XLIII CILAMCE
21–25, November, 2022
FOZ DO IGUAÇU – PR – BRAZIL

A numerical scheme for solving a mathematical model derived from larvae-algae-mussel interactions

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Abstract. In this work we present a numerical formulation for solving a mathematical model, derived from larvae-algae-mussel interactions in aquatic environments, proposed in [1]. 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 in the finite element method context for solving 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 first stage, the nonlinear stabilized finite element method CAU and the two-step Backward Differentiation Formula of second order are employed in the spatial and time discretizations. The nonlinear process is solved by a Picard fixed point iteration. In the second stage, the system of ordinary differential equations for reactions is approximated by the fourth-order Runge-Kutta scheme. The numerical formulation proposed is used to simulate the 3D dynamics of species proliferation and quantify the golden mussel population in a stretch of the Pereira Barreto channel, located in Brazil, with a focus on population control actions. The preliminary results as well as other considerations related to the problem and the numerical model are discussed.

Keywords: golden mussel, larvae-algae-mussel model, Navier-Stokes equations, numerical methods, nonlinear system of PDEs

1 Introduction

The presence of the invasive species *Limnoperna fortunei*, known as golden mussel, in rivers and reservoirs can result in several impacts on the environment and economic activities [2]. In Brazil, this mollusk is particularly common in hydroelectric power plant reservoirs. In these areas, the animals can block the grids, pipes and heat exchangers, a particularly favored spot where the temperature contributes to the reproduction and growth of the bivalve. To deal with the problem, a larvae-algae-mussel interactions two-dimensional model in aquatic environments was proposed in [1]. In this work we present the three-dimensional model to illustrate the population dynamics of mussels, where we consider the densities of the adult mussels, mussel larvae, and algae which is its main source of food, in a stretch of the Pereira Barreto channel, located in Brazil, with a focus on population control actions. The channel was elected as the study area because is an artificially constructed channel which connects the reservoirs of two main hydroelectric power plants of the Complexo de Urubupungá (Brazil) to maximize energy production: the Ilha Solteira and the Três Irmãos HPPs. Both power plants suffer greatly with the golden mussel infestation and the channel itself is entirely occupied by these species. 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. Then 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 [3] in the finite element method context for solving the transport problem in two steps. The first step stands for 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 - ODE for the reactions terms. In the firs step, the nonlinear stabilized finite element method SUPG - Streamline Upwind Petrov–Galerkin [4] plus CAU - Consistent Approximate Upwind [5] and the BDF2 - two-step Backward Differentiation Formula of second order [6] are employed in the spatial and time discretizations. The nonlinear process is solved by a Picard fixed point iteration [7]. In the second step, the system of ODEs for reactions is approximated by the fourth-order Runge-Kutta scheme [7], as will be seen in the next section. The numerical simulation associated with a local verification of environmental information and biological variables can be used to provide a more complete and clear view of the ecological and hydrological dynamics of the studied environment, as well as provide crucial information for the infestation management by HPP operators of the region. Thus, the results can serving as an additional tool for environmental agencies and operators to manage the golden mussel in Pereira Barreto channel.

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

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

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

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

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

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

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

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

are the reactive terms.

The first part of the dynamics corresponding to larvae variation, Eqs. (1) and (4), admits that the growth of larvae is related to adult mussel population, due to external reproduction as indicated by Cataldo & Boltovskoy [8]. Besides, the logistical growth function [9] that depends on an intrinsic growth rate of the larvae population r_1 and the carrying capacity for the larvae population, K_L, which is the limit of individuals of a particular species (density) that the environment can sustain due to limiting factors [10]. In addition, the losses of larvae are understood as mortality in a rate of b_1, and the maturation, which represents the larvae that successfully turns into adult golden mussel in a rate of λ_M. Finally, to model the spatial propagation in a certain domain, a diffusion parcel and an advection term due to the suspension of larvae in the water column [8] were considered, being $\boldsymbol{u}$ the velocity field and D_L the diffusion coefficient of larvae. For the second part (adult mussels), Eqs. (2) and (5) of the model, it is admitted that mussel growth depends on the larvae maturation and algae availability, since the seaweed algae is the golden mussel's main source of food as some studies indicated [11]. Accordingly, the model associates mussel population growth directly with mature larvae and a function related to algae predation. The equation also highlights the logistical growth rate [12, 13], being K_M the carrying capacity for the golden mussel, c_1 the half saturation constant for the adults, and b_2 the mortality rate due to fish predation. Furthermore, a diffusion term is considered, admitting D_M as a measure of mussel motility caused by their pedal locomotion mechanism and its concomitant byssal thread deployment [14]. For the algae variation, Eqs. (3) and (6), this can be directly modelled assuming an r_2 growth rate and the logistical growth limited by a carrying capacity for algae, K_A. Besides, the terms of diffusion and advection were considered, with D_A being the diffusion coefficient of algae and b_3 its mortality due to predation by golden mussels. For more details of this model see [1].

