A Numerical Scheme for Solving a Mathematical Model Derived from Larvae-Algae-Mussel Interactions

Ramoni Z. S. Azevedo[1], Charles H. X. B. Barbosa[2], Isaac P. Santos[1,3(✉)], José C. R. Silva[4], Dayse H. Pastore[4], Anna R. C. Costa[4], Claudia M. Dias[2], Raquel M. A. Figueira[5], and Humberto F. M. Fortunato[5]

[1] Federal University of Espírito Santo, Vitória, Espírito Santo, Brazil
ramoni.sedano@aluno.ufes.br
[2] Federal Rural University of Rio de Janeiro, Seropédica, Rio de Janeiro, Brazil
mazza@ufrrj.br
[3] Federal University of Espírito Santo, São Mateus, Espírito Santo, Brazil
isaac.santos@ufes.br
[4] Federal Centers of Technical Education Celso Suckow da Fonseca, Rio de Janeiro, Rio de Janeiro, Brazil
{jose.rubianes,dayse.pastore,anna.costa}@cefet-rj.br
[5] hubz, Rio de Janeiro, Rio de Janeiro, Brazil
{raquel.figueira,humberto.fortunato}@hubz.com.br

Abstract. In this work is proposed the use of a numerical strategy based on the operator splitting technique, for solving a mathematical model for the population of the golden mussel in its adult stage, larval stage and algae (its food source) in aquatic environments, presented in [1,19]. The model is composed of three unsteady and nonlinear advective-diffusive-reactive equations for species dynamics and the Navier-Stokes equations to simulate the water velocity field. We employ the operator splitting technique in order to effectively handle the reaction terms and the stiff processes associated with the model. The numerical methodology solves the transport problem in two stages: first, given the velocity field, we solve the advective-diffusive problem to obtain the densities of larvae, algae and mussels; then, we use this first step approximation as initial condition for solving the system of ordinary differential equations for the reactions terms. The new numerical formulation is then used in a 3D simulation of golden mussel proliferation in a section of the Pereira Barreto channel (Brazil), with a focus on population control actions. Preliminary results are discussed, as well as other considerations related to numerical strategy.

Keywords: Golden Mussel · Numerical Methods · Operator Splitting Technique

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1 Introduction

The existence of the non-native species *Limnoperna fortunei*, also known as the golden mussel, in rivers and reservoirs can result in several impacts to the environment and economic activities [2]. In Brazil, this mollusk species is notably abundant within hydroelectric power plant reservoirs. Within these reservoirs, the mollusks possess the tendency to obstruct pipes, grilles, and heat exchangers, as these locations provide optimal conditions for their growth and reproductive activities due to the favorable temperature settings. To deal with this problem, a two-dimensional model capturing the interactions between larvae, algae, and mussels within aquatic environments was proposed in [19]. In this work we present the three-dimensional model to illustrate the population dynamics of mussels, considering the densities of adult mussels, mussel larvae, and algae in a stretch of the Pereira Barreto channel, located in Brazil, with a focus on population control actions. This channel was chosen as the study area because it artificially connects the reservoirs of two main hydroelectric plants in the Urubupungá Complex (Brazil) in order to maximize energy production, the Ilha Solteira HPP and the Três Irmãos HPP. Both plants have an advanced degree of golden mussel infestation, as does the channel itself. The extension of the model to the three-dimensional version is challenging since a new numerical treatment is necessary to avoid oscillations and deal with the computational complexity.

A numerical formulation for solving the mathematical model is presented. As the model is composed of three unsteady and nonlinear advective-diffusive-reactive equations for species densities coupled with the Navier-Stokes equations to simulate the velocity field of the water, we employ the operator splitting technique [20] in the finite element method context in order to effectively handle the reaction terms and the stiff processes associated with the model. The numerical methodology solves the transport problem in two stages: first, given the velocity field, we solve the advective-diffusive problem to obtain the densities of larvae, algae and mussels; then, we use this first step approximation as initial condition for solving the system of ordinary differential equations for the reactions terms. In the firs step, the nonlinear stabilized finite element method SUPG - Streamline Upwind Petrov-Galerkin [3] plus CAU - Consistent Approximate Upwind [6] and the BDF2 - two-step Backward Differentiation Formula of second order [8] are employed in the spatial and time discretizations. The nonlinear process is solved by a Picard fixed point iteration [4]. In the second step, the system of ODEs for reactions is approximated by the fourth-order Runge-Kutta scheme [4], as will be seen in the next section. Numerical simulations associated with a local validation of biological and environmental variables can be used to provide a more assertive and complete view of the hydrological and ecological dynamics of the studied environment. Thus, the results can serving as an additional tool for environmental agencies and operators to manage the golden mussel in Pereira Barreto channel.

