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Editorial

Differential Models, Numerical Simulations and Applications

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Abstract: Differential models, numerical methods and computer simulations play a fundamental role in applied sciences. Since most of the differential models inspired by real world applications have no analytical solutions, the development of numerical methods and efficient simulation algorithms play a key role in the computation of the solutions to many relevant problems. Moreover, since the model parameters in mathematical models have interesting scientific interpretations and their values are often unknown, estimation techniques need to be developed for parameter identification against the measured data of observed phenomena. In this respect, this Special Issue collects some important developments in different areas of application.

Keywords: applied mathematics; numerical methods; computational mathematics; differential and integro-differential models; inverse problems

Citation: Bretti, G. Differential Models, Numerical Simulations and Applications. *Axioms* **2021**, *10*, 260. https://doi.org/10.3390/axioms10040260

Received: 12 October 2021
Accepted: 13 October 2021
Published: 19 October 2021

1. Special Issue Overview

The Special Issue contains 12 contributions covering a fan of methodology and applications that can be summarized as follows:

1. Numerical methods, simulations and control for particles dynamics [1–4].
2. Modeling and numerical methods for traffic [5,6] and manufacturing problems [7].
3. Inverse problems for biomedical applications [8,9].
4. Theoretical study and numerical solutions for integro-differential equations [10–12].

The main results of the papers are described below.

1.1. Numerical Methods, Simulations and Control for Particles Dynamics

In [1] the authors developed a hybrid PDE–ODE mathematical model mimicking the mechanisms observed in cancer-on-chip experiments, where tumor cells are treated with chemotherapy drugs and secrete chemical signals into the environment, attracting multiple immune cell species. The in silico model proposed here goes towards the construction of a "digital twin" of the experimental immune cells and allows the reconstruction of the chemical gradients in the chip environment in order to better understand the complex mechanisms of immunosurveillance. The development of a trustable simulation algorithm, able to reproduce the dynamics observed in the chip, requires an efficient tool for the calibration of the model parameters. In this respect, the present paper represents a first methodological work to test the feasibility and the soundness of the calibration technique here proposed, based on a multidimensional spline interpolation technique for the time-varying velocity field surfaces obtained from cell trajectories.

The authors in [2] studied a relaxation limit of the so-called aggregation equation with a pointy potential in one-dimensional space. The aggregation equation is today widely used to model the dynamics of a density of individuals attracting each other through a potential. When this potential is pointy, solutions are known to blow up in final time. For this reason, measure-valued solutions have been defined. The convergence of this approximation was studied and a rigorous estimate of the speed of convergence in one dimension with the Newtonian potential was obtained; moreover, the numerical discretization of this relaxation limit by uniformly accurate schemes was investigated.

In [3] a Mean Field Games model where the dynamics of the agents is given by a controlled Langevin equation, and the cost is quadratic, was addressed. An appropriate change of variables transforms the Mean Field Games system into a system of two coupled kinetic Fokker–Planck equations and an existence result for the latter system, obtaining consequently a solution for the Mean Field Games system.

In [4] a tailored version of the Cellular Potts model, a grid-based stochastic approach where cell dynamics are established by a Metropolis algorithm for energy minimization, was developed. The proposed model allowed for quantitatively analyzing selected cell migratory determinants (e.g., the cell and nuclear speed and deformation, and forces acting at the nuclear membrane) in the case of different experimental setups. Most of the numerical results show a remarkable agreement with the corresponding empirical data.

1.2. Modeling and Numerical Methods for Traffic and Manifacturing Problems

In [5], two models describing the dynamics of heavy and light vehicles on a road network were introduced, taking into account the interactions between the two classes. Such models are tailored for two-lane highways where heavy vehicles cannot overtake. The first model couples two first-order macroscopic LWR models, while the second model couples a second-order microscopic follow-the-leader model with a first-order macroscopic LWR model. Numerical results show that both models are able to catch some second-order (inertial) phenomena such as stop and go waves. Models are calibrated by means of real data measured by fixed sensors placed along the A4 Italian highway Trieste–Venice and its branches, provided by Autovie Venete.