Dirichlet boundary conditions for larvae and algae are imposed on the inflow of the channel, whereas homogeneous Neumann boundary condition are imposed in the remaining part of the boundary. The homogeneous Neumann boundary condition means that there is no population movement of larvae and algae across the boundary. To simplify the computational implementation, we consider $M = 0$ in $\Omega \backslash \Omega_M$. The mathematical model (1)-(3) is completed by assuming the initial conditions,

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

where L_0, M_0, A_0 are given non-negative functions representing the initial densities of larvae, mussels and algae, respectively. The velocity field $\boldsymbol{u}$ in the advective terms of (1) and (3) is obtained from the unsteady incompressible Navier-Stokes equations [15].

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 [3, 16]. 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 [16].

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) [17], 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 [18].

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 [19] to generate the mesh and to solve the transient incompressible Navier-Stokes equations to obtain the velocity field. A code in *MATLAB*© platform [20] 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 $3,200m$ 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 4 months to evaluate the beginning of the golden mussel infestation. The following initial values were used for the populations: $L(\boldsymbol{x}, 0) = 0.0194115\ gl^{-1}$, $M(\boldsymbol{x}, 0) = 1\ gm^{-3}$ and $A(\boldsymbol{x}, 0) = 0.001\ gl^{-1}$. 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	$m^2 day^{-1}$	[14]
D_M	0.0012	$m^2 day^{-1}$	[21]
D_L	0.012	$m^2 day^{-1}$	[12]
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 Figure 1.

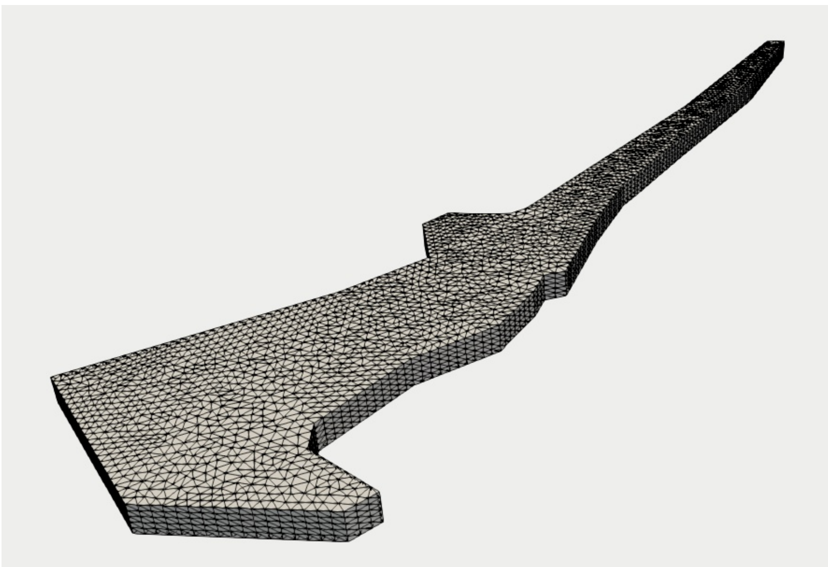

Figure 1. Discretization of the spatial domain.

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

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.