This work is organized as follows. Section 2 is devoted to present the mathematical model. In Sect. 3, we present the numerical formulation. The results of the numerical simulations are shown in Sect. 4 and Sect. 5 concludes this paper.

2 Mathematical Model

The larvae-mussel-algae model consists of finding $L = L(\boldsymbol{x}, t)$, $M = M(\boldsymbol{x}, t)$ and $A = A(\boldsymbol{x}, t)$, the densities of larvae, mussels and algae, respectively, such that

$$\frac{\partial L}{\partial t} - D_L \Delta L + \boldsymbol{u} \cdot \boldsymbol{\nabla} L = R_L(L, M, A), \text{ in } \Omega \times [0, t_F], \tag{1}$$

$$\frac{\partial M}{\partial t} - D_M \Delta M = R_M(L, M, A), \text{ in } \Omega_M \times [0, t_F], \tag{2}$$

$$\frac{\partial A}{\partial t} - D_A \Delta A + \boldsymbol{u} \cdot \boldsymbol{\nabla} A = R_A(L, M, A), \text{ in } \Omega \times [0, t_F], \tag{3}$$

where $\Omega \subset \mathbb{R}^3$ is an open and bounded domain with a Lipschitz boundary Γ, $[0, t_F]$ is the temporal interval, with $t_F > 0$, $\Omega_M \subset \Omega$ is the spatial domain for the mussels, representing a layer close to the boundary walls (solid substrates and side walls), and

$$R_L(L, M, A) = r_1 M \left(1 - \frac{L}{K_L}\right) - (b_1 + \lambda_L) L, \tag{4}$$

$$R_M(L, M, A) = \lambda_M L \left(\frac{A^2}{c_1^2 + A^2}\right)\left(1 - \frac{M}{K_M}\right) - b_2 M, \tag{5}$$

$$R_A(L, M, A) = r_2 A \left(1 - \frac{A}{K_A}\right) - b_3 \left(\frac{A^2}{c_2^2 + A^2}\right) M \tag{6}$$

are the reactive terms.

The first component of the dynamics, described by Eqs. (1) and (4), pertains to the variation in larvae population. It accounts for the growth of larvae, which is related to the adult mussel population, conforming described in Cataldo & Boltovskoy [7]. The model further incorporates a logistic growth function, given as a function of the intrinsic growth rate of the larvae population, r_1, and the carrying capacity of the larvae population, K_L [10]. The rates of mortality and maturation of the larvae are denoted as b_1 and λ_M, respectively. In order to model the spatial propagation, the mathematical formulation incorporates diffusion and advection terms, with D_L representing the larval diffusion coefficient and $\boldsymbol{u}$ denoting the flow velocity field. The second equation in the model, Eq. (2) with R_M given by (5), characterizes the dynamics of the adult mussel population. In this case, the growth of mussels is influenced by both larval maturation and the availability of algae, with studies indicating seaweed algae as the primary food source for the golden mussel

[13]. The equation incorporates a logistic growth rate, where K_M represents the carrying capacity for mussels, c_1 denotes the half-saturation constant for adults, and b_2 signifies the mortality rate resulting from fish predation. The parameter D_M corresponds to the diffusion coefficient, a measure of mussel motility caused by their pedal locomotion mechanism and its concomitant byssal thread deployment [5,14,21]. Lastly, Eqs. (3) and (6) represent the dynamics of algae. This model assumes a growth rate, denoted as r_2, with logistic growth dynamics constrained by a carrying capacity, K_A, and a mortality rate due to predation by mussels, expressed as b_3. Additionally, the mathematical formulation incorporates diffusion and advection terms, where D_A signifies the diffusion coefficient governing algae dispersal. For a comprehensive understanding of this model, we refer the interested reader to Silva et al. (2022) [19].

