the change of use of some spaces for leisure activities, waterfront redevelopment, development of entrepreneurial activities [25].

The Authority's constant efforts on sustainable matrix guidelines such as the ecological, energy and digital transition for the pursuit of socio-economic development integrated with the territory has allowed it to receive awards on a national scale, such as the recent 'Smart Ports Award' (September 2023). In this way, the Authority works to establish a balance and positive relations, from an economic and urban planning point of view, mainly with the Municipal Authority. Therefore, below we highlight peculiarities and projects activated in the two island ports that are on which the study focuses.

Port of Cagliari. The port is divided into three areas [25].

1. The 'Porto Vecchio' is developed on a 333,250 square meter land area (coastal development over 11,000 m including 4,800 m of quay). The port area is delimited by

two external breakwaters (western and eastern breakwaters) and by the Molo Ichnusa (internal breakwater). Three areas are identified between the two breakwaters - Levante Basin, Inner Harbour, Ponente Basin - for a total of around 7 km of waterfront (Fig. 2).
2. 'Porto Canale' is delimited by two converging outer breakwaters, each 2,020 m long, and is configured with five berths for transshipment and Ro-Ro traffic.
3. Porto Foxi' (Municipality of Sarroch) is Cagliari's liquid bulk port.

In 2023, plans are underway to build a new marina in the 'Porto Vecchio' area. Here it is planned to overhaul the berthing system for yachts and private boats and the restyling of the ex-maritime station, which will be converted into a multifunctional center (recreational boating services and tourist hub) and of the additional public spaces.

Fig. 2. The Port of Cagliari. Source: Authors' elaboration [22]

Port of Olbia. The port it is divided into three areas with different functionalities (Fig. 3).

The 'Porto Cocciani' (industrial), which a land area of about 270,000 square meters is located in the industrial area to the north of the city and is used for Ro-Ro traffic and traditional goods - stone material, cement, frozen tuna, cereals and fertilizers; the 'Pontile Isola Bianca' is a commercial area consisting of a strip of land artificially formed for a total of 107,894 square meters - including parking areas for commercial vehicles and semi-trailers - in which there are 11 quays. Ten quays are destined for Ro-Pax ferries for passenger and commercial transport; the 'Porto Interno' (inner harbor), located to the south of the Pontile Isola Bianca, which is reserved for recreational activities.

The Port of Trieste within the Eastern Adriatic Sea Port System Authority. The port of Trieste is part of the Eastern Adriatic Sea Port System Authority, that includes also the Port of Monfalcone, while integrates also the presence of inner ports and dry

Fig. 3. The Port of Olbia. Source: Authors' elaboration

terminals, as Bagnoli - Fernetti and Cervignano, as well as including the consortium for the industrial development of Trieste area (COSELAG) located in close proximity to the docks of the Port of Trieste, in the Southern part of the port area. The Port of Trieste (Fig. 4) is characterized by interesting dynamics particularly in terms of the maritime - land connections, with a high percentage - 30% - of freight share moved by train towards European inland destinations. Furthermore, a mixed role of hub & gateways functions characterize the port. 35 to 40% of freight traffic is generally transshipped - originating mainly through pendulum routes with Far East Asia, although this share dropped down dramatically at the beginning of 2024, due to the Suez - Bab el Mandeb traffic limitations, while the rest of the traffic is directed towards the port of Trieste's hinterland, at short range - in Friuli Venezia Giulia Region - and at medium and longer ranges - to European destinations.

In the national framework of the Italian System Port Authorities, the Port of Trieste is characterized by being mainly a rail port and the only true international port, with a predominance of international destinations for freight. Pier VII in particular is dedicated to the container movements, while several terminals are nowadays multipurpose ones, hosting a mixed container and ro-ro traffic. Noticeable is also the liquid oil movement, still representing the lion share - more than 70% - in terms of the overall tonnage moved.

Fig. 4. The Port of Trieste. Source: Authors' elaboration [22]

4 Results and Discussion

The recent changes occurring in the port systems are relevant and having consequences on the spatial patterns and balances among the different kinds of uses. Namely, port and urban ones, bringing with them together activities as people and freight movements, residential, services and industrial activities, tend to compete both on the waterfronts and in inner areas for gaining access to the most suitable areas for their exploitation.

The different cases considered are interesting in terms of how peculiar they are in tackling these issues, descending from different urban evolution's histories and port ones.

The analysis applied to the three cases with the aid of the analytical matrixes (Figs. 2, 3, 4). The planning tools were considered, particularly those insisting on the different areas of the port-city. The planning tools are related to urban and port planning, extended also to consider the industrial plans and the mobility ones. The urban/metropolitan scale was also considered, together with the evaluation concerning the presence and operation of Free Zones. The analysis applied to the three cases with the aid of the analytical matrixes. The different stages of adoption of the planning instruments were related to differences in the 'cities and ports' performances in matching and meeting urban and port planning issues [22].

4.1 The Ports of Cagliari and Olbia

As highlighted above, the ports of Cagliari and Olbia belong to the same Port System Authority, although with considerable differences in terms of their performances and characteristics, both from the city and from the port points of view. The characters of accessibility are the most relevant ones. In the case of Sardinia, of course, it has to be

considered that maritime transport - together with air transport - is the only one really connecting high volumes of passengers and freight traffic.

From the urban point of view, Cagliari represents the regional capital and also a metropolitan city with higher order functions and services. Given the presence of a wide urban area, extending to a wide metropolitan city and area, potential pressures and symbiosis are important. In the case of Cagliari, the aspects related to the implementation of the industrial areas are advanced in most of the geographical framework - port, semi-periphery and periphery. The free zone in the port area is also present and available, although not yet fully implemented (Fig. 5).

Cagliari faces a complex challenge. Despite a large metropolitan area, establishing Free Zones – a key development tool for the city and its region – has been slow. The city's substantial population, industries, and service sectors further complicate planning, which currently prioritizes central urban and port infrastructure. Additionally, delays in implementing specialized customs regimes for industrial zones could hinder future progress [22].

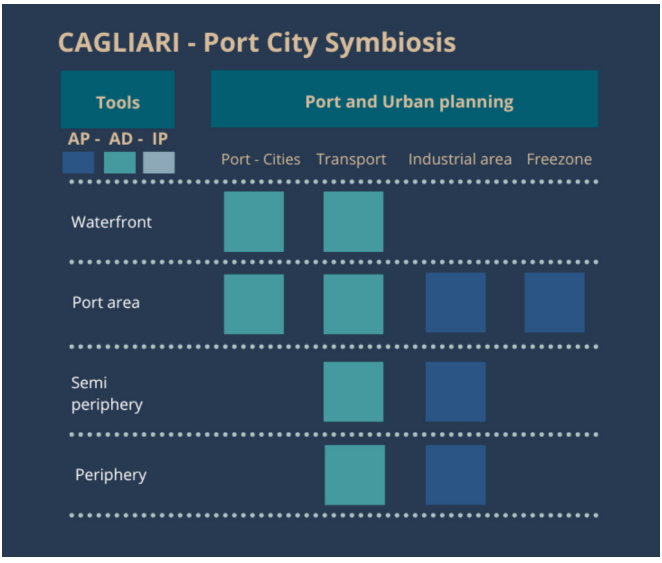

Fig. 5. Cagliari: Analysis matrix. Source: Authors' elaboration

Olbia has been an important port city in the Mediterranean since ancient times. The port favored trade and exchange with other Mediterranean civilizations, contributing to the economic growth of the city and the island's territory. The port-city relationship has not always been harmonious: the port was born and established a conflictual relationship with the city, relegating it to the margins and depriving it of direct contact with the sea, and only in recent decades can it be considered integrated into the urban context. Infrastructure and services help to establish a close relationship with the local community (port services, shipbuilding, yachting, tourism, logistics, etc.). In its role as a passenger gateway in particular, with a constant flow of people it enhances the fruition of the two

areas (urban and port) thus also contributing to the development of the local and regional tourism sector. Following the commitments to achieve Agenda 2030 sustainability goals, in recent years there has been a growing awareness on the importance to develop the port compatible with environmental protection and the wellbeing of residents and guests. In this perspective, for instance, investments and projects are being made in the reconversion of the waterfront and in new redevelopment projects in the port areas that are more open to the city: an area of about 3,500 square meters along the 'Pontile Isola Bianca' will see the creation of spaces equipped with street furniture, greenery, and lighting for leisure enjoyment (Fig. 6).

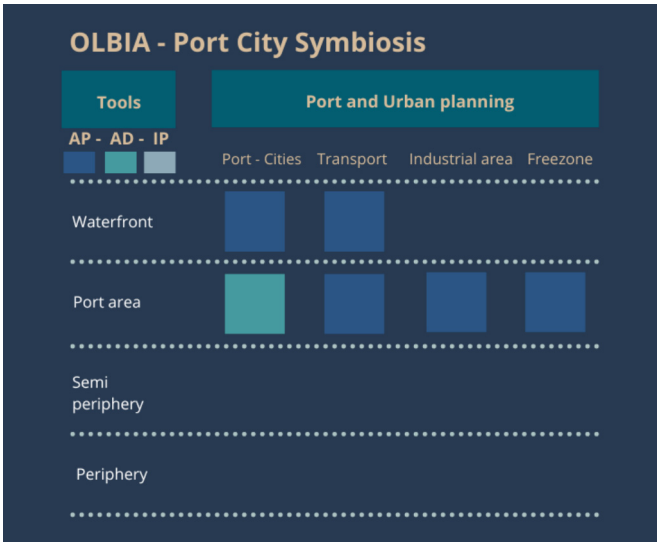

Fig. 6. Olbia: Analysis matrix. Source: Authors' elaboration

4.2 The Port of Trieste

Trieste, encompassing the city and port, holds a set of planning tools applicable across its territory – central core, port zones (including expansions), inner and outer suburbs – nonetheless gap remains. Conventional transportation planning instruments haven't sufficiently tackled the needs of the peripheral areas.

If the previously analyzed ports represent important gateways for a region isolated from other transport systems point of view, in the case of Trieste the maritime - land connections are tightly linked and all the efforts have been put, particularly in more recent times, to make this set of long-range flows be operational and functional. In such a sense, the planning tools were considered particularly for fostering the logistic and transport functions, together with the re-exploitation of the industrial components, after a period of deindustrialization. The overall picture coming out from the observation of the matrix analysis displays an area whose level of maturity of the planning instruments

for the transport, logistics and industry sectors is advanced and presents an important framework for further developing the area. The port masterplan, the integration with industrial planning and a one-of-a-kind jurisdiction of international free port, allowing eased set up of transport and industrial activities, hold potentials for a full exploitation of the area. The development of port-related and extra activities out of the strictly-related port area is not however yet exploited and planned, living room for further planning implementation (Fig. 7).

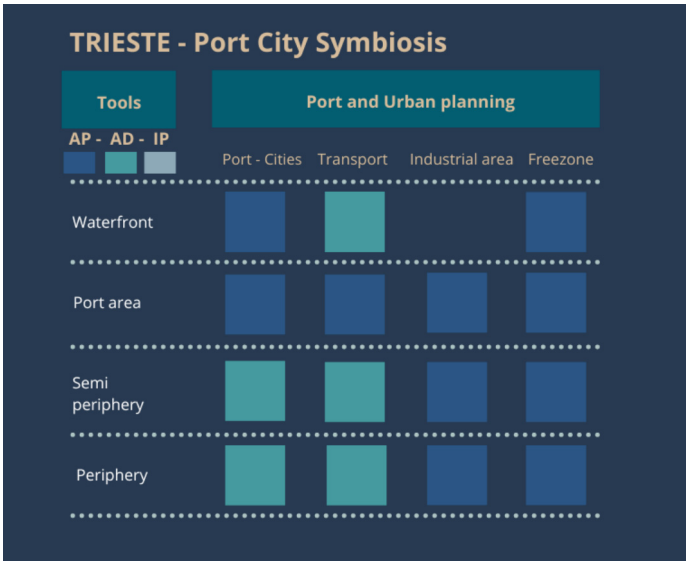

Fig. 7. Trieste: Analysis matrix. Source: Authors' elaboration

5 Conclusions

The port-city symbiosis is a phenomenon that aims to create a relationship of mutual collaboration between port and city. Symbiosis is a phenomenon borrowed from the plant system and consists of a close mutualistic and long-lasting relationship between two organisms of different species that benefit from their interaction.

In this sense, for the port and city symbiosis, the sharing of knowledge and information between the port and the city is fundamental, from port operations and development plans: The city must be informed on how the port operates and what its development plans are for the future, thus allowing us to plan in symbiosis.

The port-city symbiosis is therefore an interdependent relationship between the port and the city of which it is part. In this relationship, the port provides the city with access to the sea and trade routes, while the city provides the port with labor, infrastructure, and services, with economic development created for both parties. The port can create jobs and attract investment, while the city can benefit from increased trade and tourism

and demand for goods and services. Furthermore, the port-city symbiosis can promote environmental sustainability, including through reducing the environmental impact of the port and promoting the circular economy and energy transition.

However, there are also areas of conflict of interest between the port and the city, such as the land use of the waterfront quays which are often used for parking cars, occupying vast central and attractive areas. In this sense, the port-city symbiosis requires multi-level governance to facilitate the creation of a common reference framework for the planning and development of the port and the city, which must include a common vision for the port-city symbiosis, as well as objectives and indicators of measurement.

6 Future Developments

The port-city symbiosis is a desirable alternative to parasitic dynamics, in which one of the two actors exploits the other to its own advantage. Symbiosis can manifest itself both through the development of shared strategic plans that take into account the needs and objectives of both parties and the establishment of consultation tables and multilevel governance bodies. Flexibility and adaptation to changing global and local circumstances are crucial to maintaining a lasting symbiotic relationship.

The port-city symbiosis is not a static model, but a continuously evolving process that requires the active involvement and support of the public and private actors involved. Over the centuries, the relationship between port and city has evolved in parallel with economic, social and technological changes. However, the port-city symbiosis must face the challenge of economic-environmental sustainability, to face global and local challenges.

The development of research on the port-city symbiosis which is constantly evolving, will be oriented towards implementing pilot experiences capable of: overcoming regulatory barriers and facilitating the adoption of symbiotic management models capable of innovating to improve its efficiency, security, sustainability and life quality [26–28].

Acknowledgments. The paper descends from the common aim of the three authors. However, Giuseppe Borruso wrote paragraphs 1, 3.2 “The Port of Trieste…” and 4.2. Ginevra Balletto realized paragraphs 3.1 and 3.2 “Port of Cagliari” and 5. Silvia Battino realized paragraphs 2, 3.2 (a part from the above-mentioned paragraphs), 4 (a part from paragraph 4.2) and 6. This study is part of a larger Research Project “Osservazioni e analisi regionali dello yachting e dei porti turistici della Sardegna” funded by the Regione Autonoma della Sardegna (R.A.S.), Department of Tourism.

Disclosure of Interests. The authors have no competing interests to declare that are relevant to the content of this article.

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Literature Review on the Smart Port: Evolution, Technological Development, Performance Indicators of Smart Ports

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Abstract. Boost in the global supply chain in the post-industry 4.0 revolution has amplified the demand for maritime ports, triggering their operational capacities, competitiveness, and sustainability concerns. Maritime ports are undergoing a paradigm shift, an evolution from goods loading and unloading terminals to highly intelligent hubs in the logistic supply chain.

Existing literature on smart ports focuses on different aspects such as evolution stages, bibliometrics analysis, feasible technologies, and Key Performance Indicators (KPI).

This review complements the existing ones by investigating the term "smart port" definition, the technology use, the Key Performance Indicators (KPIs), and providing bibliometric analysis across major databases, sourcing from journals, conferences, official websites, and books in various disciplines.

Results show that the definition of "smart port" is still under development. Moreover, the major driver of transformation is the technology use, some technologies are mature enough for implementation and the rest are in the early stages. Importantly, along with innovative technologies, management skills play a crucial role in successful implementation. The Smartness of the port is difficult to answer but an accurate quantification of Key Performance Indicators (KPIs) can assist the ports in gauging their level of "smartness".

From the bibliometric perspective, there is a growing trend of smart port research, particularly in recent years. This trend is interestingly almost uniformly distributed in different geographic locations.

The findings underscore the kernel role of technology in shaping smart port evolution, and performance indicators for quantifying the smartness. The investigation of the challenges for ports to implement technologies is a key area for future research.

Keywords: Smart Port · Smart Port KPIs · Container Terminal Digital transformation · Industry 4.0 · Port Sustainability

1 Introduction

Ports are regional multimodal intersections of global supply chains (Molavi et al., 2020), a complex system that provides a logistic distribution hub for domestic and foreign trades, acting as a primary driver in the functioning of an open economy and social well-being.

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O. Gervasi et al. (Eds.): ICCSA 2024 Workshops, LNCS 14823, pp. 340–357, 2024.
https://doi.org/10.1007/978-3-031-65329-2_23

Maritime transportation accounts for 80% of goods carriage in the world, which makes it a vital part of the global supply chain (Belmoukari et al., 2023a; UNCTAD 2021). European ports in the third quarter of 2023 handled 807 million tons of goods (Eurostat 2023).

On the other hand, shipping is responsible for 3% of greenhouse gas emissions; an increase of 20% over the last decade has been observed, and no counteraction can cause a 130% shoot-up by 2050 to their 2008 level (UNCTAD 2023). These challenges are directly influencing the port's role in the industry. Environmental, business, social, and operational challenges for ports made governments, port authorities, and stakeholders rethink the operational design of the port. Port challenges are congestion, delays, operating errors, and lack of information sharing (Molavi et al., 2020). Issues related to the environment are water and waste management, energy demand and consumption, and their impact (i.e., noise pollution and greenhouse gas emissions), and safety and security issues (Belmoukari et al., 2023a). Moreover, ports are battling cutthroat competition due to their homogenization (Chen et al., 2019).

Therefore, the concept of smart port has evolved; it provides environmental compliance, financial efficiency, and technology support to ports. A smart port is, by definition, more connected, safe, and green. The term "smart" applies to more innovation in a competitive sense. Smart ports are more effective and offer greater performance. They provide real-time information and, an effective and collaborative management style. Successful technology involvement and a proper gauging of smartness through Key Performance Indicators (KPIs) are two essential elements of the transition from simple terminals to smart ports. Among the review studies available on smart ports, Li et al. (2023) laid a smart port foundation research on technologies used, and port performance indicators. However, how can smartness be defined for ports? Is a digitalized port smart? How can technology drive the ports to smartness? This research review tries to answer these questions, which include bibliometrics evolution stages of smart ports, technologies for ports, and Key Performance Indicators (KPI) and tries to elaborate on how these integrate for the development of smart ports.

This paper is organized as follows: the Sect. 2 analyses the bibliometric trends in smart port research, the Sect. 3 discusses smart port evolution and definition, Sect. 4 describes the literature on technologies for smart ports, Sect. 5 focuses on the key performance indicators for smart ports, and Sect. 6 is dedicated to the conclusion.

2 Bibliometrics

Bibliometric analysis was conducted using multiple approaches in the smart port area. Keywords such as smart port or smart ports, maritime ports, digital transformation, port sustainability, and container terminal were utilized. 76 articles were ultimately selected for synthetic analysis from 160 downloaded. The review includes 4 review papers and 69 novel experiments, case studies, reports, official websites, and books that advocate smart ports. VOSviewer software version 1.6.20, a tool developed by VN Eck and Waltman (2022) (Martins et al. 2022), was utilized for mapping keyword co-occurrence (Fig. 3), and data in RIS (Research Information Systems) format was extracted from Mendeley reference manager and used as VOSviewer's input. The concept of the smart port was

raised after 2010, nevertheless, we analyzed the papers from 2000 because of their technological involvement that founded the smart port concept. However, more weight was given to top journal papers (Table 1), bibliometric trends in publication years (Fig. 1), the geographic distribution of publications (Fig. 2), types of technologies for smart port and their use case (Sect. 4), macro and micro areas of key performance indicators, and contributing authors (Sect. 5). These are discussed as follows:

2.1 Annual Publication Trends

A positive trend has been observed in line with smart port research. The technological revolution and smart port development concept are key components of this tendency. Figure 1 shows publications from 2000–2023 in smart port. The graph shows a rapid development in recent years. 2020–2023 shows constant and maximum publications in the preceding years. It is noteworthy that exact smart port articles were found beyond 2016, and prior publications were somehow the building blocks and technologies that founded the smart port concept.

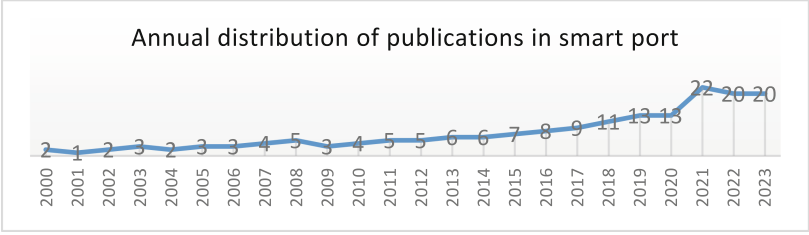

Fig. 1. Annual distribution of publications in smart port

2.2 Geographic Distribution

Interestingly, smart port research is distributed all over the world, as shown in Fig. 2. Europe and Asia have greater contributions. Specifically on smart ports, most research has been conducted in mainland China, with 16 publications, followed by Spain (11), Germany (8), Italy (7), Singapore (5), and Indonesia (5). The USA, Taiwan, Morocco, and Egypt have published 4, respectively. The UK, Thailand, Estonia, and Brazil contributed to 3 articles, respectively. Authors affiliated with France, South Korea, Russia, Poland, Croatia, and Belgium have each contributed to 2 articles on the smart ports area. Other nations, such as Vietnam, Ukraine, UAE, Turkey, Tunis, Srilanka, Portugal, Netherlands, Malaysia, Pakistan, Iraq, India, Greece, Finland, Slovenia, Canada, Chile, Bangladesh, Australia, and Albania have each one paper in the smart port domain.