The results for the densities of larvae, mussels and algae, in the period of 4 months, are shown in Figures

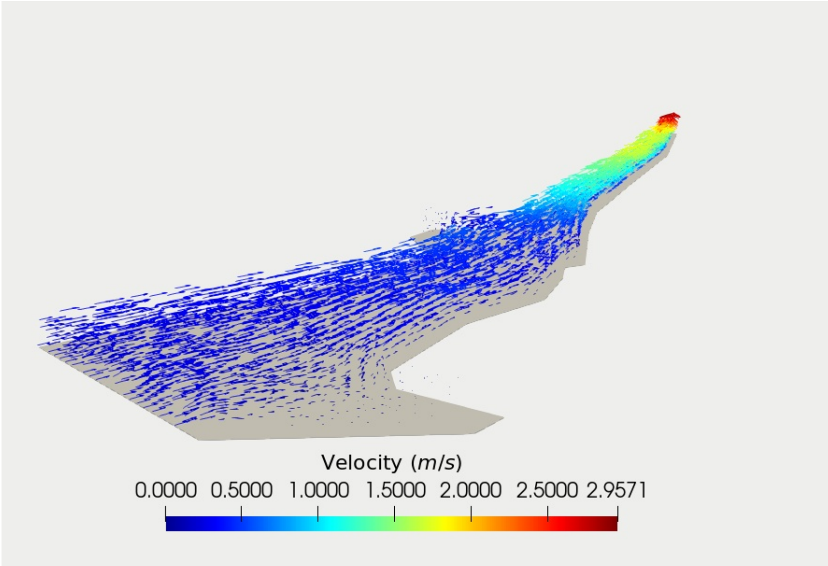

Figure 2. Velocity field obtained from incompressible transient Navier-Stokes equations.

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.

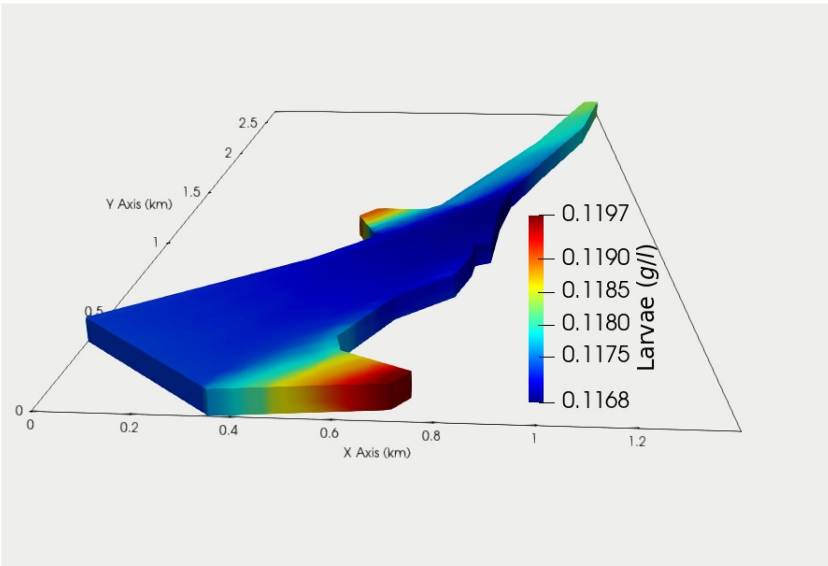

Figure 3. Densities of Larvae after 4 months of infestation.

5 Conclusions

We presented a numerical formulation, based on the finite element method in space and finite difference schemes in time, for solving a complex 3D system of transient and nonlinear transport PDEs arising from larvae, algae and mussel interactions. The operator splitting technique was employed for solving the problem in two stages: first, the advective-diffusive transport problems are solved, using the nonlinear stabilized finite element method, CAU, in space and the BDF2 scheme in time. Then, this first step approximation is used as initial condition for solving the system of ordinary differential equations for the reactions terms, using the fourth-order Runge-Kutta scheme.

