



Editorial

Mathematical and computational modeling of biological systems: advances and perspectives

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Abstract: The recent developments in the fields of mathematics and computer sciences have allowed a more accurate description of the dynamics of some biological systems. On the one hand new mathematical frameworks have been proposed and employed in order to gain a complete description of a biological system thus requiring the definition of complicated mathematical structures; on the other hand computational models have been proposed in order to give both a numerical solution of a mathematical model and to derive computation models based on cellular automata and agents. Experimental methods are developed and employed for a quantitative validation of the modeling approaches. This editorial article introduces the topic of this special issue which is devoted to the recent advances and future perspectives of the mathematical and computational frameworks proposed in biosciences.

Keywords: differential equations; complexity; agents; validation; system biology

Biological systems are usually composed by a large number of elements which are able to interact each others and with the outside environment [1]. The evolution of a biological system is thus characterized by interactions which can trigger the onset of complex phenomena [2]. Indeed complexity is a key element which needs to be investigated before developing a modeling tool for a complex biological system. Among the many properties charactering a complex biological system, the ability of performing strategies is an important issue which complicates the modeling and requires a

special attention [3]. Moreover some components of biological systems can be able to proliferate or mutate thus modifying the number and the type of elements.

The observation scale is another issue which needs to be taken into account; some phenomena occur at a specific scale (micro, meso or macro), e.g. molecular, cellular. The temporal and the spatial scales thus need to be investigated [3]. The modeling approaches need to be proposed in order to avoid gaps among the scales.

In the last two decades, many scholars have been involved in the modeling of complex biological systems. Different models have been proposed coming from the mathematical sciences and computational sciences. A brief overview of these approaches follows.

Mathematical models. Biological systems have been firstly investigated by constructing models based on ordinary differential equations, briefly ODE-based models [4]; accordingly the time evolution of the density of the composing elements is obtained by analyzing the density of the all elements. The only independent variable is time. This approach is usually suitable at the macroscopic scale where the interacting populations can be reduced to the main actors. However this approach could be expensive if the number of the main actors is large.

The methods of the continuum mechanics have been also suggested usually for the growth of biological matter and its behavior to physics/biological stress and strain [5]. This approach consists in partial differential equations where space and velocity are also independent variables. The evolution equations are obtained by employing conservation laws and constitutive relations.

Recently kinetic theory models have been proposed for the modeling of a biological system at the cellular level, see [6] and the references cited therein; the evolution of the distribution function of cell populations is the main modeled element. The independent variables consist of an internal variable (strategy, function), velocity and space variables. The evolution equations, obtained by balancing the interactions into the elementary domain of the microscopic states, consist of partial-integro differential equations where the degree of nonlinearity is at least two. The definition of cellular interactions is at the base of this approach. It is worth stressing that in this approach the elements are also called structured population.

Hybrid models, combining the above mentioned different mathematical approaches, is an interesting perspective and it is an important key of this special issue. Indeed any mathematical framework presents advantages et disadvantages which could be relaxed by coupling the mathematical frameworks at different scales.

Computational models. The interest towards the development of computational models for biological systems is twofold. On the one hand a computational model could be of support of a mathematical model based on differential equations; on the other hand a computational model could be directly based on the methods of the information sciences. In this context the agent-based model has been the main approach largely employed in the last decade and recently the employment of multi-agent modeling have gained much attention [7,8].

The derivation of computational methods for the construction of the numerical solution to a mathematical model follows the methods of numerical analysis. Different numerical approaches exist in the pertinent literature which span from classical numerical methods for ordinary differential equations [9] to finite element/spectral methods [10,11] for partial differential equations. However this is a research domain which constantly increase then advances and perspectives in the context of biological systems constitutes an important part of this special issue.

Concurrently, the information sciences has increased their interest in the modeling of biological

systems. On the one hand the information sciences contributes to the numerical simulations of mathematical models by proposing a research activity in the development of computer and memory; on the other hand the information sciences has developed its computational models by employing agent-based models and recently multi-agent-based models [12]. In an agent-based model the actions and interactions of autonomous agents are defined; the interplay with game theory [13] and other computational sciences appears in the heuristic principles of the decisions and in the adaptation and learning processes. The advances and perspectives of these research fields are part of this special issue.

In between the mathematical and computational models for biological systems, an important role is covered by the experimental methods. Empirical and experimental data play a crucial role in the quantitative validation of a modeling approach. This aspect cannot be neglected considering that the main scope of a modeling approach is the reproduction of the data and the prediction of future events or phenomena [14]. This is for instance the case of the COVID-19 pandemic which has shown the importance of new experimental methods for the detection and screening of the infection. Accordingly the advances in this research direction are also part of this special issue.

It is worth stressing that the biosciences mentioned in this special issue are concerned with cellular biophysics, biomechanics, bioenergetics, and some applications in bioengineering such as biophysics membranes, neuro-biophysics, biophysical technology.

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