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Computational Science and Its Applications – ICCSA 2023 Workshops

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Preface

These 9 volumes (LNCS volumes 14104–14112) consist of the peer-reviewed papers from the 2023 International Conference on Computational Science and Its Applications (ICCSA 2023) which took place during July 3–6, 2023. The peer-reviewed papers of the main conference tracks were published in a separate set consisting of two volumes (LNCS 13956–13957).

The conference was finally held in person after the difficult period of the Covid-19 pandemic in the wonderful city of Athens, in the cosy facilities of the National Technical University. Our experience during the pandemic period allowed us to enable virtual participation also this year 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 2023 was another successful event in the International Conference on Computational Science and Its Applications (ICCSA) series, previously held as a hybrid event (with one third of registered authors attending in person) in Malaga, Spain (2022), Cagliari, Italy (hybrid with few participants in person 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 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 2023 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 61 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 workshop proceedings we accepted 350 full papers, 29 short papers and 2 PHD Showcase papers. In the main conference proceedings we accepted 67 full papers, 13 short papers and 6 PHD Showcase papers from 283 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 2023 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 2023

Osvaldo Gervasi
Beniamino Murgante
Chiara Garau

Welcome Message from Organizers

After the 2021 ICCSA in Cagliari, Italy and the 2022 ICCSA in Malaga, Spain, ICCSA continued its successful scientific endeavours in 2023, hosted again in the Mediterranean neighbourhood. This time, ICCSA 2023 moved a bit more to the east of the Mediterranean Region and was held in the metropolitan city of Athens, the capital of Greece and a vibrant urban environment endowed with a prominent cultural heritage that dates back to the ancient years. As a matter of fact, Athens is one of the oldest cities in the world, and the cradle of democracy. The city has a history of over 3,000 years and, according to the myth, it took its name from Athena, the Goddess of Wisdom and daughter of Zeus.

ICCSA 2023 took place in a secure environment, relieved from the immense stress of the COVID-19 pandemic. This gave us the chance to have a safe and vivid, in-person participation which, combined with the very active engagement of the ICCSA 2023 scientific community, set the ground for highly motivating discussions and interactions as to the latest developments of computer science and its applications in the real world for improving quality of life.

The National Technical University of Athens (NTUA), one of the most prestigious Greek academic institutions, had the honour of hosting ICCSA 2023. The Local Organizing Committee really feels the burden and responsibility of such a demanding task; and puts in all the necessary energy in order to meet participants' expectations and establish a friendly, creative and inspiring, scientific and social/cultural environment that allows for new ideas and perspectives to flourish.

Since all ICCSA participants, either informatics-oriented or application-driven, realize the tremendous steps and evolution of computer science during the last few decades and the huge potential these offer to cope with the enormous challenges of humanity in a globalized, 'wired' and highly competitive world, the expectations from ICCSA 2023 were set high in order for a successful matching between computer science progress and communities' aspirations to be attained, i.e., a progress that serves real, place- and people-based needs and can pave the way towards a visionary, smart, sustainable, resilient and inclusive future for both the current and the next generation.

On behalf of the Local Organizing Committee, I would like to sincerely thank all of you who have contributed to ICCSA 2023 and I cordially welcome you to my 'home', NTUA.

On behalf of the Local Organizing Committee.

Anastasia Stratigea

Organization

ICCSA 2023 was organized by the National Technical University of Athens (Greece), the University of the Aegean (Greece), the University of Perugia (Italy), the University of Basilicata (Italy), Monash University (Australia), Kyushu Sangyo University (Japan), the University of Minho (Portugal). The conference was supported by two NTUA Schools, namely the School of Rural, Surveying and Geoinformatics Engineering and the School of Electrical and Computer Engineering.

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Plenary Lectures

A Multiscale Planning Concept for Sustainable Metropolitan Development

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Urban sprawl has often been pointed out as having an important negative impact on environment and climate. Residential zones have grown up in what were initially rural areas, located far from employment areas and often lacking shopping opportunities, public services and public transportation. Hence urban sprawl increased car-traffic flows, generating pollution and increasing energy consumption. New road axes consume considerable space and weaken biodiversity by reducing and cutting natural areas. A return to "compact cities" or "dense cities" has often been contemplated as the most efficient way to limit urban sprawl. However, the real impact of density on car use is less clear-cut (Daneshpour and Shakibamanesh 2011). Let us emphasize that moreover climate change will increase the risk of heat islands on an intra-urban scale. This prompts a more nuanced reflection on how urban fabrics should be structured.