The authors of [6] use empirical traffic data collected from three locations in Europe and the US to reveal a three-phase fundamental diagram with two phases located in the uncongested regime. Model-based clustering, hypothesis testing and regression analyses are applied to the speed–flow–occupancy relationship represented in the three-dimensional space to rigorously validate the three phases and identify their gaps. Accordingly, a three-phase macroscopic traffic-flow model and a characterization of solutions to the Riemann problems are proposed. In this work, critical structures in the fundamental diagram that are typically ignored in first- and higher-order models are identified, which could significantly impact travel-time estimation on highways.

In [7], the input-to-state stability (ISS) of an equilibrium for a scalar conservation law with nonlocal velocity and measurement error arising in a highly re-entrant manufacturing system was studied. A numerical discretization of the scalar conservation law with non-local velocity and measurement error was introduced and a suitable discrete Lyapunov function was analyzed to provide ISS of a discrete equilibrium for the proposed numerical approximation.

1.3. Inverse Problems for Biomedical Applications

In [8] a new framework for optimal design was developed, by introducing new protocols for estimating soft tissue parameters in biaxial experiments. This framework is based on the information-theoretic measures of mutual information, and conditional mutual information and their combination is proposed. In particular, the information gain about the parameters from the experiment as the key criterion to be maximized is considered and directly used for optimal design. Information gain is computed through k-nearest neighbor algorithms applied to the joint samples of the parameters and measurements produced by the forward and observation models. For biaxial experiments, the results show that low angles have a relatively low information content compared to high angles. The results also show that a smaller number of angles with suitably chosen combinations can result in higher information gains when compared to a larger number of angles which are poorly combined.

The authors of [9] study the problem of functional connectivity by quantifying the statistical dependencies among time series describing the activity of different neural sources from the magnetic field recorded with magnetoencephalographic (MEG) exam. This problem can be addressed by utilizing connectivity measures whose computation in the frequency domain often relies on the evaluation of the cross-power spectrum of the neural time series, estimated by solving the MEG inverse problem. Recent studies have focused on the optimal determination of the cross-power spectrum in the framework of regularization theory for ill-posed inverse problems, providing indications that, rather surprisingly, the regularization process that leads to the optimal estimate of neural activity does not lead to the optimal estimate of the corresponding functional connectivity. Along these lines, the present paper utilizes synthetic time series, simulating the neural activity recorded by a MEG device to show that the regularization of the cross-power spectrum depends on the spectral complexity of the neural activity.

1.4. Theoretical Study and Numerical Solutions for Integro-Differential Equations

In [10] a prey–predator system with logistic growth of prey and hunting cooperation of predators is studied. The introduction of fractional time derivatives and the related persistent memory strongly characterize the model behavior, as many dynamical systems in the applied sciences are well described by such fractional-order models. Mathematical analysis and numerical simulations are performed to highlight the characteristics of the proposed model. The existence, uniqueness and boundedness of solutions is proved; the stability of the coexistence equilibrium and the occurrence of Hopf bifurcation is investigated. Some numerical approximations of the solution are finally considered; the obtained trajectories confirm the theoretical findings.

The work in [11] is devoted to the study of dynamical models, such as the Rothamsted Carbon (RothC) model, used predict the long-term behavior of soil carbon content for the achievement of land degradation neutrality as measured in terms of the Soil Organic Carbon (SOC), a key indicator of land degradation. Indeed, a reduction in the SOC stock of soil results in degradation and it may also have potential negative effects on soil-derived ecosystem services. In this paper, continuous and discrete versions of the RothC model were compared, especially to achieve long-term solutions. The original discrete formulation of the RothC model was then compared with a novel nonstandard integrator that represents an alternative to the exponential Rosenbrock–Euler approach in the literature.

The authors in [12] studied the asymptotic behavior of the numerical solution to the Volterra integral equations. In particular, a technique based on an appropriate splitting of the kernel is introduced, which allows one to obtain vanishing asymptotic (transient) behavior in the numerical solution, consistent with the properties of the analytical solution, without having to operate restrictions on the integration steplength.

Funding: This research received no external funding.

Conflicts of Interest: The author declares no conflict of interest.

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