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Editorial

Importance of modelling and simulation in biophysical applications

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Abstract: Mathematical modelling and simulation in biophysics and its applications in terms of both theoretical and biological/physical/ecological point of view arise in a number of research problems ranging from physical and chemical processes to biomathematics and life science. As known, the modeling of a biophysical system requires the analysis of the different interactions occurring among the different components of the system. This editorial article deals with the topic of this special issue, which is devoted to the new developments in the modelling and simulation in biophysical applications with special attention to the interplay between different scholars.

Keywords: mathematical models; system biology; computational ecology; nonlinear phenomena in biophysics; validation of biophysical models

Preface

Biophysics is defined as a branch of science that uses the laws of physics, chemistry, mathematical analysis methods, and computer modeling to understand how biological systems work. In short, biophysics is defined as the physics of living organisms. It is obvious that the structure and functions of living beings cannot be explained by a single discipline. For this reason, more disciplines need to come together and look for a solution to the problem. New perspectives of the recent theoretical developments in mathematical modelling in biophysics and its illustrative

applications/analysis in biology, ecology, ecosystem functioning, and health sciences have gained much attention and the interplay among mathematicians, physicists and information science scholars. For the favorable reception of models, a systematic accrual of a good knowledge base is crucial for both science and decision-making. As the roles of models grow in importance, there is an increase in the need for appropriate methods with which to test their quality and performance. For biophysical models, the heterogeneity of data and the range of factors influencing usefulness of their outputs often make it difficult for full analysis and assessment. As a result, modelling studies in the domain of natural sciences often lack elements of good modelling practice related to model validation, that is correspondence of models to its intended purpose [1].

A biophysical model is a simulation of a biological system using mathematical formalizations of the physical properties of that system. Such models can be used to predict the influence of biological and physical factors on complex systems. Areas of interest of biophysical models include the dynamics of complex and active materials, and aspects of collective behavior and self-assembly in both natural systems (e.g., inside the cell) and synthetic ones.

The biophysical modeling approach is based on mathematical modeling and analysis, the development and application of software tools for large-scale biophysical simulation, and close collaboration with experimentalists. Modelling in biophysics, ecology and biology has been widely applied by scientists. This approach has been adopted by the decision-makers and the number of illustrative and practical applications in these areas is increasing over time [2–9]. On the other hand, model evaluation is an essential step in the modelling process because it indicates if the implementation of the calculations involved reproduces the conceptual model of the system to be simulated (model reliability) and the level of accuracy of the model in reproducing the actual system (model usefulness) [10].

Meanwhile, biophysical, process-based models (unlike statistical models) are made up of mixtures of rate equations, comprise approaches with different levels of empiricism, aim at simulating systems which show a non-linear behaviour and often require numerical rather than analytical solutions. In general, two types of modeling can be identified: a conceptual model and a computerized model. The conceptual model is composed of information (input data, parameters and equations) that describes the physical system or process of interest. The computer program includes technical issues and possible errors. In practice, the computer program is tested, rather than the mathematical model representing the system [11].

This Special Issue has published a total of six high-quality papers. In [12], Valkova et al. have probed the effect of the endogenous heptapeptide VV-hemorphin-5 (valorphin) on the bending elasticity of biomimetic lipid membranes of 1-palmitoyl-2-oleoyl-sn-glycero-3-phosphocholine (POPC) by analysis of thermal shape fluctuations of nearly spherical giant unilamellar vesicles. In a wide concentration range covering valorphin concentrations applied in nociceptive screening in vivo, they have reported alterations of the bilayer bending rigidity in a concentration-dependent non-monotonic manner. They have also performed quantitative characterization of VV-hemorphin-5 association to POPC membranes by isothermal titration calorimetry in order to shed light on the partitioning of the amphiphilic hemorphin between the aqueous solution and membranes. The calorimetric results correlate with flicker spectroscopy findings and support the hypothesis about the strength of valorphin-membrane interaction related to the peptide bulk concentration. A higher strength of valorphin interaction with the bilayer corresponds to a more pronounced effect of the peptide on the membrane's mechanical properties. The presented study features the comprehensive

analysis of membrane bending elasticity as a biomarker for physicochemical effects of peptides on lipid bilayers. The reported data on thermodynamic parameters of valorphin interactions with phosphatidylcholine bilayers and alterations of their mechanical properties is expected to be useful for applications of lipid membrane systems in pharmacology and biomedicine.

In [13], Lefebvre has given general formulas for the probability that a given increase in the number of daily new cases is due to the normal variations of the continuous part of the process or rather to a jump of this process. Based on these formulas, the probability of observing the likely start of a new wave of infections is calculated for the application to the COVID-19 pandemic. Mallick et al. [14] have presented a robust methodology to establish an accurate process to estimate Cole parameters and relaxation time from measured BIS data. Six nature inspired algorithms, along with NLS are implemented and studied. Experiments are conducted to obtain BIS data and analysis of variation (ANOVA) is performed. The Cuckoo Search (CS) algorithm achieved a better fitment result and is also able to extract the Cole parameters most accurately among all the algorithms under consideration. The ANOVA result shows that CS algorithm achieved a higher confidence rate. In addition, the CS algorithm requires less sample size compared to other algorithms for distinguishing the change in physical properties of a biological body.

In another study, Almiala and Kuikka have previously presented a model for simulating the spreading of infectious disease throughout a social network and another one for simulating the connectivity of data traffic in an information network. They have argued that these models are similar in that they produce equivalent results with appropriate parameters when run on the same network. They have also explained this by reasoning that the manners in which the models carry out their calculations, although devised from different assumptions, turn out to be equivalent. Moreover, they have shown empirical results of applying the models to calculate the spread of contagion and information connectivity on two complex networks suitable for the models. Based on the results, they have calculated centrality metrics reflecting the outcome of the application, highlighting its important properties [15]. Mala et al. [16] have discussed the passivity analysis for Markovian jumping Neural Networks of neural-type. The results are demonstrated using phases of linear matrix inequalities as well as an improved Lyapunov-Krasovskii functional (LKF) of the triple integral terms and quadruple integrals. The information of the mode-dependent of all delays have been taken into account in the constructed Lyapunov–Krasovskii functional and novel stability criterion is derived. The value of selecting as many Lyapunov matrices that are mode-dependent as possible is demonstrated. The effectiveness and decreased conservatism of the aforementioned theoretical results are eventually demonstrated by a numerical example.

Finally, in [17], Anjam et al. have focused on examining the dynamics of a fractional-order model involving three interconnected lakes, utilizing the Caputo differential operator. The aim is to investigate the issue of lake pollution by analyzing a system of linear equations that represent the interconnecting waterways. To numerically solve the model, they have employed two methods: The Laplace transform with the Adomian decomposition method (LADM) and the Homotopy perturbation method (HPM). They have compared the obtained numerical solutions from both methods and present the results. The study encompasses three variations of the model: the periodic input model, the exponentially decaying input model, and the linear input model. The numerical results are further supported by informative graphical illustrations. Through simulation, they have validated the suitability of the proposed model for addressing the issue at hand. The outcome of this research is considered as it contributes to the understanding and management of water pollution, aiding

policymakers and researchers in formulating effective strategies for maintaining water quality and protecting our environment.

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