Moreover, urban planning cannot ignore social demand. Lower land prices in rural areas, often put forward by economists, is not the only reason of urban sprawl. The quality of the residential environment comes into play, too, through features like noise, pollution, landscape quality, density etc. Schwanen et al. (2004) observe for the Netherlands that households preferring a quiet residential environment and individual housing with a garden will not accept densification, which might even lead them to move to lower-density rural areas even farther away from jobs and shopping amenities. Many scholars emphasize the importance of green amenities for residential environments and report the importance of easy access to leisure areas (Guo and Bhat 2002). Vegetation in the residential environment has an important impact on health and well-being (Lafortezza et al. 2009).

We present here the Fractalopolis concept which we developed in the frame of several research projects and which aims reconciling environmental and social issues (Bonin et al., 2020; Frankhauser 2021; Frankhauser et al. 2018). This concept introduces a multiscale approach based on multifractal geometry for conceiving spatial development for metropolitan areas. For taking into account social demand we refer to the fundamental work of Max-Neef et al. (1991) based on Maslow's work about basic human needs. He introduces the concept of satisfiers assigned to meet the basic needs of "Subsistence, Protection, Affection, Understanding, Participation, Idleness, Creation, Identity and Freedom". Satisfiers thus become the link between the needs of everyone and society

and may depend on the cultural context. We consider their importance, their location and their accessibility and we rank the needs according to their importance for individuals or households. In order to enjoy a good quality of life and to shorten trips and to reduce automobile use, it seems important for satisfiers of daily needs to be easily accessible. Hence, we consider the purchase rate when reflecting on the implementation of shops which is reminiscent of central place theory.

The second important feature is taking care of environment and biodiversity by avoiding fragmentation of green space (Ekren and Arslan 2022) which must benefit, moreover, of a good accessibility, as pointed out. These areas must, too, ply the role of cooling areas ensuring ventilation of urbanized areas (Kuttler et al. 1998).

For integrating these different objectives, we propose a concept for developing spatial configurations of metropolitan areas designed which is based on multifractal geometry. It allows combining different issues across a large range of scales in a coherent way. These issues include:

- providing easy access to a large array of amenities to meet social demand;
- promoting the use of public transportation and soft modes instead of automobile use;
- preserving biodiversity and improving the local climate.

The concept distinguishes development zones localized in the vicinity of a nested and hierarchized system of public transport axes. The highest ranked center offers all types of amenities, whereas lower ranked centers lack the highest ranked amenities. The lowest ranked centers just offer the amenities for daily needs. A coding system allows distinguishing the centers according to their rank.

Each subset of central places is in some sense autonomous, since they are not linked by transportation axes to subcenters of the same order. This allows to preserve a linked system of green corridors penetrating the development zones across scales avoiding the fragmentation of green areas and ensuring a good accessibility to recreational areas.

The spatial model is completed by a population distribution model which globally follows the same hierarchical logic. However, we weakened the strong fractal order what allows to conceive a more or less polycentric spatial system.

We can adapt the theoretical concept easily to real world situation without changing the underlying multiscale logic. A decision support system has been developed allowing to simulate development scenarios and to evaluate them. The evaluation procedure is based on fuzzy evaluation of distance acceptance for accessing to the different types of amenities according to the ranking of needs. We used for evaluation data issued from a great set of French planning documents like Master plans. We show an example how the software package can be used concretely.

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Graph Drawing and Network Visualization – An Overview – (Keynote Speech)

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Abstract. Graph Drawing and Network visualization supports the exploration, analysis, and communication of relational data arising in a variety of application domains: from bioinformatics to software engineering, from social media to cyber-security, from data bases to powergrid systems. Aim of this keynote speech is to introduce this thriving research area, highlighting some of its basic approaches and pointing to some promising research directions.