Thus, smart port research is comparatively new, but the trend is growing uniformly throughout the world. The predominance of China in Smart Port Research could be due to the fact that China has the highest impact on global shipping and the special universities in China dedicated to maritime research e.g. Shanghai Maritime University

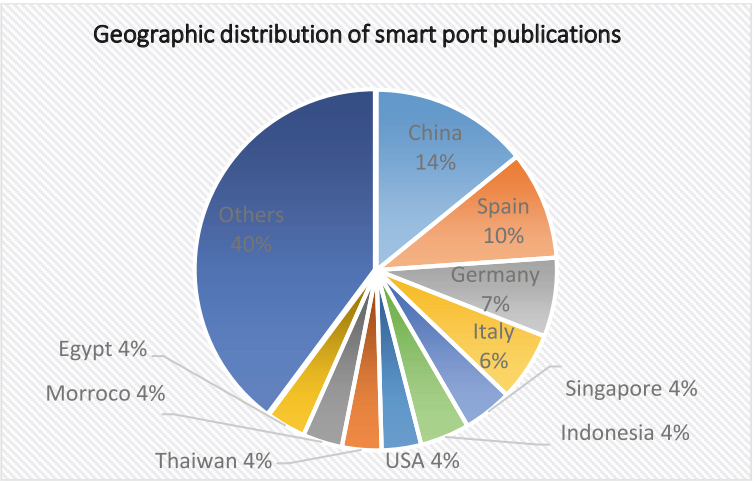

Fig. 2. Geographic Contribution to Smart Port Research

(SMU). It is noteworthy that this geographic quantification is based specifically on smart ports. Other areas that indirectly support smart ports i.e., use of technology in general transportation or supply chain, and research on ports in general are vast and not part of this spatial survey.

2.3 Top 10 Journals on Smart Port Research

Smart port research is a multidisciplinary field, maritime or marine journals, transportation-related journals, logistics, and technological or sustainability journals have an equal interest in smart port research. Table 1 lists the top 10 journals, out of 38, where smart port works are published more frequently. Thus, a selection of 24 out of 73 papers analyzed for this review are on this list.

Table 1. Top journals on smart port research

Journals	Publications
Maritime Policy & Management	4
Journal of Marine Science and Engineering	3
Sustainability	3
Environmental and Climate Technologies	2
Ocean and Coastal Management	2
IEEE Power & Energy Society General Meeting (PESGM)	2

(*continued*)

Table 1. (*continued*)

Journals	Publications
Case Studies on Transport Policy	2
Journal of Advanced Transportation	2
Logistics and Transportation Review	2
Ports and Network	2

2.4 Keywords Co-occurrence

The co-occurrence of keywords is a very useful tool to map the frequency of the occurrence of keywords within an article and the association of various topics. VOSviewer can illustrate this feature in clusters of keywords that represent the wholesomeness of the research topic. Figure 3 shows the keyword co-occurrence of this analysis. The map was created based on bibliometric data extracted from the Mandeley reference manager. The full counting method was selected, and a minimum number of occurrences of the keyword was taken as 2, given the fact that the port concept is very new and limited contributions are likely. Results show 74 items grouped in 12 clusters, with 204 links and a total link strength of 321.

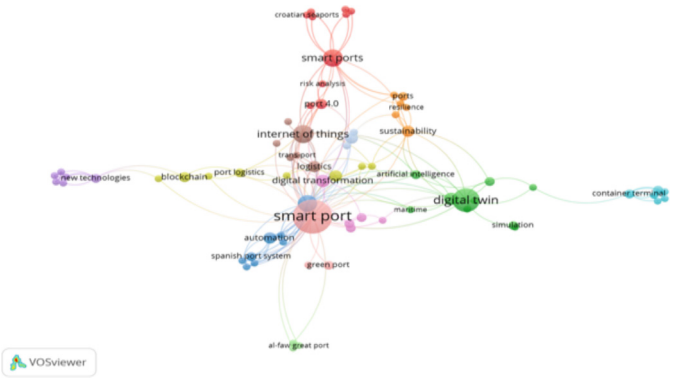

Fig. 3. Keywords Co-occurrence Map. VOSViewer (self-elaboration)

The sections described above deliver a clear idea of how smart port is injected into the research ground. The growing trend (Fig. 1) indicates the novelty of this discipline and its spreading trend, especially in the preceding years. Technological evolution (Sect. 4) is playing an important role in this trend. A very interesting part of this research is, that smart port research does not concentrate on a single geographic location but is widely distributed (Fig. 2). However, smart port indicators (Table 3) for a smart port may be different in various ports depending on many factors, such as education, environmental regulations, and the financial health of the port and country. In conclusion, the recent

and multidisciplinary nature of the smart port research area needs greater exploration, meanwhile making this area very interesting for further insights.

3 Smart Port Evolution and Definition

Smart ports are rooted in systematic, strategic, and social viewpoints that integrate modern technology use, constant interconnection, intelligent integration, coordinated operation, information sharing among interested parties, and creating an ecosystem that is smarter, safer, efficient, greener, flexible, resilient, and sustainable. Smart ports got the dominant attention for port development, representing the highest level of modern port transformation development, as reported by Chen et al. (2019). Currently, there are no universal definitions of what 'smart ports' are, since the 1990s, there has been an increasing trend for worldwide ports to invest in information and communication technology in operations (Du et al., 2023).

Yang et al. (2018) and Yau et al. (2020) defined smart ports as fully automated ports in which all devices are connected via IoT. Belmoukari et al. (2023b) define a smart port as a connected, sustainable, safe, and automated port, that relies on smart infrastructure and equipment, skilled personnel, and smart managerial practices to ensure customer satisfaction, environmental protection, and better quality of life for the citizen. Li et al. (2023) claim that smart ports enhance operational efficiency, communication, and crew satisfaction. Mi & Liu (2022) define the smart port as a system with cyber-physical systems as the structural framework, in which logistics suppliers and demanders are involved in the integrated system of collection, distribution, and transportation through the innovative application of high and new technologies. Smartness of ports can also be traced back to technology-driven automation and should be an integrated and coordinated system composed of knowledgeable and skilled work, intelligent infrastructure, automation, optimized port operations, enhanced productivity, energy efficiency, safety, and sustainability (J. Gao et al., 2022; Molavi et al., 2020b).

In this context, **five ports generation** may be distinguished by Yau et al. (2020):

First-generation ports were nodal points between sea and land and served as loading and unloading points for goods. *Second-generation* ports deployed equipment and infrastructures to reduce manpower dependency. *The third generation* provided value-added services such as warehousing, packaging, and distribution. *Fourth-generation* ports networked the physically separate ports. *Fifth-generation* ports, which are the latest version of ports, that provide services such as vessel and container management, are technology-driven by ICT and automation, connected, and integrated with the entire supply chain, and pursue sustainability goals. Jović et al., (2019) the transition process of ports towards smartness needs the mutual interest of governments and stakeholders.

In conclusion, it is quite evident from the above description that ports have evolved; indeed, traditional ports were just cargo loading and unloading terminals, and industrial ports were ports equipped with more advanced handling means, whereas smart ports are logistic nodes in which technologies have shifted the business into a service (Philipp, 2020a). The key driver of this transformation is technological evolution, as explained in the next section. Some technologies are mature enough for implementation, and some are at the research and development stage. However, a unified definition is still under

development, but the smart port concept revolves around the Key Performance Indicators (KPIs) described in Sect. 5.

4 Technologies for Smart Port

This section first synthesizes different technologies that may be implemented in a commercial port, then proposes an overview of the most significant case studies in which such technologies have been implemented. Finally, their effectiveness has been evaluated, followed by a discussion where various factors are examined for the successful implementation of technologies in the port industry.

4.1 Sensors, Internet of Things (IoT), and Digital Twins

Sensors are part of IoT-embedded systems that collect data such as temperature, and humidity, and structural health monitoring (SHM) for metal structures (Mi & Liu, 2020). Actuators work on the contrary, they take user input and trigger the system for action. Internet of Things, which consists of sensors, actuators, and embedded systems, is the foundation of smart ports (Bouhlal et al., 2022). Interconnection provides an excellent information-sharing platform among heterogeneous infrastructure and equipment. Digital twins in the port sector can be defined as a real virtual representation of a real scenario, which includes the actual layout of the system, design characteristics, and other relevant parameters. Cyber-physical systems and digital twins, integrated with IoT-embedded systems, could be used for the emulation or port operation for evaluation, prediction, and optimization of port systems (Rudskoy et al., 2021). Digital twin-based Q-learning algorithms are used to optimize the path planning for AGVs (Gao et al., 2022). The digital model is set with the desired algorithms; it generates instructions through fitted actuators to trigger the physical system, which is subjected to human intervention. Szpytko & Salgado Duarte, (2021) presented a model capable of organizing the maintenance scheduling strategy in the container terminal. Researchers such as Lind et al. (2020), Kirchhof et al. (2021), Y. Zhou et al. (2022), Wang et al. (2021), and Skuba & Janota. (2020) also studied digital twins for ports.

4.2 Information and Communication Technologies (ICTs) and 5G

ICTs can reduce the delay due to documentation and enhance transparency and trust (Kapkaeva et al., 2021). The IT-supported system uses modern technologies for efficient information flow throughout the entire transport supply chain. Information systems consist of data acquisition devices, data centers, and networking and communication (Yau et al., 2020). 5G technology is 100 times faster than 4G, this quick transition of data leads to lower power consumption and provides support for IoT. Sohaib et al. (2021) highlighted automated rail-mounted gantry cranes that have recently been deployed at Singapore's Pasir Panjang Terminal 5, where cranes can stack containers 6 high and 10 broads. Up to five cranes may be under the control of one operator from the control room. These cranes increase production by over 10% by moving more than 30 containers per hour; improved safety is a side benefit of the increase in production.

4.3 Artificial Intelligence (AI)

Artificial intelligence is used for programming machines to replicate and imitate human decision-making and monitoring processes. AI, through machine learning, uses big data to predict the future scenarios of operations and logistic chains. AI is used for the estimated time of arrival (ETA), and the average reliability of a global carrier arriving on time across 34 different trade lines fell to 50.1% ('Report Sea-Intelligence', 2020). da Silva et al. (2023) used a machine learning algorithm to study dynamic scheduling for the Truck Appointment System (TAS) at the gate, achieving 95% accuracy, a 90.4% improvement in truck waiting time, and an 80% reduction in the entrance queue.

4.4 Blockchain

Blockchain-based applications provide transparent visibility of information to involved parties to build trust reduce interdependency and reduce the chance of fraud and tampering inside the chain by disintermediating the traditional chain and enhancing end-to-end process visibility. Giant corporations such as MAERSK and IBM applied blockchain technology by introducing TRADELENS, which involves broader supply chain insight, not limited to shipping activity (Kapnissis et al., 2022). It is applicable to document exchange, cargo tracking, and tracing. Paperwork in the shipping industry is responsible for 15%–50% of transportation costs. Blockchain technology can replace those hassles by providing a paperless environment (Yau et al., 2020).

4.5 Computer Vision Application for Container Identification

For administration in terminals, yards, and customs, serial numbers are the fundamental information about containers. Computer vision can be used to automatically recognize a container's number and collect this data as part of automatic real-time logistics, resolving the crucial problem of automated container management as it is practiced in several Chinese ports (Yang et al., 2018).

4.6 Automation

The primary drivers for port automation are enhancements in operational effectiveness, reduction in the per container handling cost, the shift from labor to capital costs, increased land productivity, increased environmental sustainability, safety, and security, and application of cutting-edge technology (Rodrigue & Notteboom, 2021). Shanghai Yangshan Port Phase IV is a fully automatic port except few operations (Luo, 2019).

4.7 Cyber Security of Smart Ports

Interconnected physical systems with digital technology in cyberspheres leave crucial security risks; thus, a cyber security plan is an essential component of smart ports (Yau et al., 2020). Cybersecurity skill shortages in ports are one of the critical vulnerabilities for cyber attackers. Data infrastructure needs a concrete security architecture in the port support system. Cybercriminals may target data-rich integrated electronic platforms,

such as systems related to Maritime Single Windows (MSW) and Port Community Systems (PCS) (Tusher et al., 2022). New methods of hardware hacking in barcode scanners and other equipment are utilized to launch cyber-criminal activities in port operations, in addition to security flaws in radio transmission and software. Integrated systems of devices, agents, and activities and a holistic ecosystem of connectivity inside smart ports have raised the cyber risk (de la Peña Zarzuelo, 2021).

4.8 Technology Use-Success Examples

Technology is practiced in many ports around the world. The Valencia port uses an LED lighting system, and 73% less electricity consumption is recorded since devices only illuminate when vehicles are nearby (Valencia port). Port of Rotterdam (Digital Report) showed digitalization of customs documents reduced processing time by 30%, and the OnTrack application resulted in a more accurate Expected Time of Arrival (ETA) of ships, which is a major issue for terminal operators. Port of Gdynia, Poland uses the navigation tool developed by NavSim (Navigation). Port of Gothenburg utilizes a bunkering App that synchronizes the bunkering data, which is incredibly useful for operators to plan and execute bunkering operations (Bunkering App). Port of Antwerp uses sensors to measure the tension on the bollard (Port of Antwerp), the Port in 2017 installed devices, called iNose for measuring and monitoring the air composition (Port of Antwerp-Bruges). In addition, Limas et al. (2022) in their case study on the Port of Balikpapan found that minimal technology use in ports causes inefficient operations. Triska et al., (2019) studied smart port-hinterland integration using 5 Brazilian ports, substantiating that smart port logistics systems enhance the reliability and efficiency of port-hinterland integration, minimizing disruption throughout the supply chain. It contributed to a reduction of at least 78% in the truck queues at the analyzed ports. Llaha & Rista (2021) recommended implementing Vessel Traffic Service (VTS) and Vessel Traffic Management Information Service (VTMIS) systems as the "Single Window" with the help of blockchain and IoT, establishing a communication hub among stakeholders in Albanian ports. Ortiz et al. (2022) worked on an IoT microservice architecture for air quality monitoring and alerting in smart ports. Jin, (2023) suggests a selection of virtual team members for smart port development projects. Jun et al. (2018) used a combination of Delphi surveys and input-output analysis to evaluate the impact of the smart port industry on the Korean economy, and a field survey was carried out. Jović et al. (2019) studied ICTs for port efficiency. Rüßmann et al. (2015) summarized nine technological advancements in industry that paved the foundation for further research and development. To summarize the analysis performed in Sect. 4, various technologies explored by the authors have been clustered. However, some technologies have proven success (i.e., automation and ICTs) and few (i.e., augmented reality and blockchain) are at an infant stage for industry use (Table 2).

Table 2. Technologies explored by various authors.

Area	Authors
Internet of things (IoT)	Rüßmann et al. (2015), Li et al. (2023), Muñuzuri et al. (2020), Bouhlal et al. (2022), J. Gao et al. (2022)
Artificial intelligence	Rüßmann et al. (2015), de la Peña Zarzuelo et al. (2020), da Silva et al. (2023)
Automation	Li et al. (2023), Rodrigue & Notteboom (2021), Luo (2019), Zhao et al. (2021), Rüßmann et al. (2015)
Cyber security	Rüßmann et al. (2015), de la Peña Zarzuelo et al. (2020), Li et al. (2023), Yau et al. (2020)
Bigdata	Li et al. (2023), Rüßmann et al. (2015)
Simulation modeling	Rüßmann et al. (2015), de la Peña Zarzuelo et al. (2020)
ICTs	Molavi et al. (2020), Yau et al. (2020), Kapkaeva et al. (2021), Yang et al. (2018)
Additive manufacturing	Li et al. (2023)
Blockchain	Kapnissis et al. (2022), Yau et al. (2020), de la Peña Zarzuelo et al. (2020)
Digital twins	Szpytko & Salgado Duarte (2021), Wang et al. (2021), Szpytko & Salgado Duarte (2021), Lind et al. (2020), Kirchhof et al. (2021), Skuba & Janota (2020), Y. Zhou et al. (2022), Y. Gao et al. (2022), Rudskoy et al. (2021)
Machine vision	Yang et al. (2018)
5G	Sohaib et al. (2021)

5 Key Performance Metrics

In addition to technological aspects, another important part of the literature is devoted to key performance indicators. Successful implementation of technology is a primary pillar of "smart ports". An important reference is the "Port Performance Measurement," derived from the "United Nations Conference on Trade and Development" (UNCTAD-1976), from where the Port Performance Indicators originated (Philipp, 2020a). Traditionally, Port Performance Indices were mainly focused on operational efficiency and the annual throughput. However, the recent digitization revolution added novel indicators (Ha et al., 2019). Due to the rising interest in digitalization, the recent Port Performance Measurement (PPM) concept exhibits novel indicators like IT systems, databases, networks, integrated Electronic Data Interchange (EDI) for communication, and integrated IT to share data. Smart Port Indicators (SPIs), derived from Port Performance Metrics, refer to measuring tools that indicate port performance in terms of several operational, environmental, energy, security, functional, and social domains. Numerous research efforts have been conducted to assess smart ports from one or more perspectives. Iris & Lam (2019) indicate the ecological environment such as energy consumption, renewable energy, and water pollution, as primary parameters for smart ports. According to Gunes et al.

(2021), technological environments such as digital transformation, cyber security, and operation infrastructure are smart port indicators. Policy environments such as port-city integration, policy support, and cooperation with government departments are studied by D'amico et al. (2021). The education level of the workforce, logistic services, and production management were discussed by Meyer et al. (2021). Philipp (2020b) established a readiness index assessment for smart port development. Table 3 summarizes key authors who specifically studied Key Performance Indices of smart ports clustered by domains.

Table 3. Authors contributions in key performance domains and metrics

Domains	Indicators	Authors
Operational	Agility & Resilience and Operational efficiency	Molavi et al. (2020), Chen et al. (2019), Bichou & Gray (2004), Li et al. (2023)
Energy	Consumption	Iris & Lam (2019), Battino & del Mar Muñoz Leonisio (2022),(Gervasi et al. (2022)
Ecological Environmental	Water	Iris & Lams, (2019), Molavi et al. (2020), Battino & del Mar Muñoz Leonisio (2022), Gervasi et al. (2022)
Technological Environment	Cyber security, Operational infrastructure	Gunes et al. (2021), Philipp (2020b), Ha et al. (2019), Chen et al. (2019), Du et al. (2023)
Policy Environment	Port-city integration; Policy support, Collaboration with environment department	D'amico et al. (2021)
Education & Training	Workforce education	Meyer et al. (2021)
Logistic Services		Meyer et al. (2021), Chen et al. (2019),
Management	Productional management, Crew, and Customer satisfaction	Meyer et al. (2021), Belmoukari et al. (2023b), Li et al. (2023)
Safety and Security		Molavi et al. (2020), Battino & del Mar Muñoz Leonisio (2022), Chen et al. (2019)
Socioeconomics	Quality of life for citizen	Battino & del Mar Muñoz Leonisio (2022), Gervasi et al. (2022), Chen, Xue, et al. (2019)

Molavi et al. (2020) assessed port performance indicators in five aspects: operation, environment, energy, safety, and security. According to D. Zhou et al. (2022), the indicators are mainly composed of eight categories: market, technology, production,

finance, service, manpower, and safety production supervision and inspection. Chen, Xue, et al. (2019) categorize the smart port evaluation indicators in the following major domains: port production and operation system, port financial, port logistic supply chain system and trade service technologies, port energy conservation, and emission reduction capacities. Makkawan and Muangpan (2021) identified the SPIs and developed a conceptual model of port performance using the subject of Thailand's Eastern Economic Corridor (EEC) in 29 indicators. Lakhmas & Sedqui (2020) and Maglić et al. (2021) surveyed 78 marinas to understand their level of smartness using KPIs. The Port of Hamburg and Singapore are good examples of ports as smart, developing economic, social, and environmental improvement (Rajabi et al., 2019). Hsu et al. (2023) studied the service quality of smart ports' key factors for success during the post-pandemic era, SERVQUAL service quality scale 25 evaluation indicators. Jun et al. (2018) studied the impact of the smart port industry on the Korean national economy using input-output analysis. Chen et al. (2019) applied a single-valued neutrosophic exponential similarity measure to enable quantitative evaluation of port integrity for setting smart port KPI. Wu et al. (2010) analyzed the model to test the sensitivity of the individual input and output of a decision-making unit (DMU), results indicated the number of berths, investments, and location of the container terminal are fundamental for performance. Campisi et al. (2022) in their case study on the port of Ravenna, Italy, stressed a locally integrated partnership framework. Botti et al. (2017) studied Salerno port and found port as a smart service system through the lens of service science.

Pham (2023) studied the indicators, and challenges of smart port development. Li et al. (2023) studied available publications on smart ports from 2002 to 2021. However, the actual research on smart ports began after 2010. Studies and reports indicate that the primary driver of smart port evaluation is the increasing involvement of technology. However, as described in Sect. 4, numerous factors guarantee the successful implementation of technology in the port.

In conclusion, Key Performance Indicators are not just a measure of port efficiency but a strategic move that leads to optimization of operations, sustainability, and maritime logistics enhancement. Technology implementation is a crucial figure in performance indicators, but it's not the whole picture of performance. Interestingly, KPIs can be defined in a customized way; a parameter that is crucial for one port may not be for another. A port can achieve a maximum level of its own set of KPIs, but in this case, significant metrics such as sustainability cannot be ignored. Finally, all the above-described KPIs serve the port to gauge their level of smartness, guiding the port industry towards resilience and innovation.

6 Discussion and Conclusion

Maritime ports are crucial actors in the global economy. However, associated environmental, operational, social, and safety concerns in the port industry have gained prominence in recent years. These challenges made the terminal operators and authorities rethink on operational design of the port. Therefore, the smart port concept emerged. This research revealed the emerging trend of smart port research, a shoot-up in publication has been observed in recent years (2021–2023) uniformly distributed throughout

the globe. Maritime Policy & Management, Journal of Marine Science and Engineering, and Sustainability were the top three journals with 4, 3, and 3 publications respectively. Smart port(s) was the most used keyword in literature, followed by digital transformation and the Internet of Things.