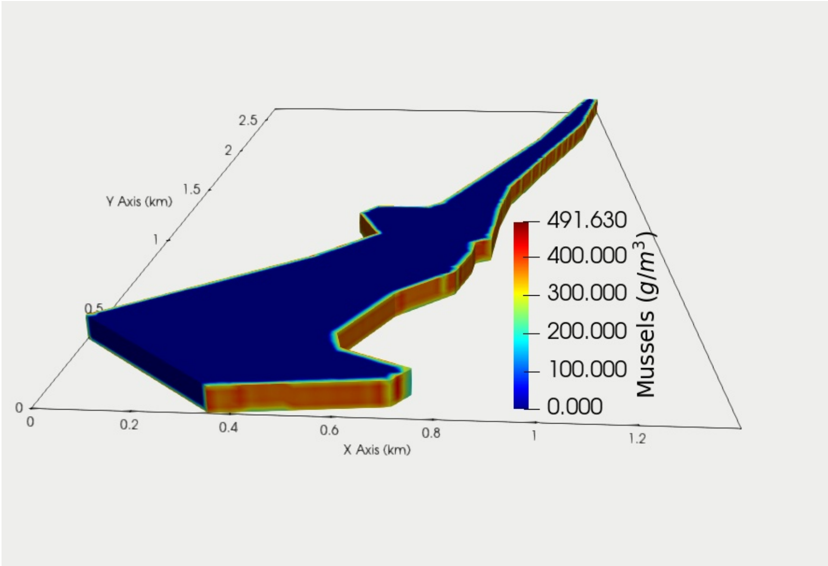

Figure 4. Densities of Mussels after 4 months of infestation.

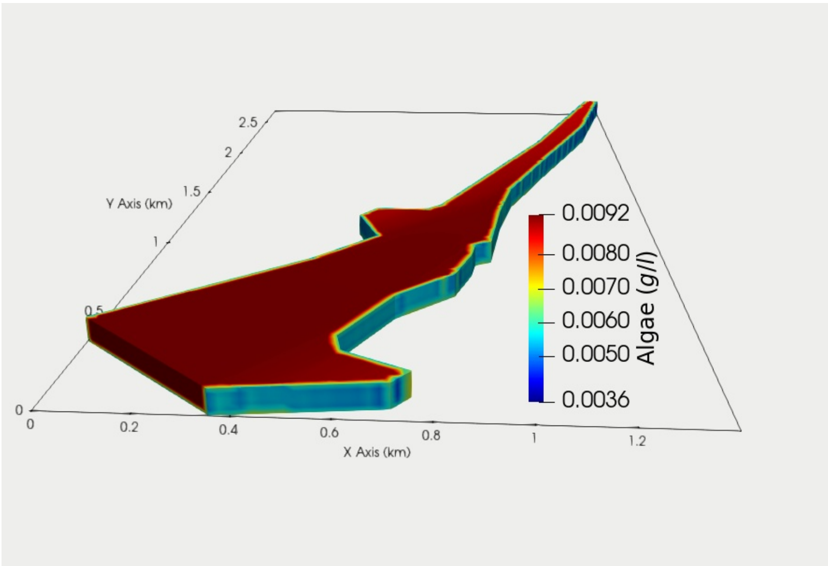

Figure 5. Densities of Algae after 4 months of infestation.

The population dynamics of larvae, mussels and algae were evaluated in a short period of time of only 4 months. These preliminary results indicate that the model represents well the interaction between the populations in this initial period of infestation. The increase in mussel density corroborates the proposition that the Pereira Barreto channel has been serving as a nursery for the species, and that the infestation of the reservoir at Ilha Solteira HPP is mainly due to the arrival of larvae from the Três Irmãos HPP (already heavily infested), which through the channel, reach the São José dos Dourados river and then the Ilha Solteira HPP, thus forming a route for mussel infestation in the region.

A more complex computer simulation is being implemented, evaluating a longer period of time, using more refined meshes and a more extensive spatial domain. This will allow more accurate comparisons between the numerical solutions and *in situ* data, as well the evaluation of the convergence of the numerical process. Furthermore, the numerical experiments indicate that the two-stage division scheme can lead to a considerable reduction in computational time.

Acknowledgements. Research carried out within the scope of the project “Biotechnology for Golden Mussel Control in Brazil” (PD-10381-0419/2019) with funding from CTG Brasil, SPIC Brasil and Tijoá Energia, within the Research & Development Program of ANEEL. This study was financed in part by the Coordenação de

Aperfeiçoamento de Pessoal de Nível Superior - Brasil (CAPES)- Finance Code 001.

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