1 Introduction

Graph Drawing and Network Visualization is at the intersection of different disciplines and it combines topics that traditionally belong to theoretical computer science with methods and approaches that characterize more applied disciplines. Namely, it can be related to Graph Algorithms, Geometric Graph Theory and Geometric computing, Combinatorial Optimization, Experimental Analysis, User Studies, System Design and Development, and Human Computer Interaction. This combination of theory and practice is well reflected in the flagship conference of the area, the *International Symposium on Graph Drawing and Network Visualization*, that has two tracks, one focusing on combinatorial and algorithmic aspects and the other on the design of network visualization systems and interfaces. The conference is now at its 31st edition; a full list of the symposia and their proceedings, published by Springer in the LNCS series can be found at the URL: http://www.graphdrawing.org/.

Aim of this short paper is to outline the content of my Keynote Speech at ICCSA 2023, which will be referred to as the "Talk" in the rest of the paper. The talk will introduce the field of Graph Drawing and Network Visualization to a broad audience, with the goal to not only present some key methodological and technological aspects, but also point to some unexplored or partially explored research directions. The rest of this short paper briefly outlines the content of the talk and provides some references that can be a starting point for researchers interested in working on Graph Drawing and Network Visualization.

2 Why Visualize Networks?

Back in 1973 the famous statistician Francis Anscombe, gave a convincing example of why visualization is fundamental component of data analysis. The example is known as the *Anscombe's quartet* [3] and it consists of four sets of 11 points each that are almost identical in terms of the basic statistic properties of their x– and y– coordinates. Namely the mean values and the variance of x and y are exactly the same in the four sets, while the correlation of x and y and the linear regression are the same up to the second decimal. In spite of this statistical similarity, the data look very different when displayed in the Euclidean plane which leads to the conclusion that they correspond to significantly different phenomena. Figure 1 reports the four sets of Anscombe's quartet. After fifty years, with the arrival of AI-based technologies and the need of explaining and interpreting machine-driven suggestions before making strategic decision, the lesson of Anscombe's quartet has not just kept but even increased its relevance.

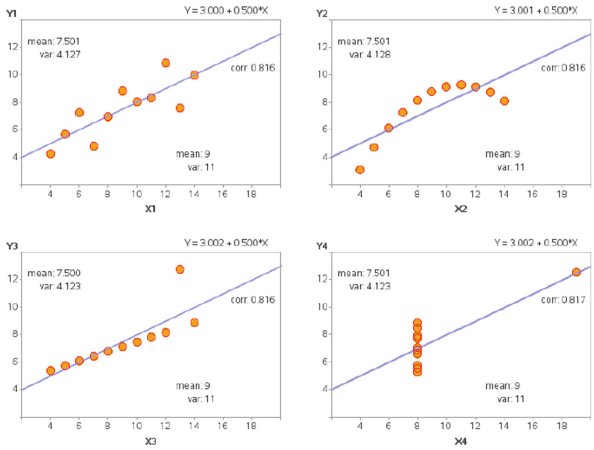


Fig. 1. The four point sets in Anscombe's quartet [3]; the figure also reports statistical values of the x and y variables.

As a matter of fact, nowadays the need of visualization systems goes beyond the verification of the accuracy of some statistical analysis on a set of scattered data. Recent technological advances have generated torrents of data that area relational in nature and typically modeled as networks: the nodes of the networks store the features of the data and the edges of the networks describe the semantic relationships between the data features. Such networked data sets (whose algebraic underlying structure is a called graph in discrete mathematics) arise in a variety of application domains including, for example, Systems Biology, Social Network Analysis, Software Engineering, Networking, Data Bases, Homeland Security, and Business Intelligence. In these (and many other) contexts, systems that support the visual analysis of networks and graphs play a central role in critical decision making processes. These are human-in-the-loop processes where the

continuous interaction between humans (decision makers) and data mining or optimization algorithms (AI/ML components) supports the data exploration, the development of verifiable theories about the data, and the extraction of new knowledge that is used to make strategic choices. A seminal book by Keim et al. [33] schematically represents the human-in-the-loop approach to making sense of networked data sets as in Fig. 2. See also [46–49].