Dirichlet boundary conditions for larvae and algae are imposed on the inflow of the channel, whereas homogeneous Neumann boundary condition are applied to the remaining portions of the boundary. The homogeneous Neumann boundary condition signify the absence of larvae and algae movement across the boundary. To simplify the computational implementation, we consider $M = 0$ in $\Omega \backslash \Omega_M$. The initial conditions are given by

$$L(\boldsymbol{x}, 0) = L_0(\boldsymbol{x}), \quad M(\boldsymbol{x}, 0) = M_0(\boldsymbol{x}), \quad A(\boldsymbol{x}, 0) = A_0(\boldsymbol{x}), \tag{7}$$

where L_0, M_0, A_0 are given non-negative functions representing the initial densities of larvae, mussels and algae, respectively. In the larvae and algae equations, Eqs. (1) and (3), the velocity field $\boldsymbol{u}$ is obtained from the unsteady incompressible Navier-Stokes equations [18].

3 Numerical Formulation

The model (1)–(3) is a unsteady and nonlinear system of advective-diffusive-reactive equations coupled through reactive terms. The free divergence velocity field, $\boldsymbol{u}$, which appears in the larvae and algae equations, is obtained from the unsteady incompressible Navier-Stokes equations. To solve the system of three transport equations, we use operator splitting technique, presented in [17,20]. This numerical scheme consists of solving the advection and diffusion terms separately from the reaction terms. This decomposition of operators is computationally efficient in solving advective-diffusive-reactive transport problems with complex reactive terms, especially in the common case when the timescale of reactive processes is much smaller than the timescale of advective/diffusive processes [17].

Thus, the approximate solution of (1)–(3), with suitable initial and boundary conditions, is obtained in two stages, which can be solved with different time steps. In the first stage the system of homogeneous advection-diffusion equations, given by (8)–(10), is solved by the finite element method in space, coupled with the nonlinear stabilized method, Consistent Approximate Upwind (CAU) [11], and by the two-step Backward Differentiation Formula (BDF2) in time. The resulting system of nonlinear equations is solved by a Picard fixed point iteration.

In the second stage the system of ODE's for the nonlinear reactions terms, Eqs. (11)–(13), is solved by the the fourth-order Runge-Kutta scheme. These stages are shown as follow.

Stage 01: solve the system of advective-diffusive equations:

$$\frac{\partial L}{\partial t} - D_L \Delta L + \boldsymbol{u} \cdot \boldsymbol{\nabla} L = 0, \tag{8}$$

$$\frac{\partial M}{\partial t} - D_M \Delta M = 0, \tag{9}$$

$$\frac{\partial A}{\partial t} - D_A \Delta A + \boldsymbol{u} \cdot \boldsymbol{\nabla} A = 0. \tag{10}$$

Stage 02: solve the ODE's system of reactive equations:

$$\frac{\partial L}{\partial t} = R_L(L, M, A), \tag{11}$$

$$\frac{\partial M}{\partial t} = R_M(L, M, A), \tag{12}$$

$$\frac{\partial A}{\partial t} = R_A(L, M, A). \tag{13}$$

The intermediate solution obtained in each time step, Δt, in the first stage, is used as initial condition for the reaction equations in the second stage, also calculated in Δt using a much more refined time step, $\Delta t_R = \Delta t / N_R$, where N_R is the number of small time steps for the Runge-Kutta scheme in each Δt. The numerical formulation for the Navier-Stokes model is based on the Characteristic Galerkin method [9].

4 Numerical Experiments

In this section we present the numerical experiments in order to evaluate the quality of the obtained solutions, comparing it to the densities observed in the field. Recent *in situ* measurements were carried out in December 2020 and August 2021, obtaining a mussel density of 3,936 gm^{-3} and 7,546 gm^{-3}, respectively.

We used the *FreeFEM++* software [12] to generate the mesh and to solve the transient incompressible Navier-Stokes equations to obtain the velocity field. A code in *MATLAB*© platform [15] was developed to solve the system of partial differential equations, given in Eqs. (1)–(3). The 3D domain Ω represents a stretch of the Pereira Barreto channel, corresponding to one third of its total length, that is 3, 200 m long, close to the Três Irmãos HPP reservoir, located in the Tietê river basin, next to the municipalities of Pereira Barreto (SP) and Andradina (SP).