The growth and success of a smart port depend on several factors, most of them not depending on the technologies but on where, how, and when they are implemented and integrated. However, some indications explained in Sect. 5 highlight the key success elements that enable the growth of smart ports. Philipp (2020a) studied the readiness of port smartness, concluding that the current strategic position and benchmarking the measurement induces are dominant factors. Only innovative technologies do not safeguard digital transformation, but management measures, knowledge, and skills play important roles. Heilig et al. (2017) highlighted the role of digital transformation in ports since it will make it possible to inter-, intra-, and meta-organizational dimensions, but pointed out that digital initiatives cannot succeed in obtaining their purpose if the customized requirements of individual actors are not properly addressed in seaports. According to Castellano et al. (2019), Investments in Digital communication Technologies (DCTs), asset efficiency monitoring (DEA), and port competitiveness improvement are three crucial success elements that enable the growth of creative smart ports as *The Port of the Future*. Finally, it has been widely demonstrated the need to invest massively in digital data-based technologies should be extended to the whole logistic chain and, thus, also to smaller ports that are often either reluctant or limited in their knowledge (Philipp, 2020a). In these streams, digital transformation is fundamental for the strategic alignment and cooperation among stakeholders. However, it is the attitude, management skills, stakeholders' motivation, and vision that guarantee the success of digital transformation.

In conclusion, the recent development and multidisciplinary nature of the smart port research needs greater exploring, meanwhile, it makes this area very interesting for further investigations. Our analysis delved into smart port definition and evolution. Findings suggest that smart port definition is still under development due to technological evolution but a set of KPIs helps to figure out the concept. Technology plays an important role in ports' transformation from traditional terminals to smart ports. However, the growth and the success of a smart port rely on numerous factors, most of them not depending on the technologies, but on where, how, and when they are implemented and integrated. Some successful examples of European ports (i.e., Port of Antwerp, Rotterdam, and Hamburg) have shown very positive results such as minimizing custom processing by 30% in Rotterdam and Port of Valencia reducing energy consumption by 78% after installing light systems sensors. One of the important areas of smart ports explored in this study is the Key Performance Indicator (KPIs). These indices refer to measuring tools that indicate port performance in terms of several operational, environmental, energy, security, functional, and social domains. KPIs are very useful sets of metric ports that can be used to gauge their level of smartness, not only economic, and operational boost but enhancement in whole port logistics and sustainability.

This research insights into the useful understanding of smart ports definition, feasible technology, use-cases, factors for successful implementation, and KPIs to gauge the level of smartness.

Practical applications of smart port measures still lacking in medium and small-size ports around the world. A study that evaluates the challenges and barriers terminal operators face in implementing these measures is worth exploring.

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Theoretical and Computational Chemistry and its Applications (TC-CMA 2024)

A Computational Analysis of the DMSO-Water Interaction: Toward the Implementation of an Accurate Force Field

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Abstract. Molecular dynamics (MD) simulations represent an essential tool for the investigation of the chemical and physical properties of a large variety of systems, with a plethora of possible applications ranging from medicine to the development of new nanomaterials for energy purposes and carbon neutrality. The implementation of an accurate force field represents a key step in the overall theoretical analysis, allowing a correct representation of all the non-covalent interactions in the target system. The Improved Lennard-Jones potential (ILJ), developed to have a better representation of van der Waals interactions, represents a feasible methodology for the implementation of accurate force fields. The validity of the proposed methodology has been assessed by performing a theoretical investigation considering a mixture of dimethyl sulfoxide (DMSO) in water, which represents a strong cryoprotecting agent for biological samples. The ease of implementation and the low computational cost makes ILJ an excellent technique for the analysis of non-covalent interactions and the production of accurate MD force fields.

Keywords: Molecular Dynamics · Force Field · Improved Lennard-Jones

1 Introduction

Molecular dynamics represents a powerful tool in order to model the structure and predict properties of big systems which are difficult, or even impossible, to study through accurate ab initio investigations and/or experimental analysis. Molecular dynamics (MD) simulations allow to predict the position of the different atoms in a system as a function of time, by calculating the forces applied

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O. Gervasi et al. (Eds.): ICCSA 2024 Workshops, LNCS 14823, pp. 361–374, 2024.
https://doi.org/10.1007/978-3-031-65329-2_24

using simple formulations based on Newton's laws of motion. For this reason, MD simulations are widely spread in a variety of different fields, ranging from molecular biology and medicine to nanomaterials for energy and carbon neutrality. A clear example is represented by graphene, a carbo-nanostructure composed of a single atomic layer organized in an hexagonal lattice structure. In the last years, MD simulations unveiled the importance of graphene and graphene-like structures (such as carbon nanotubes and γ-graphynes) as possible precursors for the design of materials able to capture and selectively adsorb small molecules, including carbon dioxide and methane [1–4].

One of the main challenges in molecular dynamics simulations is represented by the implementation of a force field, which must be able to correctly reproduce the interactions of the systems under investigation. Force fields are a variety of interatomic potentials. More precisely, the force field refers to the functional form and parameter sets used to calculate the potential energy of a system at the atomistic level. The parameters for a chosen energy function may be derived from classical laboratory experiment data, calculations in quantum mechanics, or both. Force fields utilize the same concept as force fields in classical physics, with the main difference that the force field parameters in the MD simulations describe the energy landscape on the atomistic level. From a force field, the acting forces on every particle are derived as a gradient of the potential energy with respect to the particle coordinates. Typically, a MD force field, which is necessary to treat non-covalent interactions, is composed by two main components: the electrostatic (Coulombic) contribution between atoms and the non-electrostatic one. One of the most challenging task in developing accurate force fields is represented by the correct modeling of intermolecular interactions (non electrostatic contribution), in particular the van der Waals component, which is always present and plays a pivotal role in the overall dynamics.

From the non-electrostatic part, a new formulation of the classical Lennard-Jones (LJ) potential has been provided in the last years in order to have a better representation of both long-range attraction and short-range repulsion in the analysis of non-covalent interaction. The so called Improved Lennard-Jones (ILJ) [5] potential represents, indeed, an extension of the previously mentioned LJ treatment, formulated considering additional parameters which can be easily calculated on the basis of atomic and molecular properties (such as dipole moment and polarizability) [6]. Different investigations have been performed to assess the viability of the ILJ formulation and to check the correctness of the predicted results, considering the outcomes coming from both high level ab initio calculations and experimental investigations, performed through molecular beams scattering techniques [7,8].

The excellent agreement between theoretical predictions and experimental results confirmed the accuracy of the new implementation. Recently, the same formulation has been used to characterize the nature of the initial interaction between the reactants of gas phase bimolecular reactions [9,10]. The remarkable results obtained helped to clarify the reaction micro-mechanism and allowed a better understanding of how long-range non-covalent interactions drive the

chemical reactivity. The use of simple formulations, such as the semiempirical ILJ model, allowed to obtain values of rate constants in agreement with the experimental results, showing how the method is portable and can be easily adapted to different cases.

In the present contributon, the ILJ model has been used to develop an accurate preliminary force field to run MD simulations in order to characterize the interaction of dimethyl sulfoxide (DMSO, CH_3SOCH_3) in water, with pivotal applications in the field of medicine and biology [11–14]. Dimethyl sulfoxide is, indeed, a key species in medicinal chemistry and biology and shows a strong pharmacological potential. In the last decades, CH_3SOCH_3 showed important features in different fields, including analgesia, but also as possible anti-viral and anti-bacterial agent. It is also considered important in the field of anti-inflammatory and radioprotection. Together as a possible agent for the increasing of membrane permeability [15,16, & references therein], DMSO is considered an important cryoprotectant. The extreme drop in the freezing point of solutions of DMSO in water, leads to a very efficient action of dimetyl sulfoxide to preserve biological samples in extreme conditions, such as very low temperatures, increasing the possibility of survival of cryoconserved cells. Despite the strong effect of DMSO in the field has been extensively investigated, the main mechanism of action is still lacking. For this reason, different investigations have been already performed, both through experimental analysis and molecular dynamic simulations [15,17–23].

The present work is focused in order to implement an accurate preliminary force field using the Improved Lennard-Jones potential to describe the intermolecular interactions to run MD simulation of DMSO-water mixtures. Here, we will present, only, the Force Field.

2 Theoretical Methods

The preliminary force field to be used in molecular dynamics (MD) simulations, has been built considering a global potential (V_{tot}) composed of two main contributions: a first term representing the electrostatic potential (V_{elec}) and a second term (V_{nelec}), accounting for the non-electrostatic contribution of the interaction. The electrostatic contribution has been evaluated considering the atomic charges of the two interacting molecules, as expressed by the Coulomb laws. The non-electrostatic contribution has been defined exploiting proposed semi-empirical potential (ILJ), described in the next sections.

2.1 Electronic Structure Calculations

In details, an initial geometry optimization on the two separated molecules has been performed at the DFT level, using the B3LYP functional [24,25] in conjunction with the correlation consistent valence polarized set aug-cc-pVTZ [26–28]. Previous works on reactions involving small organic/inorganic molecules

showed the robustness and affordability of the functional for geometry optimizations [29–31]. Harmonic vibrational frequencies calculations have been performed at the same level of theory, in order to check the accuracy of the optimized molecules, i.e. a minimum shows all real frequencies. Finally, the optimized geometry has been used to evaluate the electrostatic potential atomic charges (ESP). In this regard, a benchmark analysis has been performed considering the same B3LYP functional and different basis sets: the Pople basis sets 6-31 G and 6-311++G(d,p) and four difference correlation consistent valence polarized sets aug-cc-pVDZ, aug-cc-pVTZ, aug-cc-pVQZ and aug-cc-pV5Z. All the calculations have been performed using GAUSSIAN09 [32] while the analysis of the molecular structures has been carried out using Avogadro [33].

2.2 Potential Energy Surface to Describe the Intermolecular Interactions

The intermolecular forces of interest in this work are those occurred between H_2O molecules pair and between the H_2O and the DMSO. For each pair, the total intermolecular interaction energy component is further decomposed in terms of molecule-molecule pair contribution, which are non-electrostatic and electrostatic contributions.

$$V_{tot}(r) = V_{nelec} + V_{elec} \tag{1}$$

The non-electrostatic contribution (V_{nelec}) is measured by taking into consideration the strength of induced dipoles attraction and the average molecular sizes repulsion. This can be done by assigning a value of polarizability to both interacting centers. On the other hand, the electrostatic contribution (V_{elec}) is evaluated by employing the Coulomb's law.

The non electrostatic contribution has been then evaluated considering the previously mentioned Improved Lennard-Jones (ILJ) model [5,34–37].

In details, (V_{nelec}) is considered as a sum of pairwise ILJ potential energy functions, formulated as:

$$V_{nelec} = V_{ILJ} = \varepsilon \left[\frac{m}{n(r) - m} \left(\frac{r_m}{r} \right)^{n(r)} - \frac{n(r)}{n(r) - m} \left(\frac{r_m}{r} \right)^{m} \right] \tag{2}$$

where ε and r_m represents the well depth and its location, respectively, while m assumes the value of 6 for neutral-neutral systems and 4 in the case of ion-neutral interactions. The values are estimated on the basis of the value of the polarizability, evaluated considering each interaction center at a certain distance r. The term $n(r)$ shows a dependence on the distance r, defined as:

$$n(r) = \beta + 4 \left(\frac{r}{r_m} \right)^2 \tag{3}$$

where the β parameter represents the hardness of the two interacting fragments and can be properly modulated. This newly introduced parameter is what makes ILJ potential (Eq. 3) able to indirectly take into account some effects of

atom clustering, induction and charge transfer and to improve the Lennard-Jones function at asymptotic regions. Nevertheless, while ILJ improves the description of the present system, other effects should be included in the intermolecular potential for enhancing the model of the system.

3 Results

Geometry Optimization

As reported in the previous section, the geometry of the two interacting molecules has been optimized through density functional theory calculations. In Fig. 1 are reported the main geometrical parameters obtained for dimethyl sulfoxide and water at the B3LYP/aug-cc-pVTZ level of theory. As already seen in several cases before, the use of the B3LYP functional, in conjunction with the aug-cc-pVTZ basis set, represents a good compromise between computational cost and chemical accuracy [38]. The same level of theory has been used for geometry optimization and frequencies calculations in several works [39–41].

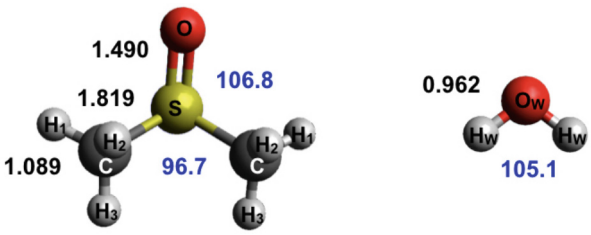

Fig. 1. Structural details of the molecular models of water and DMSO system. The optimized structure of the dimethyl sulfoxde and water molecules have been obtained at the B3LYP/aug-cc-pVTZ level of theory. In this figure appears labeled the different pair centers for the potential interaction.

In order to check the validity of the present calculations, the obtained data have been compared with standard reference values present in the NIST chemistry database [42]. The comparison is reported in Table 1.

As can be seen from the data reported in Table 1, the values of bond distances obtained at the B3LYP/aug-cc-pVTZ level are in very good agreement with the ones reported in the NIST database, being the differences negligible. The maximum deviation is, indeed, represented by the C-S bond, which differs from the reference in 0.02 $\mathring{A}$. As a consequence, the present level of calculation can be considered a good compromise between chemical accuracy and computational cost.

Table 1. Comparison between bond distances (in Å) and angles (in degrees) derived through DFT calculations and values present in the NIST database.

Bond Distance	B3LYP/aug-cc-pVTZ	NIST
C-H	1.089	1.092
C-S	1.819	1.799
S-O	1.490	1.485
O_W-H_W	0.962	0.958
Angles		
O_W-O_W-H_W	105.1	104.5
C-S-C	96.7	96.56
O-S-C	106.8	106.65

Atomic Charges Analysis

ElectroStatic Potential atomic charges (ESP) have been calculated at the DFT level, using the B3LYP functional and considering different basis sets, in order to identify the one which allows a better analysis and a correct representation of the dipole moment and polarizability values, which are essential for the derivation of the Improved Lennard-Jones parameters. The data obtained for the six different cases are reported in Table 2, where H_1, H_2 and H_3 are referred to the three hydrogen atoms of each methyl group, while the atoms of the water molecule are labelled as O_W and H_W (see Fig. 1).

Table 2. Atomic charges (in a.u.) obtained for the H_2O and DMSO molecules, evaluated at different levels of theory (see text for details).

Atom	6-31G	6-311+ +G(d,p)	aug-cc -pVDZ	aug-cc -pVTZ	aug-cc -pVQZ	aug-cc -PV5Z
C	−0.406	−0.465	−0.493	−0.463	−0.458	−0.456
H_1	0.151	0.158	0.170	0.160	0.158	0.158
H_2	0.180	0.195	0.205	0.195	0.193	0.192
H_3	0.164	0.187	0.195	0.186	0.184	0.183
S	0.280	0.323	0.293	0.274	0.268	0.261
O	−0.482	−0.473	−0.446	−0.431	−0.424	−0.417
O_W	−0.887	−0.800	−0.679	−0.683	−0.683	−0.683
H_W	0.444	0.400	0.339	0.341	0.341	0.342

The values of atomic charges obtained are then used to analyse the contribution of the dipole moment (μ) and polarizability (α) of the two interacting

molecules. In Table 3 are reported the values of μ and α obtained during the analysis. Atomic charges and molecular polarizabilities have been obtained through frequancies calculations, performed at the B3LYP/aug-cc-pVTZ level of theory.

Table 3. Dypole moment (in Debye) and molecular polarizability (in $Å^3$) obtained for the H_2O and DMSO molecules, evaluated at different levels of theory (see text for details).

Molecule		6-31G	6-311+ +G(d,p)	aug-cc -pVDZ	aug-cc -pVTZ	aug-cc -pVQZ	aug-cc -PV5Z	NIST
DMSO	μ (D)	4.918	4.403	4.318	4.125	4.062	4.011	3.960
	$\alpha(Å^3)$	6.619	7.602	8.252	8.126	8.094	8.067	7.969
H_2O	μ (D)	2.398	2.187	1.852	1.847	1.847	1.847	1.857
	$\alpha(Å^3)$	0.674	1.068	1.403	1.453	1.471	1.478	1.501

As can be seen from the data reported in Tables 2 and 3, the values calculated with the correlation consistent valence polarized basis sets provide a better description of the physical quantities (charges, dipole, and polarizability) with respect to the Pople basis sets. In particular, also in this case, the best compromise between accuracy of the results and computational cost is represented by the use of the triple zeta (aug-cc-pVTZ) basis set. Therefore, the data reported in column 5 of Table 2, can be used for the generation of the force field necessary to run MD calculations. The values of ESP atomic charges appear to be quite similar to those obtained by Stachura et al. [17], through the use of the AMBER force field [43].

Preliminary Force Field Atomic charges for the two interacting molecules have been calculated, allowing a correct representation of the dipole and/or quadrupole moments of the molecules in the gas phase, in accordance with the values calculated through ab initio calculations (reported in Sect. 3). In Fig. 2, are reported the final parameters of DMSO and water, together with the ESP charges to be used to model the electrostatic part of the MD force field.

The Improved Lennard-Jones potential is formulated considering the atomic and molecular polarizabilities. The ε and r_m parameters are indeed calculated on the basis of correlation formulas, which relates the values of the polarizability (α) and dipole moment (μ) of the interacting species with the main features of the potential. As a consequence, the derived parameters show a high level of portability, allowing to easily pass from a system to another. The validity of the ILJ model has been assessed considering the comparison with theoretical predictions (obtained through high level ab initio calculations) and experimental analysis, for different systems [5]. An additional advantage of the formulation is represented by the possibility to study complex systems, by simply decomposing the main molecular structure in different moieties, which are representative of

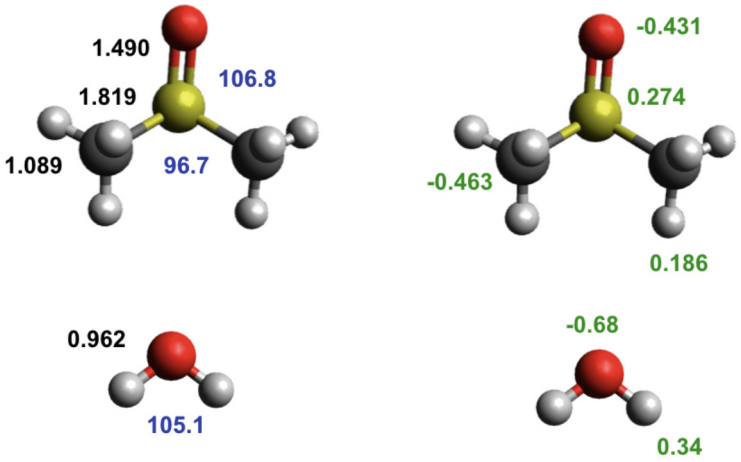

Fig. 2. Final parameters used to derive the MD Force Field. Left panel: bond lenght (in black, in Å) and angles (in blue, in degrees). Right panel: ESP charges (in green, in a.u.). All the data have been calculated at the B3LYP/aug-cc-pVTZ level of theory (Color figure online)

the interaction centers, allowing a relatively simple formulation also in the case of big interacting systems. In Table 4 are reported the ILJ parameters (in the form of ε and r_m) for the interaction of dimethyl sulfoxide with water. In details, in the case of DMSO, the methyl group has been considered as an "effective" carbon atom, which has the mass and the polarizability of a CH_3 moiety. Similarly, the interaction with the water molecules has been formulated considering only one center, represented by the O atom, reported as O_W [44].

Table 4. List of the parameters (ε and r_m) used for the representation of each interacting pair in the ILJ formulation

Interacting Centers	ε (meV)	$r_m(\AA)$
C-O_W	9.881	3.908
S-O_W	10.914	3.921
O-O_W	7.577	3.640
O_W-O_W	9.060	3.730

Usually, the β parameter is considered to be in the interval 8.5 ± 2.5 and can be properly modulated considering the fluctuations of V_{elec}. Moreover, the same parameter can be used to compensate and include the role of other different contributions which are less important and are not directly included in the formulation, such as other additive terms of the interaction at long distances which are indirectly included. Due to the relative role played by β and the dipole

moment (μ), the specific values selected for β can depend on the selected value of μ [45]. In fact, small modifications of β can be compensated by varying μ. Due to this fact, in the present paper we have analized the modulation of the β parameter as a function of various charge distributions assigned to the water molecules. The modulation of β can also partially compensate the case of different representations of the charge distributions and indirectly include other less important interaction effects at intermediate and short distances [45].

3.1 Ab Initio Calculations for the Initial Geometry

Finally, in order to have a clear idea of the initial configuration of the system, necessary to run the MD simulations, the geometry of the two interacting fragments has been preliminary optimized through DFT calculations, performed at the B3LYP/aug-cc-pVTZ level of theory. Two different cases have been considered, composed of one DMSO molecule interacting with one and two water molecules, respectively. The optimized geometry obtained for the two cases are reported in Figs. 3 and 4.

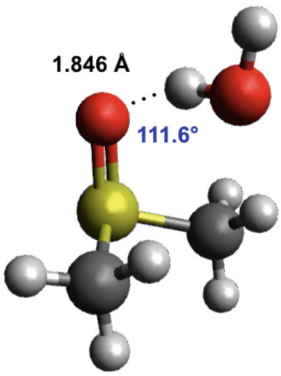

Fig. 3. Optimized geometry for the DMSO-H_2O interacting system obtained at the B3LYP/aug-cc-pVTZ level of theory

As can be seen from the structure reported, the interaction of DMSO with a water molecule is driven by the formation of an hydrogen bond between the oxygen atom of the DMSO and one of the two hydrogen atoms of the H_2O molecule. The related O-H bond distance is equal to 1.846 $\mathring{A}$ and the S-O-H angle is equal to 111.6°C. The inclusion of a second water molecule leads to the formation of a new H-bond interaction. In this case the two O-H bond distances appears to be slightly increased (reaching values of 1.898 $\mathring{A}$ and 1.875 $\mathring{A}$, respectively), while the H-O-H angle assumes a value of 106.4°C. As expected, the introduction of water molecules leads to the formation of strong H-bonds, considering the nature of the atoms in the system. This leads to a condition of

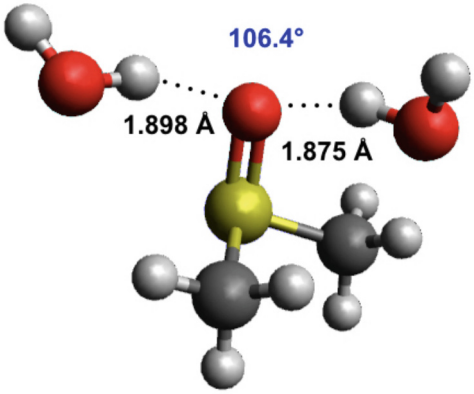

Fig. 4. Optimized geometry for the DMSO-2H_2O interacting system obtained at the B3LYP/aug-cc-pVTZ level of theory

solvation of the DMSO molecule, which can be properly analyzed through MD calculations. The main goal of the future works is investigate in a successive order the spatial solvation and structure and topological features in the different molar ratio mixture of dimethyl sulfoxide and water using the MD simulations. At this end, it is necessary an accurate force field that describes these interactions.