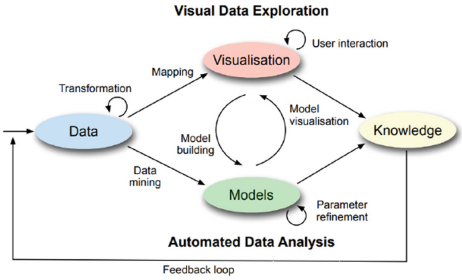


Fig. 2. Sense-making/knowledge generation loop. This conceptual interaction model between human analysts and network visualization system is at the basis of network visual analytics system design [33].

To make a concrete application example of the analysis of a network by interacting with its visualization, consider the problem of contrasting financial crimes such as money laundering or tax evasion. These crimes are based on relevant volumes of financial transactions to conceal the identity, the source, or the destination of illegally gained money. Also, the adopted patterns to pursue the illegal goals continuously change to conceal the crimes. Therefore, contrasting them requires special investigation units which must analyze very large and highly dynamic data sets and discover relationships between different subjects to untangle complex fraudulent plots. The investigative cycle begins with data collection and filtering; it is then followed by modeling the data as a social network (also called *financial activity network* in this context) to which different data mining and data analytic methods are applied, including graph pattern matching, social network analysis, machine learning, and information diffusion. By the network visualization system detectives can interactively explore the data, gain insight and make new hypotheses about possible criminal activities, verify the hypotheses by asking the system to provide more details about specific portions of the network, refine previous outputs, and eventually gain new knowledge. Figure 3 illustrates a small financial activity network where, by means of the interaction between an officer of the Italian Revenue Agency and the MALDIVE system described in [10] a fraudulent pattern has been identified. Precisely, the tax officer has encoded a risky relational scheme among taxpayers into a suspicious graph pattern; in response, the system has made a search in the taxpayer network and it has returned one such pattern. See, e.g., [9, 11, 14, 18, 38] for more papers and references about visual analytic applications to contrasting financial crimes.

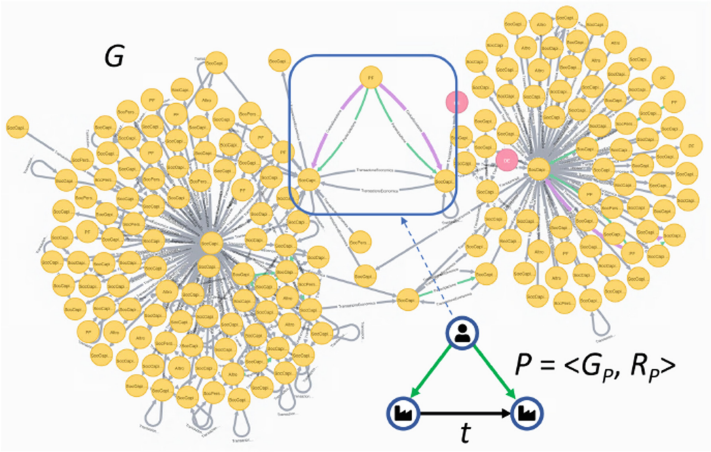


Fig. 3. A financial activity network from [10]. The pattern in the figure represents a SuppliesFromAssociated scheme, consisting of an economic transaction and two shareholding relationships.

3 Facets of Graph Drawing and Network Visualization

The Talk overviews some of the fundamental facets that characterize the research in Graph Drawing and Network Visualization. Namely:

- Graph drawing metaphors: Depending on the application context, different metaphors can be used to represent a relational data set modeled as a graph. The talk will briefly recall the matrix representation, the space filling representation, the contact representation, and the node-link representation which is, by far, the most commonly used (see, e.g., [43]).
- Interaction paradigms: Different interaction paradigms have different impacts on the sense-making process of the user about the visualized network. The Talk will go through the full-view, top-down, bottom-up, incremental, and narrative paradigms. Pros and cons will be highlighted for each approach, also by means of examples and applications. The discussion of the top-down interaction paradigm will also consider the hybrid visualization models (see, e.g., [2, 24, 26, 28, 39]) while the discussion about the incremental paradigm will focus on research about graph storyplans (see, e.g., [4, 6, 7]).
- Graph drawing algorithms: Three main algorithmic approaches will be reviewed, namely the force-directed, the layered), and the planarization-based approach; see, e.g., [5]. We shall also make some remarks about FPT algorithms for graph drawing (see, e.g., [8, 19, 20, 25, 27, 40, 53]) and about how the optimization challenges vary when it is assumed that the input has or does not have a fixed combinatorial embedding (see, e.g., [12, 13, 16, 17, 23]).
- Experimental analysis and user-studies: The Talk will mostly compare two models to define and experimentally validate those optimization goals that define a “readable”