We considered a period of time of 9 months to evaluate the beginning of the golden mussel infestation. The following initial values were used for the populations: $L(\boldsymbol{x}, 0) = 0.0194115\,\mathrm{gl}^{-1}$, $M(\boldsymbol{x}, 0) = 1\,\mathrm{gm}^{-3}$ and $A(\boldsymbol{x}, 0) = 0.001\,\mathrm{gl}^{-1}$. The parameters used in the simulations are described in Table 1.

Table 1. Parameters used in the numerical simulations.

Parameter	Value	Unit	Reference
D_A	1.2	$m^2 day^{-1}$	[5]
D_M	0.0012	$m^2 day^{-1}$	[16]
D_L	0.012	$m^2 day^{-1}$	[14]
b_1	0.015	day^{-1}	inferred
b_2, b_3	0.02	day^{-1}	inferred
λ_M, λ_L	0.03	day^{-1}	inferred
r_1	0.07	day^{-1}	inferred
r_2	0.12	day^{-1}	inferred
K_L	20	gl^{-1}	inferred
K_M	1,732	gm^{-3}	inferred
K_A	0.01	gl^{-1}	inferred
c_1, c_2	0.001	gl^{-1}	inferred

The domain was discretized with 11,184 tetrahedral elements and 50,970 nodes, conforming mesh shown in Fig. 1.

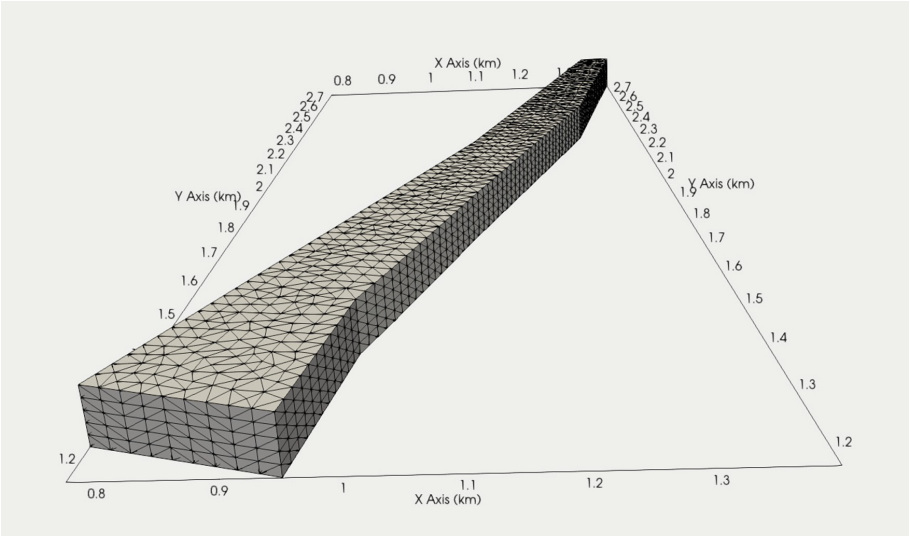

Fig. 1. Discretization of the spatial domain.

Figure 2 shows the velocity field. We use as initial condition for the Navier-Stokes equations, $\boldsymbol{u}(\boldsymbol{x}, 0) = \mathbf{0}$, in Ω. Also, a Dirichlet boundary condition on the channel inlet, for the velocity field, is given by $\boldsymbol{u} = 0.13\,\mathrm{ms}^{-1}$.