4 Conclusions

In the present contribution, a preliminary theoretical analysis has been performed in order to develop an accurate force field for the system composed of dimethyl sulfoxide in water analyzing the properties by classical MD simulations, with a plethora of possible applications, mainly in medicine and molecular biology. High-level ab initio calculations have been performed in order to assess the main geometrical parameters and evaluate the atomic charges, as well as dipole moment and polarizability for both DMSO and H_2O. The comparison between the obtained data and the standard reference, reported in the NIST database, shows very small differences, almost negligible. Therefore, according to the present results, the use of the B3LYP functional, already used for the analysis of several systems [10,39–41,46,47], in conjunction with the aug-cc-pVTZ basis set, represents the best compromise between chemical accuracy and computational cost. The non electrostatic component of the interaction, which accounts for the van der Waals long-range region of the potential energy surface has been evaluated using the semi-empirical Improved Lennard-Jones formulation, proposed to have a better representation of the forces ruling the potential at long distances. The combination of electrostatic and non electrostatic parameters allowed us to derive a new force field to be used in MD simulations, which will be the focus of a future investigation. Finally, ab initio calculations allowed to derive the optimized structure representing the initial configuration

for the system composed of a DMSO molecule interacting with one and two water molecules, respectively. Thanks to the portability of the formulation, once tested, the present methodology can be used for the development of accurate force fields, to model and derive properties of a new generation of carbon-based nanomaterials, particularly relevant for carbon neutrality applications. The work in progress is devoted to use the parameters in order to evaluate the total interaction contribution using the MD simulations to obtain the properties of the system we are studying.

Acknowledgements. This work has been funded by the European Union - NextGenerationEU under the Italian Ministry of University and Research (MUR) National Innovation Ecosystem grant ECS00000041 - VITALITY - CUP J97G22000170005. M. R and N. F-L acknowledge financial support under the National Recovery and Resilience Plan (NRRP), Mission 4, Component 2, Investment 1.1, Call for tender No. 104 published on 2.2.2022 by the Italian Ministry of University and Research (MUR), funded by the European Union - NextGenerationEU- Project Title 2022JC2Y93 ChemicalOrigins: linking the fossil composition of the Solar System with the chemistry of protoplanetary disks - CUP J53D23001600006 - Grant Assignment Decree No. 962 adopted on 30.06.2023 by the Italian Ministry of Ministry of University and Research (MUR).

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EDA-NCI: A Scientific Software to Investigate Non-covalent Interactions Combining Classical Dynamic Simulations and QM/MM Calculations

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Abstract. Simulations in biological environments such as proteins, DNA or lipids entail model systems that include a large number of atoms. Moreover, dynamic simulations, in which thermal effects are considered, sometimes require hundreds of thousands of calculations in order to reproduce a physicochemical process in a biological environment. Therefore, classical simulations based on widely parametrized force fields are employed instead of more accurate quantum methods, whose high computational requirements preclude their application. Disappointingly, although classical simulations could provide a proper sampling of the nuclear configurational space along a given process, they do not yield reliable microscopic information on the weight of different non-covalent interactions; namely, electrostatic, Pauli repulsion, induction (and charge transfer) and dispersion, in the total energy. This is mainly due to compensation of errors between different terms of the force field associated with the parametrization process, focused on getting good macroscopic properties instead of an accurate description of the interatomic interactions. As an alternative to classical and quantum methods, hybrid quantum mechanics/molecular mechanics schemes (QM/MM), where the target region is treated with a quantum method and the rest is represented by a classical force field, can be applied for large biological systems. These schemes combine the accuracy of quantum approaches and the small computational requirements of classical ones. In addition, a thorough analysis of intermolecular interactions can be carried out by means of an energy decomposition analysis (EDA), whose implementation within the framework of QM/MM schemes is known as QM/MM-EDA. In this paper, a methodology developed in our group to investigate intermolecular interactions, combining CMD simulations and a QM/MM energy decomposition analysis (QM/MM-EDA), and its implementation are presented. Finally, some applications to the study of ion solvation and membrane permeation processes are discussed.

Keywords: Non-covalent Interactions · Energy Decomposition Analysis · QM/MM · Molecular Dynamics

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O. Gervasi et al. (Eds.): ICCSA 2024 Workshops, LNCS 14823, pp. 375–386, 2024.
https://doi.org/10.1007/978-3-031-65329-2_25

1 Introduction

1.1 Classical Molecular Dynamics Simulations

Classical Molecular dynamics (CMD) simulations allow analyzing the behavior and evolution of a system (physical, chemical or biological) over time, calculating the forces between the atoms that make it up using the equations of Newton's motion [1–3]. Operationally, it is a method for generating the trajectories of a system composed of N particles by direct numerical integration of Newton's equations of motion, with specifications of an interatomic interaction potential of suitable initial and boundary conditions, also known as force field (FF). The functional form of a FF includes terms used to calculate the potential energy between atoms linked by covalent bonds (bonded terms) and between non-bonded atoms that represent the long-range electrostatic and van der Waals forces. Equation (1) represents the form of a typical polarizable FF used in CMD,

$$V\left(\mathrm{r^N}\right) = V_{bonded} + \sum_i \sum_j \left\{ \frac{q_i q_j}{R_{ij}} - \frac{1}{2} \frac{q_i \boldsymbol{\mu}_\mathrm{j} \mathrm{R_{ij}}}{R_{ij}^3} + 4\varepsilon_{ij} \left[\left(\frac{\sigma_{ij}}{R_{ij}} \right)^{12} - \left(\frac{\sigma_{ij}}{R_{ij}} \right)^{6} \right] \right\} \quad (1)$$

where the explicit form of the interatomic potential for covalently bonded atoms has been omitted since we are interested here in the non-covalent interactions. In Eq. (1), the first term included between braces corresponds to the electrostatic interactions between the atomic charges q_i and q_j separated by a distance R_{ij}, the second term is the polarization interaction between the atomic charges q_i and the induced atomic dipoles μ_j and the third term is the well-known Lennard-Jones potential, which accounts for dispersion and repulsion interatomic interactions. The Lennard-Jones parameters, ε_{ij} and σ_{ij}, as well as the atomic charges and the atomic electric polarizabilities used to calculate the induced atomic dipoles, are usually obtained from high-level quantum chemical calculations performed on simplified molecular models [4]. Simple point-charge based FFs have the same form but avoiding the second term of Eq. (1) corresponding to polarization interaction.

Different physicochemical properties of the system can be calculated by means of CMD, such as free energy, entropy, solubility, viscosity, pressure or phase change temperatures. In biological systems, it allows measuring the interaction strength between potential drugs and their biomolecular targets or receptors, and even describing the behavior of a protein and complex molecules under certain conditions. In addition, if, for example, the interaction of a drug with its receptor is analyzed, CMD makes it possible to observe conformational changes of the receptor and not only of the drug, which can yield crucial information for the design of new molecules for clinical use [5]. Another advantage is that it not only allows the simulation of the ligand-protein system, but it can also include the solvent that surrounds it (such as water), as well as possible ions present in the media, and allows the regulation of the temperature and pressure.

1.2 QM/MM Schemes

Unfortunately, the classical FFs employed in CMD simulations are sometimes not accurate enough to adequately represent the non-covalent interactions arising from non-bonded atoms, particularly dispersion and repulsion interactions. Therefore, more precise quantum chemical methods are required to describe, at least, the interaction region.

Since the computational requirements, in terms of time, memory or storage capacity, of quantum chemical methods are much higher than classical FFs, hybrid quantum/classical schemes, such as the popular QM/MM (Quantum Mechanics/Molecular Mechanics) methods, can be employed [6, 7]. The main idea behind QM/MM methods is the splitting of the system into two regions: the target and the surroundings, which are described at QM and MM levels of theory, respectively. Obviously, the QM region includes the most important part of the system, where the process takes place, whereas the MM region contains the remaining atoms. Therefore, the full Hamiltonian of the system gets separated into three parts: QM, MM and QM-MM, the latter accounting for the interactions at the interface between both regions. QM/MM methods can be grouped within two different schemes; additive [7] or subtractive [8]. In the additive scheme a term describing the interaction between the QM and MM regions is explicitly constructed, whereas in the subtractive scheme this term is avoided and the energy is calculated by combination of the energy obtained at MM level for the full system and the energies obtained at QM and MM levels for the QM region.

The methodology presented in this paper was developed to be applied in combination with additive QM/MM schemes, which are, by the way, the most widespread and accurate methods. The interaction at the interface between QM and MM regions can be represented using mechanical, electrostatic, polarizable or flexible boundary embedding schemes. The most employed embedding scheme is the electrostatic one due to its compromise between accuracy and computational cost [9, 10]. In an electrostatic embedding, the electrostatic potential created by the MM atomic charges (q) polarizes the QM region, however, the polarization of the MM region by the potential created by the QM region is not accounted for. Equation (2) represents the Hamiltonian terms corresponding to the QM-MM interaction in an electrostatic embedding, where subscripts i, k and j refer to MM atomic charges, electrons and nuclei of the QM region, respectively.

$$H^{elec}_{QM-MM} = -\sum_i \sum_k \frac{q_i}{|\mathrm{r}_{\boldsymbol{k}} - \mathrm{R_i}|} + \sum_i \sum_j \frac{q_i Z_j}{\mathrm{R_{ij}}} \tag{2}$$

In a polarizable embedding, the polarization of the MM region is also taken into account [11, 12]. Therefore, in addition to the electrostatic interaction with the MM atomic charges, the interaction of the electric potential of the QM region with the induced atomic dipole moments (μ) of the classical region is included in the Hamiltonian, so that the classical region must be described by a polarizable FF. Equation (3) represents the Hamiltonian terms corresponding to the QM-MM interaction in a polarizable embedding.

$$H^{pol}_{QM-MM} = -\sum_i \sum_k \frac{q_i}{|\mathrm{r}_{\boldsymbol{k}} - \mathrm{R_i}|} + \sum_i \sum_j \frac{q_i Z_j}{\mathrm{R_{ij}}} + \frac{1}{2}\sum_i \sum_k \frac{\mu_i(\mathrm{r}_{\boldsymbol{k}} - \mathrm{R_i})}{|\mathrm{r}_{\boldsymbol{k}} - \mathrm{R_i}|^3} - \sum_i \sum_j \frac{Z_j \boldsymbol{\mu}_\mathrm{i} \cdot \mathrm{R_{ij}}}{R^3_{ij}} \tag{3}$$

2 QM/MM Energy Decomposition Analysis (QM/MM-EDA)

2.1 Methodology

The energy involved in a non-covalent interaction between two molecules or molecular fragments A and B that form a complex AB is called interaction energy, E_{int}. At QM/MM level, this interaction energy can be calculated using the supermolecule approach as the difference between the energy of the complex and the sum of the energies of the separated molecules or fragments (Eq. (4)).

$$E_{int} = E_{AB}(\mathrm{AB}) - (E_A(\mathrm{AB}) + E_B(\mathrm{AB})) \tag{4}$$

In Eq. (4), (AB) indicates that the energies of the complex and separated molecules are all obtained with the geometry and basis set of the complex, the latter to compensate for the basis set superposition error (BSSE) within the QM region. This expression gives us the total energy involved in the interaction, but, as mentioned in the previous section, to properly test the performance of each potential energy term included in the FF it is advisable to analyze the different energy contributions separately, namely, electrostatic, Pauli repulsion and polarization. There are different interaction energy decomposition schemes proposed in the literature, also known as energy decomposition analysis (EDA), either based on variational [13] or perturbational approaches [14]. We have developed in our group a hybrid variational/perturbational methodology [15, 16]. In this method, the interaction energy is firstly partitioned into electrostatic, repulsion and polarization contributions by separating the one-electron density into isolated monomers' one-electron densities plus one-electron deformation densities associated with the repulsion and polarization interactions (Eq. (5)), and the xc-density (exchange-correlation density) into isolated monomers' xc-densities plus intermolecular x-density (exchange density) and deformation xc-density (Eq. (6)).

$$\rho(\mathrm{r}) = \rho_A(\mathrm{r}) + \rho_B(\mathrm{r}) + \Delta\rho_{Pau}(\mathrm{r}) + \Delta\rho_{pol}(\mathrm{r}) \tag{5}$$

$$\rho_{xc}(\mathrm{r}_1,\mathrm{r}_2) = \rho_{xc,A}(\mathrm{r}_1,\mathrm{r}_2) + \rho_{xc,B}(\mathrm{r}_1,\mathrm{r}_2) + \rho_{x,AB}(\mathrm{r}_1,\mathrm{r}_2) + \Delta\rho_{xc,pol}(\mathrm{r}_1,\mathrm{r}_2) \tag{6}$$

In a second step, the expression of the induction energy obtained from second order perturbation theory (PT) is employed to extract this energy from the polarization energy. For weak non-covalent interactions, where second order PT recovers most of the energy and higher-order terms are negligible, the rest of polarization energy corresponds to dispersion energy. Using this decomposition scheme, the interaction energy is partitioned as in Eq. (7),

$$E_{int} = E_{elec} + E_{Pau} + E_{ind} + E_{disp+res-pol} \tag{7}$$

where the last term of the rhs includes dispersion plus the rest of polarization energy coming from higher orders in PT.

This EDA scheme was first developed and implemented for its use in combination with pure QM methods [15, 16], either wave function based [15] or density functional theory (DFT) [16]. The method was then extended to hybrid QM/MM schemes; using

electrostatic embedding first and very recently with polarizable embedding [17, 18]. The fundamental difference with respect to pure QM methods is that the potentials corresponding to the fixed atomic charges and induced dipoles in the FF that characterizes the MM region are added to the corresponding Hamiltonians used to calculate the different energy terms of Eq. (7). Some additional details are given in the next subsection.

The reader can find full mathematical formulations of the method elsewhere, both for the pure QM version [15, 16] and the QM/MM extension [17, 18].

2.2 Implementation

The method described in the previous subsection has been implemented in a scientific software of free access (EDA-NCI) written in Fortran language [19]. The currently available version only supports pure QM calculations and QM/MM calculations using electrostatic embedding. A new version including polarizable embedding is currently in a testing stage, and some preliminary results are discussed in the next section. Moreover, the program is currently interfaced with the Gaussian 09 and Gaussian16 electronic structure software packages [20] and the AMBER20 classical molecular dynamics software [21]. The former is used to obtain the input one-electron densities of the QM region required for the EDA, whereas the latter provides the atomic charges and induced dipole moments of the MM region. Development of interfaces with other software packages, such as Terachem, ORCA and Gromacs are currently in progress.

The essential steps followed by the EDA-NCI software are summarized in the schematic flowchart shown in Fig. 1. It must be noticed that previously to the calculation of the QM electron densities with the external software (first step in Fig. 1), the corresponding input files for this software are automatically generated using a python script included in the MoBioTools toolkit [22]. For QM/MM calculations, this script also incorporates into the Gaussian input files the atomic charges and dipole moments of the MM region previously read from the topology file of AMBER.

The flowchart represents first a summary of the operations performed externally by the electronic structure software employed (currently Gaussian, versions 09 or 16). From these operations, the input information regarding the one-electron densities of the complex and the isolated molecules or fragments are generated in the form of density matrices (DMs). In the particular case of QM/MM calculations, the atomic charges and dipole moments, the latter represented by a model of two opposite point charges [18], are added to the input information required by EDA-NCI using the module charge.x, internally incorporated to the EDA-NCI program.

Once the external operations are ended, an input file containing minimal information is created to perform the EDA-NCI internal operations described at the bottom of Fig. 1. These operations include: i) diagonalization of the fragments' one-electron density matrices to obtain the eigenvectors (molecular orbitals, MOs) and eigenvalues (occupation numbers); ii) mutual orthogonalization of the MOs of the different fragments to obtain the Pauli one-electron density matrix and the intermolecular x-density matrix; iii) calculation of the polarization one-electron density matrix and the deformation xc-density matrix; iv) one- and two-electron integral evaluation for construction of the Hamiltonian matrices involved in each energy contribution; v) calculation of the different energy terms from the corresponding deformation and Hamiltonian matrices; and

finally, vi) generation of an output file containing information of the different operations and a summary of the results, and generation of separate files containing the deformation density matrices for visualization using external programs, such as Gaussview [23].

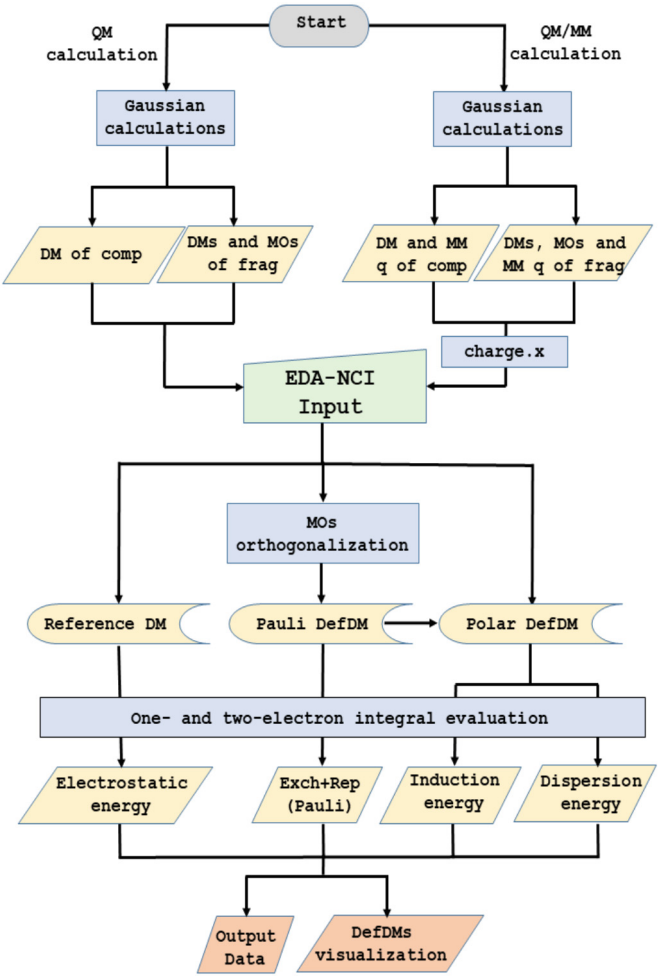

Fig. 1. Schematic flowchart of EDA-NCI

In Fig. 2, we can see on the left the representation of the Pauli and polarization electron densities obtained for an arbitrary geometry around the free energy minimum of 2,3,7,8-tetrachlorodibenzo-p-dioxin (TCDD) within a lipid membrane, and on the right a summary of the EDA results included at the end of the output file.

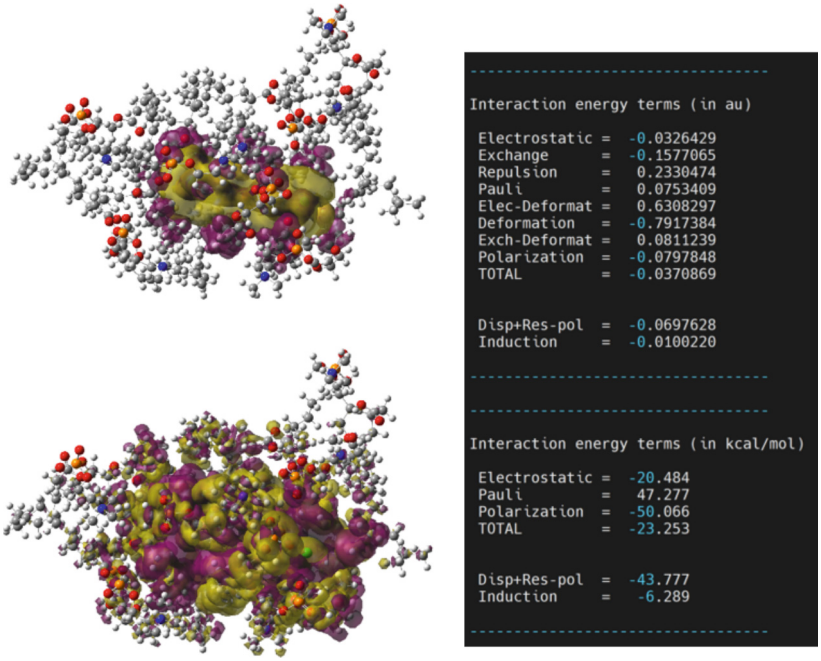

Fig. 2. Representation of the Pauli (top-left) and polarization (bottom-left) densities and the summary of the EDA results from the EDA-NCI output file (right) for the 2,3,7,8-tetrachlorodibenzo-p-dioxin embedded in a lipid membrane. A density cutoff of 10^{-5} is used, magenta and light brown colors represent positive and negative densities, respectively.

3 Examples of Application

In this section, some results of the QM/MM-EDA scheme obtained with the EDA-NCI software will be briefly summarized, namely, its application to the dynamic study of the solvation process of a zwitterion (glycine) [18] and to the dynamic study of the penetration of the TCDD pollutant through a lipid membrane [24].

3.1 Solvation of Glycine

These results presented here are part of a larger investigation where the intermolecular interactions responsible of the solvation of cationic, anionic and zwitterionic species were evaluated [18]. Zwitterions are probably the most interesting systems because, although they are globally neutral, they possess large formal positive and negative charges located on opposite sides of the molecule.

The target system was formed by a glycine molecule in its zwitterionic form ($^{+}NH_3$-CH_2-COO^{-}) surrounded by a water environment. As we intended to investigate the full dynamic process instead of a static situation, previous to the QM/MM calculations, classical molecular dynamics (CMD) simulations were carried out to generate an ensemble of geometries to subsequently perform a statistical analysis of the different interaction

energy terms. CMD simulations were run with AMBER20, a simulation box containing a total of 3250 water molecules was used. The Generalized Amber Force Field (GAFF) was employed for the glycine molecule, the simple point-charges based TIP3P and polarizable POL3 models were employed for the water molecules. Details about the results obtained from the CMD simulations can be found elsewhere [18], herein we will focus on the subsequent QM/MM-EDA analysis. The QM region was treated at DFT level, using the M062X functional and the 6-31G(d) basis set.