network visualization, i.e. a visualization that in a given application context can easily convey the structure of a relational data set so to guarantee efficiency both in its visual exploration and in the elaboration of new knowledge. Special focus will be given to a set emerging optimization goals related to edge crossings that are currently investigated in the graph drawing and network visualization community unedr the name of "graph drawing beyond planarity" (see, e.g., [1, 15, 29, 35]).

The talk shall also point to some promising research directions, including: (i) Extend the body of papers devoted to user-studies that compare the impact of different graph drawing metaphors on the user perception. (ii) Extend the study of interaction paradigms to extended reality environments (see, e.g., [21, 30, 36, 37]); (iii) Engineer the FPT algorithms for graph drawing and experimentally compare their performances with exact or approximate solutions; and (iv) Develop new algorithmic fameworks in the context of graph drawing beyond planarity.

We conclude this short paper with pointers to publication venues and key references that can be browsed by researchers interested in the fascinating field of Graph Drawing and Network Visualization.

4 Pointers to Publication venues and Key References

A limited list of conferences where Graph Drawing and Network Visualization papers are regularly part of the program includes *IEEE VIS, EuroVis, SoCG, ISAAC, ACM-SIAM SODA, WADS,* and *WG*. Among the many journals where several Graph Drawing and Network Visualization papers have appeared during the last three decades we recall *IEEE Transactions on Visualization and Computer Graphs, SIAM Jounal of Computing, Computer Graphics Forum, Journal of Computer and System Sciences, Algorithmica, Journal of Graph Algorithms and Applications, Theoretical Computer Science, Information Sciences, Discrete and Computational Geometry, Computational Geometry: Theory and Applications, ACM Computing Surveys,* and *Computer Science Review*. A limited list of books, surveys, or papers that contain interesting algorithmic challenges on Graph Drawing and Network Visualization include [5, 15, 22, 29, 31–35, 41–45, 50–52].

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Understanding Non-Covalent Interactions in Biological Processes through QM/MM-EDA Dynamic Simulations

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Molecular dynamic simulations in biological environments such as proteins, DNA or lipids involves a large number of atoms, so classical models based on widely parametrized force fields are employed instead of more accurate quantum methods, whose high computational requirements preclude their application. The parametrization of appropriate force fields for classical molecular dynamics relies on the precise knowledge of the non-covalent inter and intramolecular interactions responsible for very important aspects, such as macromolecular arrangements, cell membrane permeation, ion solvation, etc. This implies, among other things, knowledge of the nature of the interaction, which may be governed by electrostatic, repulsion or dispersion forces. In order to know the balance between different forces, quantum calculations are frequently performed on simplified molecular models and the data obtained from these calculations are used to parametrize the force fields employed in classical simulations. These parameters are, among others, atomic charges, permanent electric dipole moments and atomic polarizabilities. However, it sometimes happens that the molecular models used for the quantum calculations are too simple and the results obtained can differ greatly from those of the extended system. As an alternative to classical and quantum methods, hybrid quantum/classical schemes (QM/MM) can be introduced, where the extended system is neither truncated nor simplified, but only the most important region is treated quantum mechanically.

In this presentation, molecular dynamic simulations and calculations with hybrid schemes are first introduced in a simple way for a broad and multidisciplinary audience. Then, a method developed in our group to investigate intermolecular interactions using hybrid quantum/classical schemes (QM/MM-EDA) is presented and some applications to the study of dynamic processes of ion solvation and membrane permeation are discussed [1–3]. Special attention is paid to the implementation details of the method in the EDA-NCI software [4].

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