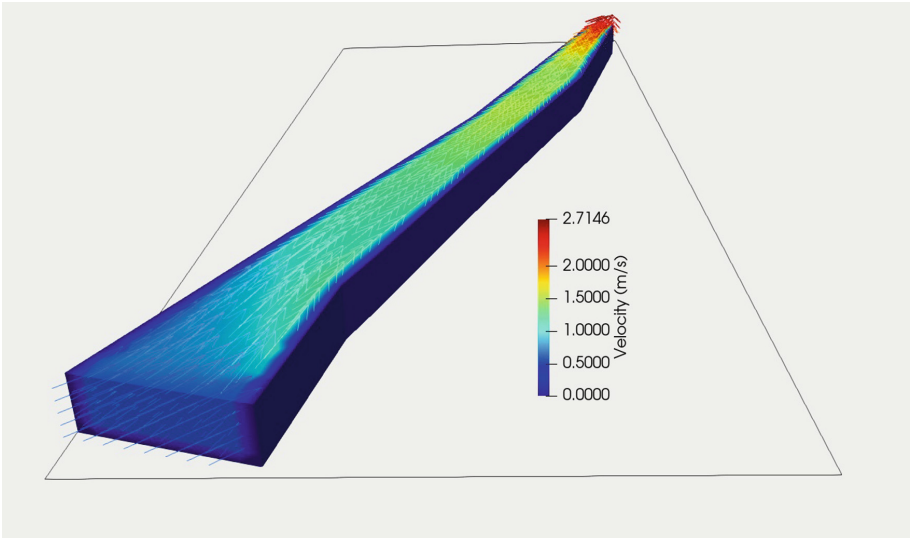

Fig. 2. Velocity field obtained from incompressible transient Navier-Stokes equations.

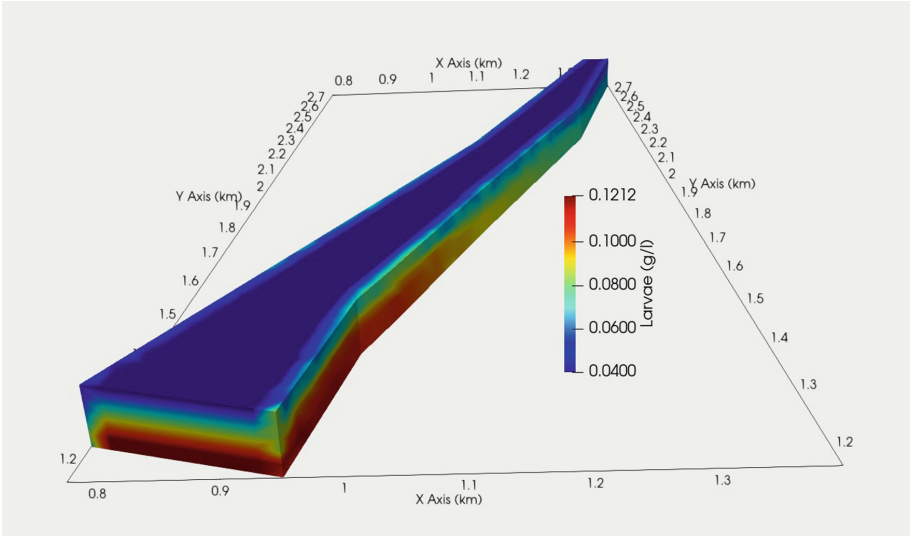

Fig. 3. Densities of Larvae after 9 months of infestation.

In the fist time step the time derivatives of the advective-diffusive equations are discretized by the Backward Euler (BDF1) method, since the BDF2 is a two-step scheme. Moreover, in each time step the algorithm performed $s_{max} = 20$ nonlinear iterations, using a Picard fixed point scheme.