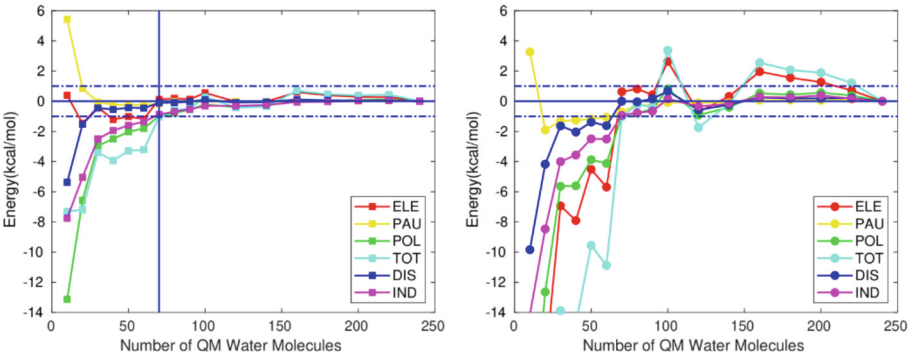

Fig. 3. Convergence of the different interaction energy terms with the number of water molecules in the QM region for hybrid QM/MM-EDA (left) and pure QM-EDA (right) calculations.

Before the statistical analysis, a geometry was randomly selected and QM/MM-EDA calculations using different QM region sizes were performed to characterize the minimum number of water molecules required for the QM region to get the EDA results converged. This is a crucial step since in the literature one can find many QM/MM calculations carried out without previous checking of the optimum QM region, with the consequent risk that the results may not be accurate enough. In Fig. 3, a representation of the interaction energy as well as its different contributions versus the number of water molecules included in the QM region is shown. In order to understand the important role played by the MM potential in the calculations, the same comparison is made by removing the MM region and keeping only the core of the glycine-water interaction represented by the QM region. As can be observed in Fig. 3, the different interaction energy terms reach convergence (within the range of 1 kcal/mol) with a QM region of 70 water molecules, being the repulsion and dispersion energies those that show a faster convergence. On the contrary, the convergence of all the energy terms is significantly slower without the MM region, with a remarkable effect on the electrostatic energy, which is not fully converged even for 200 water molecules.

Once the optimum size of the QM region was found, 200 equispaced geometries along CMD simulations carried out with the TIP3P and the POL3 models were selected to perform the statistical analysis of the relative contributions of the different energy terms. First, the statistical analysis reflected that a sample containing 20 or more geometries was sufficiently converged, as fluctuations of the sample means were in the ± 1 kcal/mol range with respect to the reference when 20 or more geometries were sampled. Therefore, Fig. 4

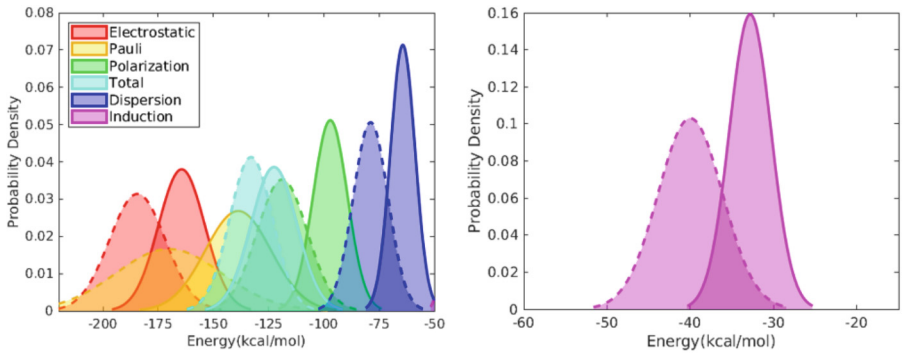

Fig. 4. Normal probability distributions for each interaction energy term obtained from a sample of 20 equispaced geometries from a CMD simulation of the solvation process of glycine carried out with the TIP3P (continuous line) and the POL3 (dashed line) models. Pauli repulsion is represented with opposite sign.

represents the normal probability distributions obtained with a sample of 20 geometries considering a QM region containing 100 water molecules.

As can be extracted from Fig. 4, the most important contribution to the stability of the zwitterion in water is by far the electrostatic energy. This energy is very large (around −190 kcal/mol and −170 kcal/mol with the POL3 and TIP3P models, respectively), reflecting the collective charge-dipole interaction established between the positive and negative charges of glycine and the dipoles of the surrounding water molecules. Regarding the polarization energy, both induction and dispersion contribute significantly, although the latter has a larger weight. On the other hand, the Pauli repulsion shows the broadest distribution among all the energy terms. This is due to the short-range character of this term, which makes it more sensitive to changes in geometry. Finally, the simple point-charge based model of TIP3P reflects a slightly lower stability of solvated glycine than the model POL3, which is based on point-charges and induced atomic dipoles. This is the expected result, as the inclusion of polarization in the CMD simulation and in the MM region for the QM/MM calculations helps to stabilize ionic and zwitterionic forms of molecules.

3.2 Membrane Permeation of TCDD

The second example of application that will be discussed is the process of penetration of polychlorinated dioxins through a cell membrane [24]. The most toxic form of polychlorinated dioxins is the TCDD, which is the one that will be analyzed here.

As in the previous example of solvated glycine, we will first perform the CMD simulation of the penetration process using a membrane model. The membrane model chosen was a lipid bilayer formed by two leaflets of 64 1,2-dioleyl-sn-glycero-phosphocholine (DOPC) molecules. This bilayer has a total thickness of 50 Å. Each DOPC molecule has a hydrophobic chain and a hydrophilic tail and the two layers are confronted each other with the hydrophobic chains pointed at the center of the bilayer. Thus, taken into

account the non-polar and aromatic character of TCDD, it is expected that the intermolecular interaction between the TCDD molecule and the lipid bilayer evolves from a small electrostatic interaction to a large dispersive one as the molecule migrates from the outer hydrophilic region to the inner hydrophobic one.

Details about the results obtained from the CMD simulation can be found elsewhere [24]. Herein, we will just mention that the penetration process was found to be thermodynamically favored and that two free energy minima (one on each side of the membrane) were found at 9 Å from the center of the membrane and a local energy maximum, very close in energy to the minima, was found at the center. As the previous example, we will focus on the QM/MM-EDA calculations. The QM region was treated at DFT level, using the M062X functional and the 6-31G(d) basis set. The first step was the characterization of the optimum size for the QM region. In Fig. 5, a representation of the interaction energy as well as its different contributions versus the number of DOPC molecules included in the QM region is shown for a geometry randomly chosen close to the energy minima. As can be observed, the convergence for all the energy terms is reached when the number of DOPC molecules in the QM region is 7. This entails a large number of atoms in the QM region since each DOPC molecule contains 54 heavy atoms and 84 hydrogens, and the TCDD molecule contains 18 heavy atoms and 4 hydrogens.

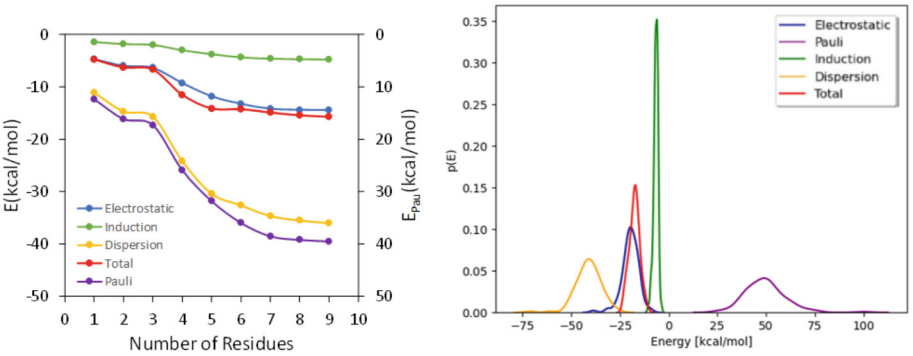

Fig. 5. Convergence of the different interaction energy terms with the number of DOPC molecules in the QM region for hybrid QM/MM-EDA calculations (left) and normal distributions of the interaction energy and its different components on 100 equispaced geometries selected from the free energy minima of the CMD simulation of the penetration process of TCDD through a lipid membrane (right).

In Fig. 5, the normal distribution of the interaction energy and its different components around the free energy minima is shown. In this case, up to 100 equispaced geometries were selected for the statistical analysis. As a remarkable difference with respect to the previous example of zwitterionic glycine in water, the dispersion energy is clearly the most important contribution. This is an expected result taken into account the non-polar character of TCDD and the hydrophobic nature of the DOPC chains. Thus, the stabilization of the TCDD molecule inside the lipid bilayer at the energy minima is due to a large dispersive interaction with these hydrophobic chains from the DOPC molecules. On the contrary, the induction energy has a residual contribution in this case.

4 Conclusions

In this short paper, a methodology to theoretically and computationally investigate the intermolecular interactions involved in biological processes and its implementation in the EDA-NCI software are presented. To illustrate its performance, some results recently published are briefly summarized. This methodology is applied in combination with CMD simulations and QM/MM electronic structure calculations. The power of this methodology is twofold: on the one hand, it allows obtaining the optimal QM size for QM/MM studies of intermolecular interactions in terms of accuracy and computational cost; on the other hand, it allows monitoring the intermolecular interactions along a dynamic process in terms of its strength and nature. Both electrostatic and polarizable embeddings can be used with the current implementation of this QM/MM-EDA scheme.

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Enhancing Low-Cost Molecular Property Prediction with Contrastive Learning on SMILES Representations

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Abstract. This paper explores self-supervised contrastive learning techniques in the Simplified Molecular Input Line Entry System (SMILES) representations. The contrastive model is responsible for pre-training the model before its downstream application on molecular property prediction. Central to our approach is the use of contrastive learning paradigms, in which pairs of distinct SMILES corresponding to the same molecule are treated as positive samples. In contrast, negative samples comprise pairs of SMILES that represent distinct molecules. This methodology aims to enrich the model's understanding of molecular structures by emphasizing the invariance of molecular properties despite permutation in the SMILES representation, thereby enhancing the robustness and predictive accuracy of the model. We conducted a series of experiments on publicly available and proprietary datasets to evaluate the efficacy of our approach. Empirical results underscore the merits of the contrastive learning model over traditional methods, demonstrating improvements in molecular property prediction tasks. This study not only validates the potential of contrastive learning in the realm of chemoinformatics, but also sets a promising direction for future research in leveraging SMILES permutations for molecular analysis.

Keywords: Contrastive Learning · SMILES · Molecular Property Prediction

1 Introduction

Accurate prediction of molecular properties is the cornerstone of numerous scientific endeavors, ranging from the design of new materials to the discovery of

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O. Gervasi et al. (Eds.): ICCSA 2024 Workshops, LNCS 14823, pp. 387–401, 2024.
https://doi.org/10.1007/978-3-031-65329-2_26

groundbreaking drugs [1]. These predictions allow researchers and developers to traverse the vast chemical space by identifying compounds with desirable properties for specific technological applications [2–4]. However, traditional methods for predicting molecular properties, such as density functional theory (DFT) and wave function methods, often face limitations due to the high computational cost and high dimensionality of the chemical space [5].

Traditionally, the determination of molecular properties has been based on experimental techniques and computational approaches such as the modern computational implementation of DFT [6]. Although experimental techniques provide a route for the characterization of the physical-chemical properties, they are often labor intensive, time consuming, and expensive. Furthermore, experimental techniques face challenges to yield an atom-level understanding of the interrelation between properties and structure. Similarly, despite providing a high degree of accuracy, DFT and other quantum mechanical calculations demand substantial computational resources, making them impractical for large-scale screenings, particularly assuming that the chemical space is practically infinite [7,8]. Consequently, while these traditional approaches remain valuable, their high costs and resource requirements present significant barriers to the rapid discovery and development of novel materials.

Machine learning (ML) has emerged as a powerful tool to bridge this gap, offering the potential to predict molecular properties quickly and accurately [5]. Several methods have been proposed in this scenario, particularly in the supervised paradigm, where molecules with target properties are used to train ML models [9–14]. For this purpose, different molecular descriptors are employed to represent chemical structures numerically, allowing ML algorithms to learn patterns and relationships between molecular features and properties. These descriptors range from simple fingerprints and text representation, such as the ECFPs (Extended-Connectivity Fingerprints) and the SMILES (Simplified Molecular Input Line Entry System), to more complex descriptors based on graph theory or quantum chemistry calculations, such as SOAP (Smooth Overlap of Atomic Positions) and MBTR (Many-body Tensor Representation) [11,15,16].

Despite the molecular representation, the properties are commonly obtained via DFT calculations, which can still be computationally expensive. For example, in [12] the authors have used a molecular descriptor extracted from SMILES using the Mordred toolkit [17] to build neural network predictors. Advanced descriptors, such as SOAP and MBTR, have been considered in other studies [13]. In both studies, the labeled data were generated by DFT calculations.

However, the effectiveness of these models is highly dependent on the quality and quantity of training data, which are often scarce or expensive to obtain in this domain [18]. Unsupervised and self-supervised learning approaches have gained attention as a means to overcome the limitations of supervised learning in the prediction of molecular properties and other downstream tasks [18–20]. In this case, an ML model is pre-trained on large datasets of unlabeled molecules and learns to capture underlying patterns and representations without explicit property labels. This pre-training step allows the model to develop a rich

understanding of molecular structures and their relationships, which can then be fine-tuned using smaller labeled datasets to make specific property predictions.

Contrastive learning, which belongs to the self-supervised learning paradigm, has shown remarkable success in domains such as Natural Language Processing (NLP) and Computer Vision [21–24]. By learning to differentiate between similar and dissimilar instances, contrastive learning facilitates the development of models that can capture complex patterns and relationships in the data, even without direct supervision. Taking into account the downstream property prediction task, in [25], the authors have proposed MolCLR, a framework based on GNNs (Graph Neural Networks). In [19], instead of using only molecular graphs, the authors proposed SmiCLR, which incorporates SMILES representations together with graphs. The SmiCLR relies on a contrastive model with two branches, one modeled by a graph neural network and the other by an LSTM (Long Short-Term Memory, to jointly learn representations from molecular graphs and SMILES strings. Overall, the use of contrastive learning techniques, such as MolCLR and SmiCLR, shows promise in enhancing molecular property prediction models by leveraging large amounts of unlabeled data to learn rich representations of molecular structures and relationships.

Here, we propose a more straightforward approach that takes only the SMILES of the molecule in the pre-training phase, thus reducing the cost of obtaining the molecular graph, atom, and bond descriptors and the geometry of the molecules. Our model learns a robust representation of molecular structures by treating pairs of distinct SMILES (permuted SMILES) that represent the same molecule as positive samples and pairs of SMILES from different molecules as negative samples. Subsequently, we deploy this pre-trained model in a downstream task to predict molecular properties, demonstrating the efficacy of our approach through computer experiments on both public and private datasets.

Our findings reveal that, compared to traditional approaches, the contrastive learning method with permuted SMILES enhances the model's performance in predicting molecular properties. Furthermore, another advantage is the elimination of the SMILES canonization process, as our model is designed to inherently recognize and interpret permuted SMILES as equivalent representations, streamlining the process and reducing preprocessing requirements. Thus, our contrastive model paves the way for more efficient and cost-effective methods for screening large chemical datasets and allows for faster exploration of the chemical space.

Our main contributions are:

- Proposing a contrastive learning approach using only the SMILES representations for pre-training a molecular property prediction model;
- This study shows the potential of contrastive learning with permuted SMILES to improve the accuracy and efficiency of screening large chemical datasets;
- We demonstrated the effectiveness of our approach through experiments on public and private datasets.

The structure of this manuscript is delineated as follows: Sect 2 elucidates the core principles that underlie this study. The methodological framework is

described in Sect. 3. Computational experiments and their corresponding discussions are presented in Sect. 4. Ultimately, Sect. 5 synthesizes the terminal insights and articulates various outstanding questions that warrant further academic exploration.

2 Background

2.1 SMILES Representation

SMILES is a notation for encoding molecular structures in a string [15]. Developed to facilitate the digital storage, retrieval, and processing of chemical information, SMILES notation represents the structure of a molecule using a series of characters including letters, numbers, and symbols. Each character or combination thereof corresponds to atoms, bonds, or specific configurations within the molecule, making SMILES a compact and versatile language for chemoinformatics [26].

The SMILES representation captures the essence of a molecule's connectivity, allowing for the depiction of complex organic structures in a straightforward and readable format. This includes the representation of cyclic structures, branching, and stereochemistry. One of the key advantages and also a disadvantage of SMILES is its ability to represent a molecule in multiple valid ways, due to permutations of chemical information within its string representation [15]. Therefore, distinct SMILES can represent the same molecule and the SMILES is not invariant to permutations. However, this property is particularly relevant for computational analyses, where the diversity of representations can be leveraged to enhance model robustness and generalizability. This process can be understood as a data augmentation method [27], in which multiple samples are generated from an available pattern, an approach analogous to rotations and translations in image classification. Figure 1 shows an illustration of the Caffeine molecule using a graph representation and also two possible SMILES that represent this compound.

The use of SMILES notation extends beyond mere structural depiction, serving as a foundation for numerous computational chemistry and molecular modeling tasks. It facilitates the application of machine learning algorithms by converting intricate molecular geometries into a form that can be easily processed by neural networks and other computational natural language processing models [28,29]. In particular, the linear nature of SMILES strings makes them amenable to processing by sequential models, such as Long Short-Term Memory (LSTM) networks, which can capture short and long dependencies and relationships within the molecular structure for various predictive and generative tasks [19].

In summary, SMILES is a powerful representation in the field of chemoinformatics, offering a concise and flexible method for encoding molecular information with low computational cost, because it does not require the geometry optimization of molecules via quantum chemistry simulations. Furthermore, its compatibility with computational and machine learning techniques has made it

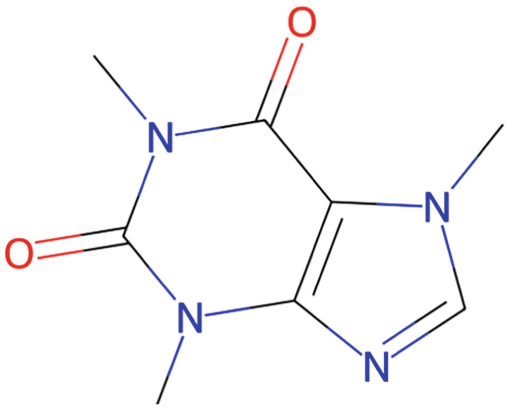

Fig. 1. Representation of the Caffeine molecule. The molecular graph representation and two possible SMILES of the caffeine are depicted on the top and bottom, respectively.

an indispensable component of modern approaches to molecular property prediction, drug discovery, and materials science.

2.2 Long Short-Term Memory

Long Short-Term Memory (LSTM) networks are a special class of Recurrent Neural Networks (RNNs) designed to address the limitations of traditional RNNs in capturing long-range dependencies within sequential data. Introduced by Hochreiter and Schmidhuber in [30], and extended by Gers et al. in [31], LSTMs have emerged as a pivotal technology in the field of deep learning, particularly for tasks involving sequences such as time series prediction, natural language processing, and more recently chemoinformatics.

The core of LSTM networks lies in their architecture, which incorporates memory cells and multiple gates (input, output, and forget gates). These components work in concert to regulate the flow of information, allowing the network to remember or forget information over long periods. This capability enables LSTMs to learn and retain complex dependencies within the data, a feature especially beneficial for processing sequential information such as the SMILES and other string-based representations.

In the context of chemoinformatics, LSTM networks have demonstrated significant potential in modeling and predicting molecular properties [19,28]. By treating SMILES strings as sequences, LSTMs can capture the intricate patterns and relationships encoded within the molecular structure, facilitating

accurate predictions of various chemical and physical properties. The adaptability of LSTM networks to handle variable-length sequences makes them particularly suited for dealing with the diverse and complex nature of chemical compounds represented in the SMILES format.

Moreover, LSTMs, as long as their competitors, such as GRU (Gated Recurrent Unit), have been instrumental in advancing the field of molecule generation and property prediction [14]. By learning the underlying rules and patterns in molecular structures, LSTM-based models can generate novel compounds with desired properties, a task of great importance in drug discovery and materials science [14].

2.3 Contrastive Learning

Contrastive learning is a form of self-supervised learning that teaches a model to understand which data points are similar or different without relying on explicit labels [32]. This approach is particularly useful for learning meaningful representations from unlabeled data, which can then be fine-tuned for a wide range of specific tasks [19].

In contrastive learning, the model is trained to distinguish between pairs of similar ("positive") and dissimilar ("negative") inputs. For example, in image processing, a positive pair could consist of two different augmentations (e.g., cropping, resizing, and color jittering) of the same image, while a negative pair would consist of augmentations from two different images [33]. The goal is to learn to project similar items closer together and dissimilar items farther apart in the embedding space [21]. This is typically achieved by minimizing a contrastive loss function, such as triplet loss [34] or the Noise Contrastive Estimation (NCE) loss [32].

A contrastive model can simultaneously use different types of input within a single model framework [35]. For example, one branch of the contrastive model could process the SMILES representation of a molecule, while another branch could handle the corresponding molecular graph [19]. Similarly, in the domain of image processing, one branch could receive an image, while another could process a textual description of that image. The choice of neural network architecture is crucial to effectively manage and learn from these varied data types. This study focuses on the Long Short-Term Memory (LSTM) architecture as it can straightforwardly handle sequential data.

3 Methodology

3.1 Datasets

In this study, three datasets were considered, two publicly available datasets (ZINC and QM9), and an in-house dataset (ionic liquid molecules). Their descriptions are depicted below:

ZINC : This dataset is a collection of commercially available compounds. It includes SMILES and XYZ representations, along with a range of calculated properties. The dataset contains 230 million molecules [36]. From the ZINC dataset, we select a subset of approximately 1.3 million molecules with atom types C, H, O, N, and F, limiting the number of heavy atoms to 14.

QM9 : This is a subset of the GDB-17 database [37], consisting of 133, 385 organic molecules with up to nine heavy atoms from four chemical species: C, O, N, and F. This dataset has previously been used as a benchmark for several machine learning studies in quantum chemistry applications. It provides two textual molecular representations (SMILES and InChI) and the XYZ files, which represents the molecule's optimized geometry via DFT (B3LYP/6-31G(2df,p)). Additionally, a set of 15 molecular properties (including geometric, energetic, electronic, and thermodynamic properties) is also presented [38].

Ionic Liquid Molecules This dataset, developed by the QTNano group [39], comprises approximately 20, 000 molecules (ions) and was generated through the combination of various cations (138) and anions (40) extracted from known literature. These molecules were generated by combining different cores and backbones derived from the selected cations and anions. The generated compounds were optimized using DFT (FHI-AIMS), and their HOMO and LUMO properties were calculated. These properties are crucial for estimating the electrochemical window of the ionic liquid, which is of paramount importance for the development of batteries and supercapacitors.

The ZINC dataset were mainly used as a pre-training dataset. The QM9 and the Ionic Liquids dataset were also considered in the molecular property prediction tasks.

3.2 Positive and Negative Pairs

Contrastive learning is based on the effective differentiation between positive and negative pairs of examples to learn meaningful representations. Here, we detail the methodology for generating these pairs.

Positive Pair Generation: Positive pairs are formed by using the inherent property of SMILES strings, where a single molecule can be represented by multiple valid SMILES notations because of the different sequences in which atoms can be traversed and written down. These variations, while representing the same molecular structure, provide an adequate opportunity to create positive samples for our contrastive learning model.

Given a molecule M, let $S(M)$ represent the set of all possible valid SMILES representations for M. A positive pair (s_i, s_j) is then defined as two distinct SMILES strings $s_i, s_j \in S(M)$, where $i \neq j$. Formally, this can be represented as:

$$(s_i, s_j) \in P \Leftrightarrow s_i, s_j \in S(M) \wedge s_i \neq s_j, \tag{1}$$

where P denotes the set of all positive pairs. Generation of $S(M)$ for a given molecule involves permuting the SMILES string to create different valid representations, ensuring that s_i and s_j are distinct, yet describe the same molecular entity. The RDKit package [40] was used for the permutation of SMILES.

Negative Pair Generation. Negative pairs are crucial for teaching the model to distinguish between different molecular structures. A negative pair consists of two SMILES strings that represent different molecules. Given two molecules M_1 and M_2 with their respective SMILES representations s_{M_1} and s_{M_2}, a negative pair is formed if and only if $M_1 \neq M_2$. Formally, a negative pair (s_{M_1}, s_{M_2}) is defined as:

$$(s_{M_1}, s_{M_2}) \in N \Leftrightarrow M_1 \neq M_2, \tag{2}$$

where N denotes the set of all negative pairs. This definition ensures that the model is exposed to a wide variety of molecular structures during training.

Pair Selection Strategy. The selection of pairs, both positive and negative, is critical for the learning process. For positive pairs, we generate two random permutations s_j from s_i of the SMILES of the same molecule, ensuring a diverse set of representations for the same molecule. For negative pairs, we randomly select SMILES strings from two distinct molecules. The balance between positive and negative pairs in the training set is crucial for effective contrastive learning. An imbalance can lead to a model that is biased towards identifying either similarities or differences, thus affecting its generalization capability. Therefore, we maintain a similar number of positive and negative pairs in our training dataset to ensure a balanced learning environment.

3.3 SMILES Tokenization

Neural networks require numerical input to operate, thus necessitating a tokenization process to convert SMILES strings into a form these models can process. This tokenization involves breaking down each SMILES string into its constituent tokens, typically representing atoms, bonds, or structural motifs. Our tokenization approach is meticulously designed to capture the details of the molecular structure, thereby facilitating the model's ability to learn from and recognize variations in molecular representations.

The tokenization process begins by identifying all valid tokens within the SMILES syntax, including single-character elements (e.g., 'C' for carbon, 'O' for oxygen), multi-character elements (e.g., 'Cl' for chlorine, 'Br' for bromine), and special characters denoting bond types or branching (e.g., '=', '#', '(',')'). In addition, ring closures are marked by digits that follow the atoms involved in the ring. Each token is then mapped to a unique identifier in our model's embedding space, enabling efficient numerical processing during the learning phase. For this project, we used the BasicSmilesTokenizer routine available in the DeepChem toolbox [41], with a modified regular expression (regex) designed to include all species present in our datasets.

3.4 Self-supervised Contrastive Pre-training

The pre-training phase of our contrastive model is designed to learn robust representations of molecular structures encoded as SMILES strings. This phase is critical for capturing the patterns and relationships inherent in the chemical space. Our model architecture employs two LSTM networks, which are particularly suited for processing the sequential nature of SMILES strings. This section outlines the architecture, the embedding process, and the training methodology of our contrastive learning model.

Model Architecture. Given a pair of SMILES strings (s_i, s_j), whether it forms a positive or negative pair, each string in the pair is independently processed by two LSTM networks. The two LSTM networks have identical architectures, but with their own set of weights. The output of each LSTM, for a given SMILES string s, is a latent representation $h_s \in \mathbb{R}^d$, where d is the dimensionality of the LSTM output.

Following extraction of latent representations h_{s_i} and h_{s_j} by the LSTMs, both are passed through a shared projection head. This projection head is an MLP (Multilayer Perceptron) neural network layer that maps the latent space h to an embedding space z, where contrastive loss is applied. The projection head is defined by a function $f : \mathbb{R}^d \to \mathbb{R}^p$, $p > d$, resulting in embeddings $z_{s_i} = f(h_{s_i})$ and $z_{s_j} = f(h_{s_j})$. The use of a shared projection head for both LSTMs ensures that the embeddings are comparable and lie in the same space, facilitating the effective application of contrastive loss.

To train our model, we employ the Normalized Temperature-Scaled Cross-Entropy Loss (NT-Xent Loss), which is widely used in contrastive learning for its effectiveness in learning discriminative features. The NT-Xent Loss for a pair of embeddings (z_{s_i}, z_{s_j}) is defined as:

$$\ell(z_{s_i}, z_{s_j}) = -\log \frac{\exp(\text{sim}(z_{s_i}, z_{s_j})/\tau)}{\sum_{k=1}^{2N} 1_{[k \neq i]} \exp(\text{sim}(z_{s_i}, z_{s_k})/\tau)}, \tag{3}$$

where $\text{sim}(u, v) = u^\top v / \|u\| \|v\|$ denotes the cosine similarity between two vectors, τ represents the temperature parameter, $2N$ is the total number of examples in the batch, half of them are samples generated from enumerated smiles from the dataset, and $1_{[k \neq i]}$ is an indicator function that equals 1 iff $k \neq i$. This loss function forces the model to produce similar embeddings for positive pairs and dissimilar embeddings for negative pairs.

Optimization and Training. For the optimization of our model, we chose the Adam optimizer. The Adam optimizer dynamically adjusts the learning rate for each parameter, based on estimates of the first and second moments of the gradients, improving the convergence rate and stability of the training process. The pre-training process involves iteratively sampling pairs of SMILES strings, processing them through the LSTMs and the projection head, and updating the

model weights based on the computed NT-Xent Loss. This iterative process continues until the model converges or a predefined number of epochs is reached. By the end of pre-training, the model is expected to have learned a rich and discriminative embedding space z, which can be leveraged for downstream molecular property prediction tasks.

3.5 Molecular Property Prediction

Upon completing the pre-training phase, the learned embeddings serve as input to a predictor neural network. For this purpose, we also use an MLP neural network, which is designed to map the embedding representation z to the target property y.

Given a labeled dataset where each molecule is associated with a specific property, the MLP is trained to minimize the prediction error between the estimated property values and the true values. In the learning phase, the predictor takes into account the mean squared error loss function. Then, the errors are backpropagated with the Adam optimizer.

The integration of the predictor neural network with the pre-trained contrastive model is straightforward. The output embedding z from the pre-trained model serves as the input feature vector for the MLP. This approach allows the predictor to utilize the knowledge distilled from the contrastive learning phase, enhancing its predictive performance on the target molecular property.

4 Experiments and Discussion

This section offers an overview of our neural models and the computer experiments conducted for the property prediction task.

4.1 Experimental Setup

To train, evaluate and report our results, we divided the datasets into training, validation, and test sets. In the supervised phase, we randomly selected a subset of 5k molecules from QM9 as the training set and two additional subsets of 10k each for validation and testing. For the cation (anion) datasets from the ionic liquid database, we defined test and validation sets of 900 (750) samples, respectively, with the remainder being used as the training set. During the self-supervised phase, we used 100k molecules from ZINC data as the validation set and assigned the rest for training. Moreover, during the self-supervised phase, we maintained the same validation and test sets as in the supervised phase and used the remaining data for training for both the QM9 and ionic liquid datasets.

The hyperparameters were empirically set to optimize the performance of the models. Specifically, the following parameters and computational infrastructure were considered in the experiments:

Computational Infrastructure: The learning phase and experiments were conducted on a high-performance workstation equipped with Dual 12-core Intel Xeon Silver 4214R processors (16.5 MB cache, 12 cores, 24 threads, up to 3.50 GHz Turbo), 256GB of RAM, and 2 NVidia RTX A6000 GPUs, each with 48GB of memory;

Optimization Parameters: The models were trained for a maximum of 100 epochs with a learning rate of $1e-3$ and no learning rate decay. The temperature was set to 0.1, and the batch size was set to 512 for the self-supervised phase. During the supervised phase, we set the number of epochs to 300 and the batch size to 256, with learning rate decay enabled;

Baseline Model Hyperparameters: The baseline model, a three-layers bidirectional Long Short-Term Memory (LSTM) network, was configured with 128 neurons. This setup was chosen to establish a foundational comparison for the performance of more complex models;

Contrastive Model Hyperparameters: After empirical experiments, we selected embedding dimensions of 64, and three LSTM layers with 128 neurons each;

Prediction Model Hyperparameters: The prediction model was designed with a 2-layer Multilayer Perceptron (MLP) neural network, with 64 neurons in the hidden layer using the hyperbolic tangent activation function and a single linear neuron for the output. This predictive head was used by both the baseline and the contrastive models.

4.2 Property Prediction

We designed four distinct tests to evaluate the performance of our models under varying conditions. Initially, a baseline LSTM model served as our benchmark, establishing a performance metric for comparison. Subsequently, we explored the impact of pre-training our contrastive model exclusively with the downstream datasets, namely QM9, to assess the direct benefits of contrastive learning in a simpler context with no external dataset. The third test, which was applied for both the QM9 and Ionic Liquids datasets, we expanded the pre-training scope by incorporating a substantial subset of the ZINC dataset, approximately 1.3 million molecules with atom types C, H, O, N, and F, limiting the number of heavy atoms to 14. This test aimed to understand the effect of a larger chemical dataset on model performance.

Table 1 shows the results with the QM9 dataset. Table 2 shows the results for the Ionic Liquids dataset. It can be observed that the contrastive model delivers results superior to those achieved with the baseline model when solely using the QM9 for both the self-supervised and supervised phase. However, the results of the model pre-trained with the ZINC dataset did not perform as expected. For instance, even in delivering results superior to the baseline model, the contrastive trained with the ZINC+QM9 was inferior than the model trained with QM9 alone.

Table 1. Test error (MAE) of 8 molecular properties from the QM9. (*i*) A baseline LSTM model; (*ii*) Contrastive model pre-trained with the QM9 dataset; (*iii*) Contrastive model pre-trained with the QM9 and a subset of the ZINC dataset (Aprox. 1.3M molecules).

Property	*i*	*ii*	*iii*
U_0 (eV)	0.3053 ± 0.0049	0.2439 ± 0.0033	0.2787 ± 0.0016
U (eV)	0.3056 ± 0.0056	0.2436 ± 0.0058	0.2858 ± 0.0019
H (eV)	0.3298 ± 0.0020	0.2475 ± 0.0075	0.2885 ± 0.0078
G (eV)	0.2987 ± 0.0046	0.2380 ± 0.0055	0.2779 ± 0.0040
Cv (cal (molK)$^{-1}$)	0.2384 ± 0.0027	0.2032 ± 0.0032	0.2271 ± 0.0062
α (a_0^3)	0.6089 ± 0.0053	0.5203 ± 0.0136	0.5860 ± 0.0140
ϵ_{HOMO} (eV)	0.1592 ± 0.0019	0.1562 ± 0.0021	0.1603 ± 0.0024
Δ_ϵ (eV)	0.2349 ± 0.0020	0.2198 ± 0.0020	0.2298 ± 0.0037

Table 2. Test error (MAE) of 2 molecular properties fromthe Ionic Liquids dataset. (*i*) A baseline LSTM model; (*ii*) Contrastive model pre-trained with the ZINC subset

Property	(*i*)	(*ii*)
Anions		
ϵ_{HOMO} (eV)	0.1361 ± 0.0008	0.1330 ± 0.0035
ϵ_{LUMO} (eV)	0.1313 ± 0.0042	0.1337 ± 0.0034
Cations		
ϵ_{HOMO} (eV)	0.2086 ± 0.0055	0.2013 ± 0.0048
ϵ_{LUMO} (eV)	0.2019 ± 0.0036	0.2011 ± 0.0041

5 Conclusion

This study proposed a contrastive learning model that takes only the SMILES representation into account for the pre-training phase. The core of our approach lies in treating pairs of SMILES strings, representing the same molecule in its original form and a permuted variant, as positive samples and contrasting them with negative samples drawn from different molecules. This methodology was designed to exploit the inherent structural and property invariance of molecular representations, facilitating the learning of robust and discriminative features critical for accurate property prediction. Furthermore, as previously mentioned, by allowing the model to learn from permuted SMILES, we eliminate the need for a canonization process.

Our experiments, conducted using publicly available and proprietary datasets, have shown superior performance of our contrastive learning model over traditional approaches, albeit contrastive models that take the molecular graph into account still deliver superior results. These findings reinforce the value of

contrastive learning in chemoinformatics and also highlight the power of SMILES permutations to capture the nuanced complexities of molecular structures.

Interestingly, the model pre-trained with a combination of the QM9 and ZINC datasets performed worse than the model pre-trained with only the QM9 dataset. Moreover, the ionic liquids dataset results were not superior to those of the baseline models. These findings were contrary to expectations and warranted further scrutiny. Owning to the promising outcomes, this study opens several avenues for future research; for instance, more powerful neural network models, such as the Transformers, together with larger unlabeled datasets, could be used to improve the learned representation in the pre-training phase.

Acknowledgements. The authors gratefully acknowledge support from FAPESP (São Paulo Research Foundation), projects No. 2017/11631-2 and 2022/09285-7, and the CNPq (National Council for Scientific and Technological Development), project No. 313680/2021-3.

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Insights into Ion Conduction Mechanisms Through the ORF3a Channel by Computational Modelling

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Abstract. Investigating the selectivity and mechanism of the SARS-CoV-2 ORF3a protein channel remains a significant challenge within the scientific community. Speculation surrounds its potential calcium ion selectivity, implicating a significant role in the pathology of COVID-19 by influencing viral replication and the cellular virus response. This study employs molecular dynamics (MD) simulations with external electric fields to examine ion conduction, focusing on the interactions between calcium, potassium and sodium ions and specific amino acid residues in the ORF3a structure. Initial findings reveal a complex framework of conductance and selectivity, characterized by distinct patterns of residue coordination. These early insights underscore the channel's selectivity and functional mechanism, laying the groundwork for further in-depth studies aimed at unravelling the ORF3a protein's role in virus-host dynamics and its therapeutic potential. Advancements in ion-residue and ion-water coordination studies, along with extended molecular dynamics simulations, are essential to deepen our understanding and uncovering essential transport mechanisms that could be pivotal in designing effective antiviral compounds.

Keywords: Molecular Dynamics · Ion Conduction · Coordination · ORF3a

1 Introduction

The cells of living organisms are perpetually under the influence of physico-chemical environmental stimuli [1–3]. Considerable progress has been made in

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O. Gervasi et al. (Eds.): ICCSA 2024 Workshops, LNCS 14823, pp. 402–414, 2024.
https://doi.org/10.1007/978-3-031-65329-2_27

unraveling how cellular receptors directly link to intracellular electrochemical signaling. These receptors encompass a diversity of ion channels activated by voltage, ligands, or mechanical sensitivity, and are pivotal for cells to detect physical and chemical stimuli from the surroundings [4–6]. Among these stimuli, mechanical forces such as osmotic pressure, gravity, touch, fluid dynamics in contact with cells, and sound waves target various types of membrane proteins, triggering intracellular changes and leading to subsequent responses in the cell nucleus-a key aspect of the discipline of mechanobiology [7]. This intricate interplay between cells and their environment becomes critically relevant in the context of respiratory diseases, where the mechanobiological responses can influence disease progression and pathology [8,9].

Research on respiratory diseases, especially those caused by the coronavirus family, has been a crucial area of study in recent decades. The emergence of diseases such as Severe Acute Respiratory Syndrome (SARS), Middle East Respiratory Syndrome (MERS), and more recently, the global COVID-19 pandemic caused by SARS-CoV-2, has underscored the importance of advancing our understanding of these pathogens [10,11]. All these viruses belong to the Beta-coronavirus and have shown the ability to cause respiratory diseases of different severity in humans, which has accentuated the need for detailed research to develop effective prevention and treatments.

Within the coronavirus genome, a key element in their study is the presence of Open Reading Frames (ORF), which encode for the structural and non-structural proteins, essential for the replication and pathogenicity of the virus. ORFs are sequences of DNA or RNA that have the capacity to be translated into proteins, playing a crucial role in the virus's biology [1,8,12]. Among all, ORF3a is the largest accessory protein encoded by SARS-CoV-2 and has emerged as a protein of interest because it performs multiple roles in the virus life cycle and its implication in the pathology of the disease. The attributed functions include modulating the release of virions, inducing apoptosis in infected cells, and manipulating the host's immune response [8,9,11,13].

ORF3a has been classified as a viroporin, belonging to a class of transmembrane proteins that form ionic channels in cellular membranes [8,12,14], facilitating the flow of ions between the inside and outside infected cells, thus altering the intracellular ionic balance and promoting various pathological processes. The structure of this protein includes an N-terminal ectodomain, three transmembrane domains (TM1-TM3), and a cytoplasmic C-terminal domain, as observed in Fig. 1. This configuration facilitates its localization in the plasma membrane and the formation of ionic pores, fundamental aspects for its function in viral pathogenicity. It is believed that ORF3a acts as a non-selective channel permeable to cations, including calcium (Ca^{2+}), which has significant implications for viral replication as well as the induction of apoptosis in infected cells. In vitro experiments suggest that ORF3a could alter cellular calcium homeostasis, a finding that underscores the need to study its mechanism of action and selectivity [10,11,13–15]. In this contribution, we simulate the ion permeation through the

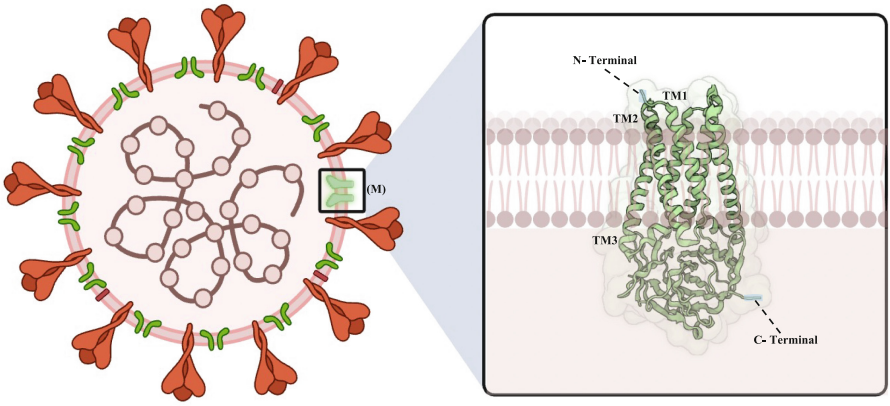

Fig. 1. Schematic structure of the ORF3a, a membrane protein (M) of the SARS-CoV-2 virus.

ORF3a channel by means of voltage-biased molecular dynamics simulations to unveil the most relevant protein residues involved in the conduction mechanism.

2 Computational Details

– **System Setup.** Protein coordinates were retrieved from the Protein Data Bank 7kjr entry [15], which delineates its structure as determined by cryo-electron microscopy at 2.1 Å resolution within a lipid environment [15]. An initial cleansing process was conducted using PyMol [16], aimed at removing all water molecules and residual ligands to purify the structure, leaving solely the ORF3a protein, thus ensuring its suitability for simulations. The preparation of the protein involved the adoption of the CHARMM36m force field [17], selected for its accuracy in modeling interactions between proteins and lipids in biomimetic contexts. Subsequently, with the assistance of CHARMM-GUI [18] and using the bilayer builder input generator [19], the protein was aligned along the Z-axis using the Orientations of Proteins in Membranes (OPM) database [20], before determining the dimensions of the simulation box. CHARMM-GUI follows a detailed procedure based on a set of parameters to define these dimensions. The process begins with the choice of a rectangular box. The length along the Z-axis is determined by the defined water layer thickness, set at 22.5 Å, which represents the minimum amount of water needed above and below the system. Dimensions along the X and Y axes are based on the lipid component ratios. The protein was then embedded in a pre-equilibrated DOPE (Dioleoylphosphatidylethanolamine) lipid bilayer, a phospholipid commonly found in biological membranes. DOPE lipid was chosen for both the upper and lower leaflets, leading to an initial estimate of the lengths of X and Y. As a result, the system was set up with dimensions of $60.288 \times 60.288 \times 127.277$ Å. Finally, to emulate physiological

conditions and maintain the system's neutrality, CHARMM-GUI automatically incorporates the necessary ions to neutralize the system (KCl is the usual choice). Additionally, specific ions of NaCl, KCl, and $CaCl_2$ were added up to a concentration of 150 mM to TIP3P water [21]. Once the system preparation was completed, NAMD inputs were generated and ready to launch the molecular dynamics simulation [22]. This simplified setup contains only one type of lipid, as this approach allows us to explore the fundamental mechanisms of ion transport and channel behavior without the computational costs associated with simulating a fully detailed lipid environment [4,5]. Such simplifications have been successfully employed in similar studies for prokaryotic voltage- activated sodium and potassium channels The generated simulation box is shown in Fig. 2.