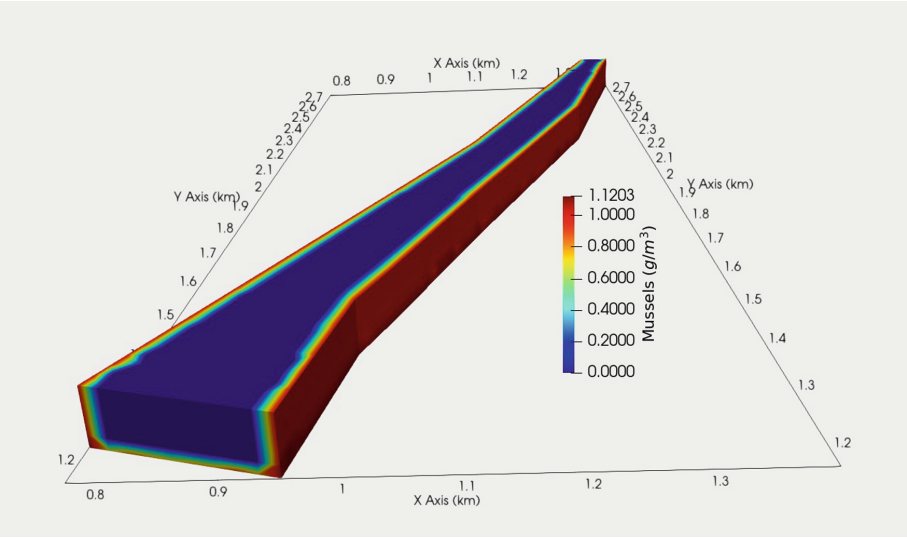

Fig. 4. Densities of Mussels after 9 months of infestation.

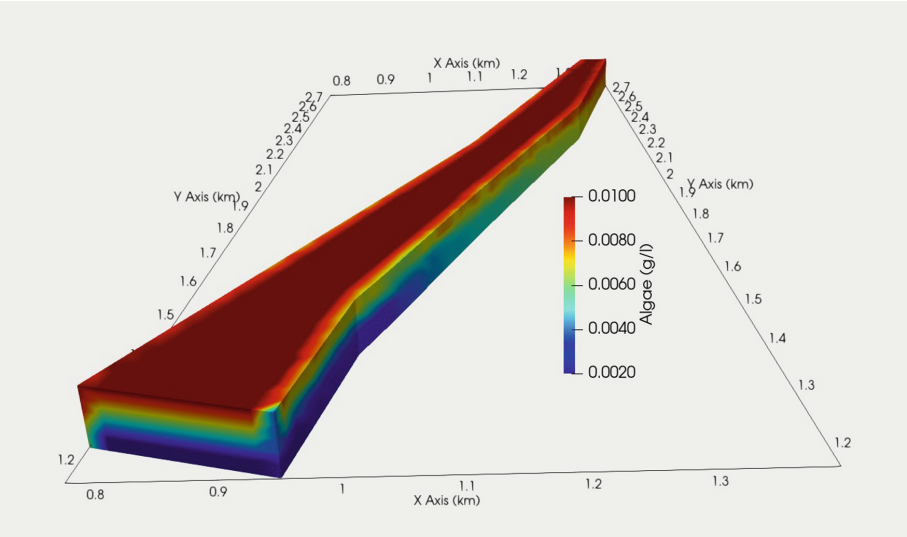

Fig. 5. Densities of Algae after 9 months of infestation.

The results for the densities of larvae, mussels and algae, in the period of 9 months, are shown in Figs. 3, 4 and 5, respectively. The larvae population at the inflow boundary is carried across the domain, due to the velocity field. In some regions far from the water flow and near the lateral boundary there is an increase in the larvae density. The mussel population, concentrated on the lateral

boundary of the domain, grows as expected. The algae population is homogeneous throughout the domain with lower density near the lateral boundaries, where the mussels reside.

5 Conclusions

We have presented a numerical formulation employing the operator splitting technique to solve a complex system that arises from the interactions between larvae, algae, and mussels. This system contains both transient and nonlinear transport PDEs, making it a difficult problem to solve. To overcome this challenge, we adopted a two-stage approach where we first solved the advective-diffusive transport problems using the nonlinear stabilized finite element method, CAU, and the BDF2 scheme in time. Then, we used the fourth-order Runge-Kutta scheme to solve the system of ordinary differential equations for the reactions terms.

The work focused on studying the population dynamics of larvae, mussels, and algae over a short period of nine months. The preliminary results indicate that the model accurately represents the interaction between the populations during this initial period of infestation. The increase in mussel density supports the hypothesis that the Pereira Barreto channel serves as a nursery for the species. Additionally, the channel can serve as a passage for mussels to infest both the Tietê River, which feeds the Três Irmãos HPP reservoir, and the São José dos Dourados River, which feeds the Ilha Solteira HPP reservoir.

The operator splitting technique was very efficient in controlling the numerical oscillations generated by the complexity of the problem. In the future, we plan to run longer simulations using more refined meshes and a larger spatial domain to allow for more accurate comparisons between our numerical solutions and *in situ* data. Additionally, the numerical experiments suggest that the two-stage division scheme can significantly reduce computational time.

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