– **Classical Molecular Dynamics**. After adjusting the default NAMD inputs provided by CHARMM-GUI, like modifications to enhance the thermal equilibration protocol, the heating process was subdivided into three distinct sequential stages. The system minimization was carried out using the conjugate gradient and line search method over 10,000 steps. Then, the system was progressively heated from 0 to 303.15 K in the NVT ensemble, using a time step of 1 fs during three distinct phases, the initial heating phase elevated the system from 0 to 100K, the second one from 100 to 200K, and the final stage reached 303.15k. This procedure, totaling 0.375 ns, allocated 0.125 ns for each phase. During the initial heating equilibration, the simulation was conducted within the NVT ensemble. Constraint scaling was initially set at 10.0kcal/(molA^2), subsequently adjusted to 5kcal/(molA^2), and then to 2.5kcal/(molA^2), applied to the alpha carbons of the protein to maintain its structural stability while allowing flexibility in other regions of the system. Temperature control was carried out using the Langevin thermostat [23], with a collision frequency of 1.0 ps^{-1}. Subsequent equilibration phases were conducted within the NPT ensemble, allowing for both temperature and pressure regulation, thereby facilitating system density adjustments. Constraints were sequentially reduced from 1, to 0.5, and finally, to 0.1kcal/(molA^2), before being completely removed (set to 0) for the production phase. Throughout these equilibration stages and the subsequent production phase, a consistent timestep of 2 fs was utilized, cumulatively amounting to an additional equilibration period of 1.5 ns. Pressure management was activated using the Langevin piston, configuring the system for pressure control through a Nose-Hoover Langevin piston [24]. A target pressure of 1.01325 bar, equivalent to 1 atmosphere, was established, with a piston oscillation period of 50 fs and an oscillation decay time of 25 fs. The Particle-Mesh Ewald (PME) method [25] was employed with a grid spacing of 1.0 Å for precise long-range electrostatic calculations, alongside a 12 Å cutoff and a 10 Å switching distance for nonbonded interactions to optimize computational efficiency and accuracy. The bonds containing hydrogen atoms were restrained using the SHAKE algorithm [26]. The first production phase, conducted in the NPT ensemble without an external electric field, lasted 100 ns, providing insights into the system's behavior under standard equilibrium conditions. Subsequently,

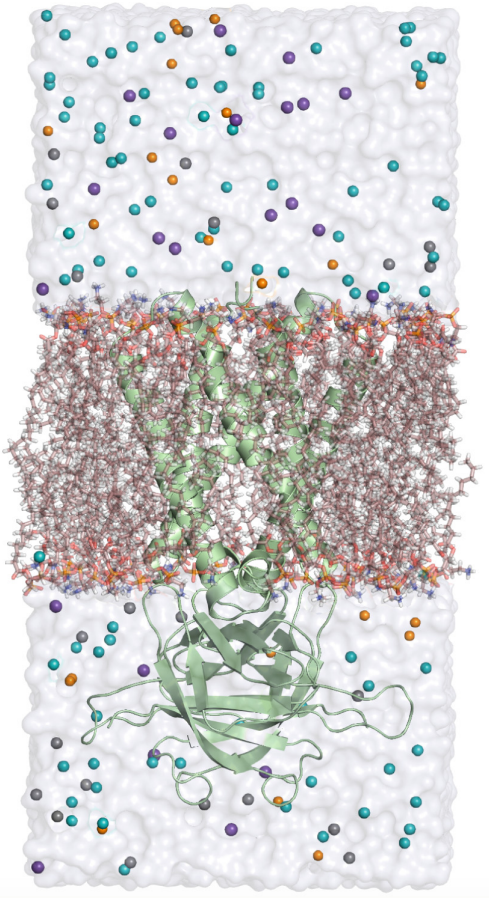

Fig. 2. The components of the simulation box. Protein is represented in green (cartoon), lipid bilayer in brown (licorice), chloride ion in cyan, sodium in orange, potassium in purple, and calcium in grey (spheres). Water is represented by the surface in light blue. (Color figure online)

a second production phase was evolved in the NPT ensemble, but this time incorporating an external electric field of 1.5 V in the Z direction (with the positive end towards the extracellular side, see Fig. 5) for another 100 ns. For a detailed explanation of the equations and their application in molecular dynamics, we recommend consulting the article [27], which is a standard reference in the field and provides a comprehensive description of the methodology and equations used. Moreover, the application of external electric fields in molecular dynamics has been previously utilized and is well described in the literature [28].

3 Results

In this section, a detailed analysis is carried out in two parts, aimed at getting insight into the mechanism of ion conduction and selectivity of the channel under study. The analysis is performed on the 100 ns production phase of the simulation, where an external electric field is applied, since it is during this stage that the ionic events occur. The application of this electric field induces an increase in the ionic mobility, which allows for the collection of a large amount of data, thus, facilitating a more accurate and rapid statistical analysis of the ion transport process. In the first part of the analysis, the ion permeation events are classified and counted for each ion type. Then, the second part of the analysis focuses on the identification of the aminoacids involved in the ion conduction by means of the characterization of the ion coordination sphere during the conduction events. Special attention has been given to negatively (GLU and ASP) and positively (LYS and ARG) charged amino acids for their ability to coordinate cations (sodium, potassium, and calcium) and anions (chloride), respectively. This analysis seeks to unveil the role of these coordinating residues on the reg-

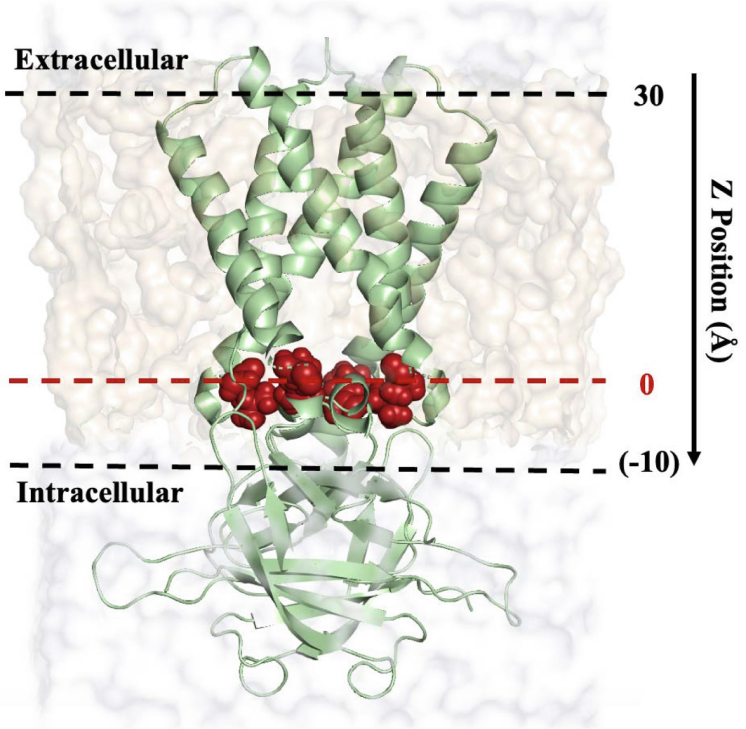

Fig. 3. Schematic representation of the transmembrane protein's orientation along the Z-axis.

ulation of ionic transport through the channel, providing valuable insights into the mechanisms underlying the channel's selectivity and efficiency.

To facilitate the understanding and visualization of the subsequent analyses, Fig. 3 presents a schematic representation of the orientation of the transmembrane protein with respect to the cellular bilayer along the Z-axis, which is the direction of the ion conduction. The extracellular and intracellular regions are differentiated by black dotted lines, while the zero reference point on the Z-axis is defined based on the geometric center of four reference amino acids, LEU 71 and ARG 126 from both chains A and B, depicted in the Fig. 3 as red spheres. The following analysis has been conducted with custom-developed Python programs, utilizing the MDAnalysis library.

– **Ion Conduction.** Figure 4 illustrates the ionic translocation events through the channel, depicted by colored dots moving from the extracellular region (Z=20 Å) to the intracellular region (Z=-20 Å). The examination of the plots reveals a higher number of conduction events for potassium ions (28) compared to sodium (17) and calcium (8). Despite the channel is supposed to be calcium selective, the simulation showcases significant activity for other cations. However, calcium events exhibit a more restricted and concentrated spatial distribution, as particularly observed in Fig. 4c around Z=10 Å, sug-

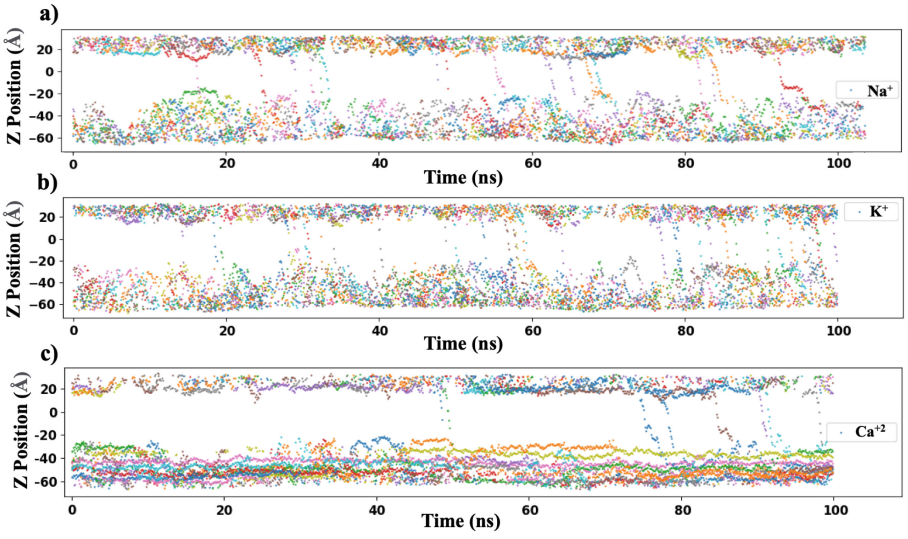

Fig. 4. Ion permeation profiles for **a)** $\mathbf{Na^+}$, **b)** $\mathbf{K^+}$ and **c)** $\mathbf{Ca^{2+}}$ along the Z-axis in Å over time in nanoseconds (ns).

gesting a potentially more specific and robust interaction with the protein. For instance, from approximately 25 ns to 40 ns, one can observe in purple that a calcium ion remains consistently in the same position, indicative of being retained. Additionally, the conduction of chloride ions was analyzed due to the observation of numerous events, but their graphical representation has been omitted. This decision was made because the individual events were not as discernible, with some occurring simultaneously or in rapid succession, as observed in simulation analysis software, in this case, PyMol.

– **Ion-Protein Coordination.** The coordination analysis elucidates the interactions between different residues and ions, providing relevant insight into their potential roles in the ion selectivity and mechanistic function of the channel. This analysis focuses on the interaction of different protein residues with calcium and the other cations, and their impact on channel dynamics. The residues that will strongly interact with the cations are the negative ones, i.e., glutamate and aspartate. Figure 5a and Fig. 5b show the coordination number of the different ions by glutamate and aspartate, respectively, with cutoff distances set at 2.5 Å for calcium, 3.0 Å for sodium, and 3.4 Å for potassium. These residues exhibit significant coordination with calcium ions and smaller coordination with sodium and potassium ions. This behaviour is likely due to the larger charge of calcium, which enhances the electrostatic interactions with the negative residues. Thus, glutamate and aspartate could be main actors in calcium conduction through the channels.

It is important to note the absence of coordination near the Z=0 point despite the presence of amino acids that might be crucial, suggesting alternative ion exit pathways from the channel or that the ions could be fully solvated by water in this region. Furthermore, positively charged residues, such as lysine and arginine displayed in Fig. 6a and Fig. 6b, respectively, show a strong coordination of the chloride anion (the cutoff distance was set at 2.5 Å), which indicate that the ion transport in this channel is a complex mechanism with different ions and residues involved. Further analysis are needed to investigate in more detail the mechanistic details. It should be noted that the coordination numbers for the ions involved in this study were determined based on the proximity of non-hydrogen atoms of the protein residues to the respective ions. Specifically, cutoff distances of 2.5 Å for calcium and chloride ions, and 3.0 Å and 3.4 Å for sodium and potassium ions, respectively, were employed. These distances correspond to the locations of the first minima observed in the ion-water oxygen radial distribution functions when the ions are in the bulk solvent.

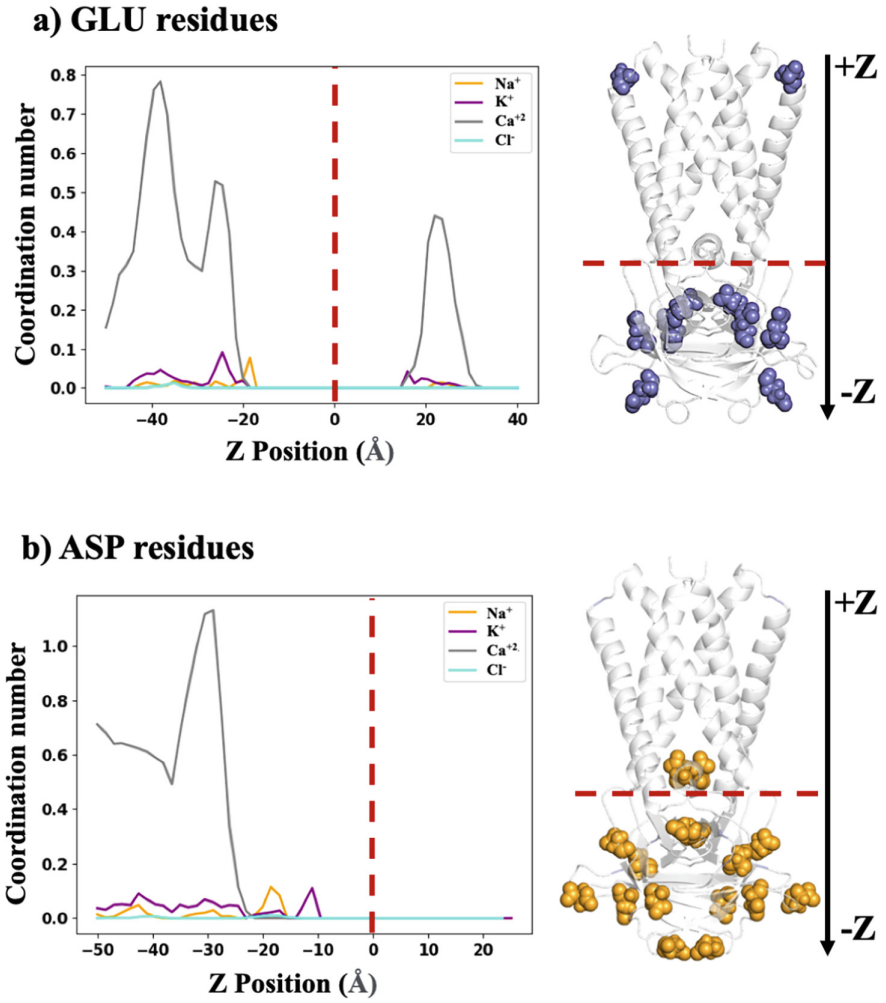

Fig. 5. Ion Coordination profiles for amino acids with negative charges along the Z-axis. **a)** GLU residues are denoted by blue spheres, **b)** ASP by orange spheres. The red dashed lines denote the zero reference point on the Z-axis. (Color figure online)

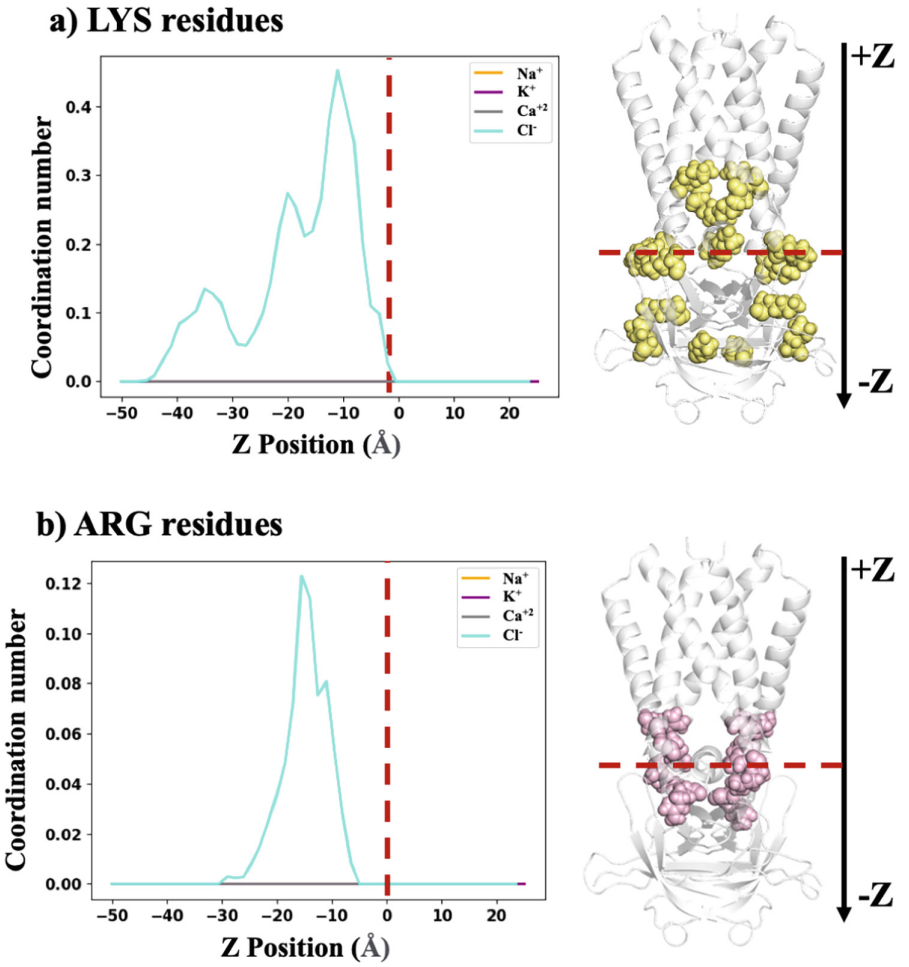

Fig. 6. Ion Coordination profiles for amino acids with positive charges along the Z-axis. **a)** LYS by yellow spheres, and **b)** ARG by pink spheres. The red dashed lines denote the zero reference point on the Z-axis. (Color figure online)

4 Conclusions

The analyses presented in this study offer a preliminary view of the ionic conduction dynamics through the ORF3a protein channel and its interaction with specific residues. The simulation has unveiled distinctive patterns in the conduction of calcium, potassium, and sodium ions, as well as coordination interactions with key residues within the protein. Specifically, the interaction between glutamate and aspartate residues with the calcium ions could be a key ingredient in the selectivity of this channel. Comparing this with the available experimental data [15], we find that, although the calcium conduction events are not predomi-

nantly high, the specific calcium coordination observed experimentally supports the selectivity and efficacy of this channel towards calcium, which is consistent with the significant coordination observed in our simulations. However, the permeation of other cations and anions and the coordination of chloride by positively charged amino acids suggest that the channel selectivity and conduction follow a very intricate mechanism that need a more thoughtful analysis and additional simulations.

The results presented here should be taken with caution due to the preliminary nature of the study. The simulations should be extended up to the microsecond timescale to enhance the statistical robustness and the reliability of the results obtained. Furthermore, it is recommended to increase the complexity of the system setup to be closer to real biological systems, even though this may entail a significant increase in computational cost. In addition, further analysis should also delve deeper into ion-water coordination and the interactions of ions with other amino acids (neutral ones) not considered in this initial analysis, but that could play a critical role in the ion conductance and selectivity of the channel. A more complete analysis based on longer simulations will allow us to unveil the factors that control the ionic dynamics through the ORF3a channel. Such relevant information will be crucial for the design of effective antiviral compounds.

Acknowledgements. The authors thank Atena Salek for preliminary calculations. We acknowledge the generous allocation of computer time at the Centro de Computación Científica at the Universidad Autónoma de Madrid (CCC-UAM). This work was partially supported by the Spanish Ministry of Science and Innovation through the project PID2020-117806GA-I00 and by the Comunidad de Madrid through the Attraction of Talent Program (Grant reference 2022-5A/BMD-24244). N. F-L and A. L thank the European Union - NextGenerationEU under the Italian Ministry of University and Research (MUR) National Innovation Ecosystem grant ECS00000041 - VITALITY - CUP J97G22000170005

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DFT+U Optical Features of Thermochromic VO_2: A Powerful Tool Towards Functional Daytime Radiative Passive Cooling Implementation

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Abstract. The structural, electronic and optical properties of both monoclinic and rutile polymorphs of vanadium dioxide, VO_2, have been determined by means of first-principles calculations based on semiempirical DFT+U method. The outcome shows that the Hubbard U scheme provides bandgap values consistent with previously reported experimental ones. The simulated optical properties for the high-temperature rutile polymorph correctly reproduce the metallic behaviour of the system. It is interesting to note that at low temperatures, the VO_2 monoclinic structure is more transparent under infrared light irradiation, while the rutile phase blocks the same IR light, as demonstrated by the simulated optical reflectance and absorption coefficient. This work aims to provide the readers with a comprehensive understanding of the complex chemistry of VO_2, paving the way to future studies addressing the doping effect on the optical and thermal behaviour of the system in view of the application of such material in devices for radiative cooling.

Keywords: Thermochromic materials · Density Functional Theory (DFT) · Hubbard U · Daytime radiative passive cooling

1 Introduction

Together with photochromic [1,2], hydrochromic [3], and electrochromic [4,5], thermochromic materials [6] are gaining enormous attention in the technological landscape. The interest towards this latter class of compounds stems from their

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O. Gervasi et al. (Eds.): ICCSA 2024 Workshops, LNCS 14823, pp. 415–426, 2024.
https://doi.org/10.1007/978-3-031-65329-2_28

unique abilities to reduce energy waste and improve indoor comfort, as response to an external natural impulse, i.e. temperature change. As consequence of such T variation indeed, these materials, largely exploited in the production of thermochromic smart windows [7] and related devices, alter their visible optical characteristics [8].

For this reason, a thorough understanding of its electronic properties at the atomistic level can aid in understanding the properties of this complex material for other applications which require enviromentally-responsive solutions, such as radiative cooling devices. Daytime radiative cooling (DRC) [9,10] is a cutting-edge technology that can be used in arid environments to address the urban heat island effect and provide passive cooling in the built environment. This technology takes advantage of the Earth's atmosphere's high transparency in the mid-infrared (MIR) wavelengths between 8 and 13 μm, also known as the "sky window" region [11] to release excess heat directly into the cold universe. Radiative coolers have remarkable potential for both local climate change mitigation and passive building cooling since they can achieve sub-ambient temperatures even during peak hours by utilizing a 3 K heat sink of the outer space. Novel models of passive daytime radiative cooling have recently been presented combining high solar reflectance with high emissivity in the atmospheric window [12], even though without deeply investigating the properties of functional materials, essential to logically develop and enhance few desired attributes which assure those devices the maximum efficiency along with wide versatility. In this regard, thermochromic materials such as VO_2 can be incorporated into a multilayered device in which the optoelectronic characteristics can be turned "on" and "off" to activate the qualities of other layers (such as the thermal emission layer's activation or deactivation) [13]. The peculiar property of thermal switch it is due to the fact that at T$\approx$ 68 °C (hereafter, T_c), the monoclinic (M1, space group $P2_1/c$) experiences a fully reversible metal-insulator phase transition (MIT), transforming into rutile-type VO_2 (R, space group $P4_2/mnm$) phase (see Fig. 1). At such temperature the MIT takes place quickly-typically in the picosecond's timescale (10^{-12} s) [14]. A lot of efforts have been spent by the community to explain the physics behind this MIT. Its occurrence is nowadays interpreted through two main competitive mechanisms: a structure-driven Peierls transition [15] or an electron-correlation driven Mott transition [16]. Several authors similarly adduce the transition to a cooperative mechanism between the two [17,18]. Our goal is to technologically exploit the fundamental thermochromic characteristic of such material (clearly associated to mentioned MIT) in order to properly regulate the emission of thermal radiation, which dissipates a significant quantity of heat connected to the incident solar energy. As consequence, the amount of energy required for cooling-related operations would massively reduce.

Before describing VO_2 application properties, however, we have to better focus on the material, describing its fundamental chemical and physical properties. Indeed, VO_2 is part of the class of the so-called *strongly correlated compounds* whose characterization has represented so far one of the most challenging fields of investigation in condensed matter physics [19]. With such terminology

we refer to those materials whose electronic behaviour (which arises from the complex chemistry of *3d* electrons in VO_2) is not properly described by standard Density Functional Theory (DFT) approaches. Polymorphism is another main feature of VO_2. Indeed, the vanadium-oxygen phase diagram displays approximately twenty stable vanadium oxide compounds, including, among the others, VO, V_6O_{13}, and V_7O_{13}. Only a very small range of partial pressures of oxygen can cause VO_2 to exist. Furthermore, over ten different types of vanadium dioxide crystalline phases have been documented [20]. These include tetragonal rutile-type VO_2 (R) ($P4_2/mnm$), monoclinic-type VO_2(M1) ($P2_1/c$), tetragonal VO_2 ($P4_2/nmc$), monoclinic VO_2 (C2/m), orthorhombic VO_2·H2O (P222), tetragonal $VO_2 \cdot 0.5H_2O$ (I4/mmm), and $V_2O_4 \cdot 2H_2O$ [14].

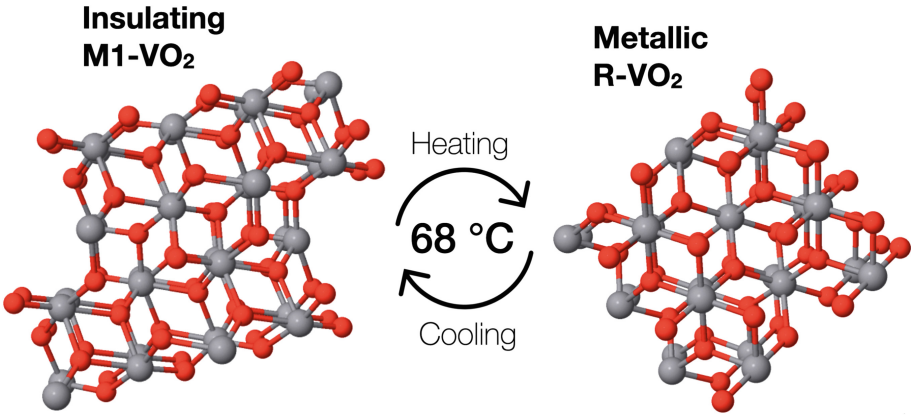

Fig. 1. Visual representation of VO_2 Metal-Insulator reversible transition at 68 °C between (left) the low temperature monoclinic (space group: $P2_1/c$) phase and (right) the high temperature rutile (space group: $P4_2/mnm$) phase.

Thus, we aim here to investigate the structural and electronic characteristics of VO_2, with a focus on optical features of M1 and R-VO_2 as prototypical investigations for future researches where we would like to address the link between the phase transition and the MIT temperature, trying to reduce it closer to room temperature (RT), thus making VO_2 more exploitable, given its potential applicability in next-generation construction materials.

Beyond the (1) high transition temperature (T_c= 68 °C) - significantly higher than RT- two other reasons motivate the fact VO_2 is not immediately employed as coatings on thermochromic materials based devices: (2) a low solar modulation efficiency (< 10%); and (3) a low luminous transmittance (∼40%) [21]. Several attempts have been made to improve them, such as element doping [22], the creation of VO_2 nanocomposites [23], the use of various substrates [24], and the alteration of structures. Element doping for VO_2 film is one of these strategies that effectively lowers T_c. It has been demonstrated that VO_2 films doped with

high valence cations, such as W^{6+}, Mo^{6+}, Ta^{5+}, Ti^{4+}, and Ru^{4+}, lower the MIT temperature [21,25]. Although its solar modulation efficiency was only 6.1%, tungsten doping has the largest MIT temperature fall-off rate among them and has been lowered to about 25 °C [26]. The optical characteristics of these films though have not significantly improved, and it is unclear how these dopants - particularly Si- affect the MIT [27]. A relevant observation is that most dopants show an upper limit in doping level to reduce the MIT temperature. In more detail, Eu^{3+}, Tb^{3+}, Nb^{5+}, P^{3+}, W^{6+}, Si^{4+}, F^{-} and Mo^{6+} are shown to produce extremely positive effects on the switching efficiency, whether Mg^{2+}, Fe^{3+}, Sb^{3+} and Zr^{4+} ions were reported to have minimal impact on the T_c as demonstrate by Wang et al. [28] In the following we report our more recent results which comprise a complete theoretical description of the electronic and optical properties of M1 and R polymorphs of VO_2, to gain insights on how this phase transition can be exploited to produce modulated optical properties. Such results represent a benchmark analysis for future investigations focusing on the doping procedure as trigger for the phase change and colour tunability.

2 Computational Details

We performed first-principles calculations in the framework of density-functional theory as implemented in the SIESTA package [29]. In particular, norm-conserving Trouillier-Martins (TM) [30] pseudopotentials for the core electrons and a triple-ζ basis set along with the generalized gradient approximation (GGA) as parametrized by Perdew-Burke-Ernzerhof (PBE) [31] for the exchange-correlation energy were employed. We have fully relaxed, lattice and ionic positions, both the structures of M1 and R-VO_2 until the maximum residual force was lower than 0.005 eV/Å, while the considered energy cutoff was of 300 Ry. Convergence in relation to the quantity of k points was thoroughly examined. Different Hubbard U [32] were tested and used to account for the electron-electron Coulomb interaction in the *3d* orbitals of V atoms.

3 Results and Discussion

The VO_2 is a monoclinic (M1) structure (shown in Fig. 2(a)) with space-group $P2_1/c$ (No. 14) at $T < T_c$. The V^{4+} ions deviate from the unit cell's center and vertex, resulting in the twist of VO_6 octahedral cages, the fundamental building blocks. The vanadium atoms tilt and dimerize to form zigzag-like chains with alternating various V-V bond lengths (see Fig. 2(b)), which is another feature specifically characterizing the M1 phase. On the other hand, the thermodynamically stable phase of VO_2 at ambient pressure and above T_c belongs to the $P4_2/mnm$ (No. 136) space group (represented in Fig. 2(c)), which has a tetragonal R structure. The tetragonal crystal cell's body center and apex are occupied by V^{4+} ions in the R-VO_2 phase. An octahedral VO_6 unit is made up of six O^{2-} ions that surround a single V^{4+} ion and vanadium atoms form equally spaced

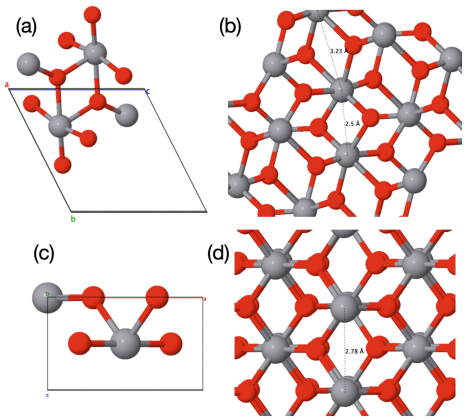

Fig. 2. DFT+U optimized crystal structure of VO_2: (a) and (c) unit cell of M1-VO_2 and R-VO_2 respectively; (b) and (d) zig-zag and linear pattern of V-V chains after metal-insulator transition (MIT). Vanadium atoms are represented with grey spheres, while red spheres are used for oxygen atoms. (Color figure online)

V-V straight chains (see Fig. 2(d)) in the c direction, while the octahedral unit creates edge-sharing chains along the c axis.

As previously mentioned, one of the relevant features of VO_2 is its strongly bound *3d* electrons. Periodic plane-wave DFT computations with standard exchange-correlation functions-like LDA or GGA-are quite successful in characterizing a wide range of materials; yet they are unable to handle systems with strong correlations. Typically, they might underestimate the band gaps and occasionally even predict a metallic ground state that is qualitatively inaccurate, such the insulating nature of M1-VO_2. The main reason is, as previously mentioned, the standard DFT failure in accounting for the correlation among *3d* V electrons. Therefore, to address this limitation and gain a better understanding of the electrical characteristics of two VO_2 phases, the present work employed the moderately computationally expensive DFT+U approach [33], which represents the electronic correlation of V-*3d* orbitals. The image below (Figs. 3(c) and 4(c)) shows the gap opening and closure due to the strong Coulomb interactions between V-*3d* electrons.

Since earlier research has demonstrated that the magnitude of effective U value, U=1.5 eV is suitable for properly describing both electronic and dynamic features of the two phases of VO_2 [34] along with its MIT temperature within the framework of the quasi-harmonic-approximation (QHA) approximation, employing this value of U, Table 1 shows the structural properties and band gaps for simulated and experimental structures. Regarding the monoclinic phase, the employed level of theory can accurately reproduce two distinct dimerized V-V bond distances: 2.50 Å and 3.23 Å in good agreement with the experimental values of 2.62 Å [35] and 3.16 Å [36]. Similarly, the optimized V-V bond length in the rutile phase is 2.78 Å, still in close agreement with the experimentally

reported value (2.85 Å) [37]. The DFT+U (U=1.5 eV) results both reproduce the insulating features of the M1 phase with a predicted bandgap (0.68 eV) perfectly in line with available experimental data [38] and the metallic behaviour of the R structure.

Table 1. DFT+U (U=1.5 eV) optimized lattice parameters, V-V bond lengths/distances and band gaps for M1 and R phase of VO_2. Experimental data are similarly reported for the sake of comparison.

Polymorph	Method	Lattice parameters (Å)	V-V distance (Å)	Bandgap (eV)
M1	DFT+U	a=4.65 b=5.47 c=5.40 α=63.0 β=90.0 γ=90.0	2.50, 3.23	0.68
	Experimental		2.62 [35], 3.16 [36]	0.67 [38]
R	DFT+U	a=4.67 b=4.67 c=2.78 α=90.0 β=90.0 γ=90.0	2.78	Metallic
	Experimental		2.85 at 360 K [37]	

To confirm the effectiveness of the selected value of U, band structures and partial density of states (PDOS) for the M and R phase of VO_2 were also computed using DFT+U (U=1.5 eV) and reported in Fig. 3(a) and Fig. 4(a), respectively. In both pictures, the zero energy is set to the Fermi energy position. The R phase metallic nature is confirmed by the DFT+U (U=1.5 eV), which, as stated before, yields an indirect band gap of 0.68 eV for the insulating M1 phase. The band dispersions around the Fermi level well reproduce the previously reported DFT findings [34]. Further proof of the distinctive characteristics of the M and R phase may be found in the partial density of states (PDOS) displayed in the right panel of Fig. 3(b) and Fig. 4(b), respectively.

The imaginary part ($\epsilon 2$) of the dielectric function in metallic species should approach infinite as photon frequency approaches zero (often referred to as the Drude tail) in accordance with Drude theory [39–41]. Since optical conductivity and $\epsilon 2$ are closely correlated, low frequencies should show a significant increase in optical conductivity. Generally, *d-d* intraband transitions and free carrier absorption are responsible for the Drude tail in VO_2. We therefore computed optical

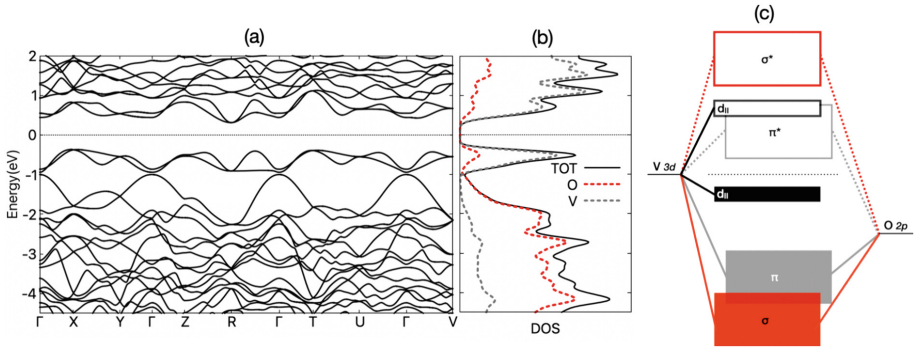

Fig. 3. DFT+U method (U=1.5 eV) calculated (a) bandstructure, and corresponding (b) density of states (DOS) along with the (c) energy-band alignment for M1-VO_2. The black dashed line represents the Fermi level.

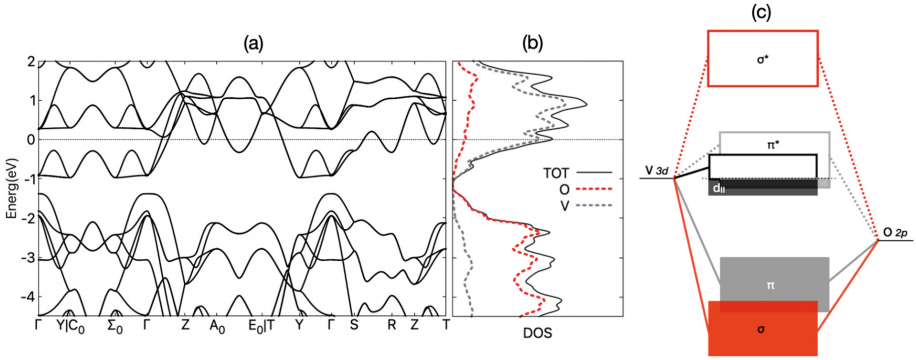

Fig. 4. DFT+U method (U=1.5 eV) calculated (a) bandstructure, and corresponding (b) density of states (DOS) along with the (c) energy-band alignment for R-VO_2. The black dashed line represents the Fermi level.

conductivity with increasing U values, finding that our optical conductivity, as determined by PBE+U calculations, reproduces correctly the Drude tail for the rutile, metallic, phase of VO_2. This is also supported by previous theoretical studies [42] where hybrid functionals are demonstrated to fail on grasping the metallic character of R-VO_2. Examining the results, we realize that the implemented U value and the Drude tail's magnitude are inversely correlated (see Fig. 5). At low frequencies, conductivity increases as the U value decreases. As frequency approaches zero, standard PBE calculations (U=0 eV) produce the largest increase in conductivity. Thus, for the metallic compounds under analysis, we conclude that the addition of the U value results in a reduction of free carrier absorption strength and *d*-*d* intraband transitions. The optical conductivity at higher energies does not show sensitive variations as function of the

U value adopted. This finding further assesses the suitability of the U value we selected for our analysis.

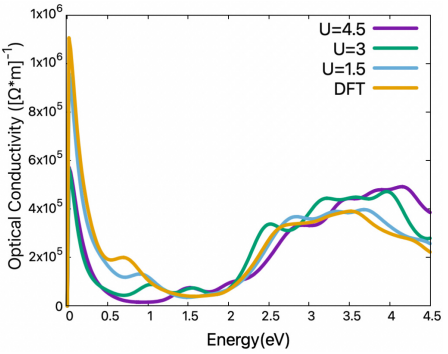

Fig. 5. DFT and DFT+U calculated optical conductivity of R-VO_2.

As previously stated, increasing temperature, VO_2 undergoes a phase transition and diffusion, allowing the material to change from an insulating to a metallic state, with consequent variation of optical properties.

Accordingly, Figs. 6, 7, 8 shows the relationship between VO_2 phase (M and R) and optical conductivity, reflectance, and absorption coefficient, respectively. In Fig. 6 the optical conductivity plot clearly indicates that R-VO_2 has high optical value around 0 eV - as expected according to the Drude model - whilst when VO_2 changes from metallic to insulating phase, the optical conductivity also decreases accordingly at frequencies close to zero. The simulated results are in good agreement with experimentally measured optical conductivity profiles found in literature [42]. The VO_2 MIT also significantly affects the optical reflectance as depicted in Fig. 7, where we observe low infrared (IR) reflectance in the insulating phase but high IR reflectance in the R metallic phase, a useful property to exploit in functional devices based on thermochromic films [43]. Finally, the absorption coefficients (reported in Fig. 8) of M1 and R-VO_2 shows that the pure M1 phase has very low absorption and reflection of IR light, whilst the pure R phase exhibits a strong absorption and reflection in the same region. These aspects clearly indicate that IR light more easily interacts with the M1 phase, but it is mostly blocked once it interacts with the R phase, an outcome in good agreement with the experimental observations and previous theoretical results [44].

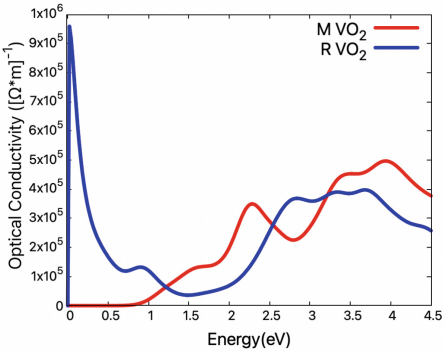

Fig. 6. DFT+U (U=1.5 eV) calculated optical conductivity of (blue) M and (red) R-VO_2. (Color figure online)

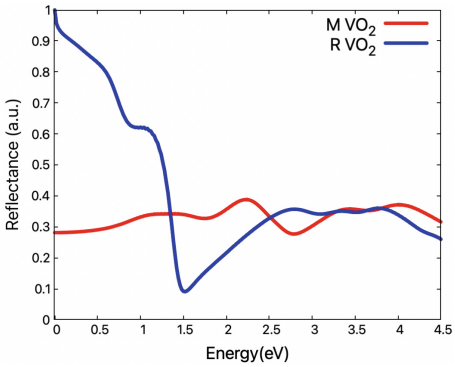

Fig. 7. DFT+U (U=1.5 eV) calculated reflectance of (blue) M and (red) R-VO_2. (Color figure online)

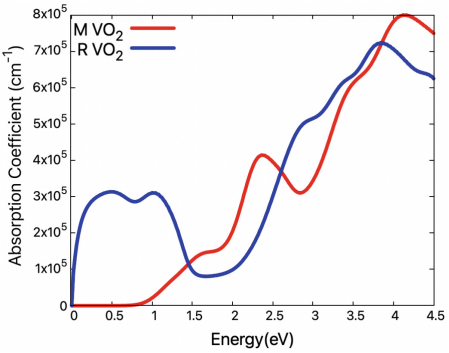

Fig. 8. DFT+U (U=1.5 eV) calculated absorption coefficient of (blue) M and (red) R-VO_2. (Color figure online)

4 Conclusions

In the present contribution the physical features of VO_2 main polymorphs, rutile and monoclinic, have been addressed in terms of their optical and electronic properties. Our results are consistent with those previously reported in literature, confirming that the DFT+U approach accurately predicts the insulating and metallic character of M1 and R phase, respectively, and further supporting the suitability of such approach for electronic structures calculation of other strongly correlated materials. Based on the obtained results, we have further noticed that increasing the U value induces a large reduction of free carrier absorption and *d*-*d* intraband transitions, therefore reducing the characteristic Drude tail for the metallic compounds. Carefully screening the Hubbard U value, we conclude that our selected one (U=1.5 eV) fairly reproduce the predicted behaviour of the two phases.

Our work paves the way towards future investigations aiming to disclose any possible relationship between VO_2 optical features and doping effects on the two polymorphs. In this framework, particular focus must be paid on the impact that do pant atoms may have in the metal-to-insulator transition temperature.

Acknowledgments. Funded by the European Research Council within the framework of the Horizon Europe Programme (ERC, HELIOS, G.A. 101041255, PI dr. A.L. Pisello). Views and opinions expressed are, however, those of the authors only and do not necessarily reflect those of the European Union or the European Research Council. Neither the European Union nor the granting authority can be held responsible for them. G.G., A.L.P. also thank the European Union - NextGenerationEU under the Italian Ministry of University and Research (MUR) National Innovation Ecosystem Grant ECS00000041 - VITALITY for funding and acknowledge Università degli Studi di Perugia and MUR for support within the project Vitality. Authors are similarly grateful to Prof. L. Latterini and her research group (Dept of Chemistry, Biology and Biotechnology, Perugia University) for the very fruitful scientific discussions.

Disclosure of Interests. The authors have no competing interests to declare that are relevant to the content of this article.

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O. Gervasi et al. (Eds.): ICCSA 2024 Workshops, LNCS 14823, pp. 427–428, 2024.
https://doi.org/10.1007/978-3-031-65329-2

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