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Mathematics, complexity and multiscale features of large systems of self-propelled particles

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To Abdelghani Bellouquid, in memoriam

This issue is devoted to complex systems in life sciences. Some perspective ideas on possible objectives of future research are extracted from the contents of this issue and brought to the reader's attention. The final ambitious aim is the development of a mathematical theory for complex living systems.

Keywords: Complexity; self-organization; nonlinear interactions; nonlocal interactions; flocking; control; stability.

1. Introduction

The interest of applied mathematicians in the modeling, qualitative analysis, and simulation of large systems of interacting living entities is rapidly growing, and is witnessed by the recent literature appeared in top level journals in several fields, both in fundamental and applied sciences, as biology, sociology, economy, and medicine. Indeed, it appears that these systems can have a paramount importance in understanding the complexity of life and social sciences.

In addition to the motivations generated by applications, mathematicians are also attracted by the challenging theoretical and computational problems generated by this new frontier of mathematical sciences, which has promoted already an intense quest toward new analytic and computational tools.

The journal M3AS has already captured the aforementioned hints by publishing several special issues appeared in recent years.[9,12,28] This present issue contributes to the research activity in the field by new contributions and authors. Section 2 deals with some discussions on the interactions between mathematical sciences and complex systems, while Sec. 3 presents the contents of the issue and looks ahead to research perspectives.

2. Toward a Mathematical Theory of Large Living Systems

Before dealing with the specific contents of this special issue let us take a look at the panorama of the scientific literature on the subject, in a very personal quest for some basic ideas on the interpretation of complex systems by eminent scientists. It is not surprising that the philosopher Immanuel Kant (1724–1804) already provided a definition of organisms viewed as "living matter"[31]:

> An organized product of nature is that in which everything is an end and reciprocally a means as well.

The concept that living entities have a purpose, which distinguish them from the inert matter, was therefore introduced long time ago. This concept was made more precise in survey paper by Hartwell *et al.*[26]:

> Although living systems obey the laws of physics and chemistry, the notion of *function* or *purpose* differentiates biology from other natural sciences. Organisms exist to reproduce, whereas, outside religious belief, rocks and stars have no purpose. Selection for function has produced the living cell, with a unique set of properties that distinguish it from inanimate systems of interacting molecules.

This forces mathematicians to invent new mathematical tools, possibly a new mathematical theory. In a similar spirit, we already learned from Schrödinger that living systems operate far from equilibrium,[45] and that they evolve in time[35,36] by a Darwinian-type dynamics.

A statement by Jona-Lasinio[30] (here translated into English from the Italian original version) captures the need of an evolutionary description:

> Life represents an advanced stage of an evolutive and selective process. To me it seems difficult to understand living entities without considering their historical evolution. Population dynamics should explain the emergence of individual living entities by selection.

The invention of a mathematical theory goes through the search for new mathematical structures. Indeed, as observed by Gromov in Ref. 25:

> Mathematics is about "interesting structures". What makes a structure interesting is an abundance of interesting problems; we study a structure by solving these problems. The worlds of science, as well as of mathematics

> itself, is abundant with gems (germs?) of simple beautiful ideas. When and how many of these ideas direct you toward beautiful mathematics?

The statement,[26] which represents the viewpoint of a biologist, motivates the search of new mathematical tools suitable to understand the complexity of biological systems. Therefore, mathematicians should go beyond traditional methods used for the inert matter, which definitely fails in the case of living entities, and introduce new ideas that can establish new frontiers for mathematics.

Moreover, the statement[25] indicates how the quest for new methods should end up with the design of mathematical structures suitable to become the background for developments important in applications. In fact, it indicates that a structure might even be richer than what is needed for a specific modeling project. Therefore, mathematicians are motivated to investigate all properties of the new structures looking for their complete predictive ability.

This historic-philosophical introduction suggests a key question, that we should pose to ourselves: *How mathematical sciences can contribute to a theory of living systems?*

Obviously, we cannot naively expect to provide, today, an exhaustive answer to such a question. But many scientists are actively working toward this target, and several new promising mathematical theories have already been developed.

The first field to be mentioned, in this framework, is the development of evolutionary game theory, which provides an important conceptual contribution to the modeling of complex systems. This topic is critically analyzed in the survey paper,[29] where the authors emphasize the substantial differences with respect to the classical game theory.[37,38] Namely rather than dealing with players involved in the game with strategies that attempt to maximize *their own payoff*, in evolutionary game theory we have a whole population that is pursuing an *individual or collective well-being*. This concept is well expressed by the following quotation extracted from Ref. 29:

> Evolutionary game theory deals with entire populations of players, all programmed to use the same strategy (or type of behavior). Strategies with higher payoff will spread within the population (this can be achieved by learning, by copying or inheriting strategies, or even by infection. The payoffs depend on the actions of the coplayers and hence on the frequencies of the strategies within the population).

In particular the authors clearly state[29] that tools of game theory must include the aforementioned features of evolution and learning dynamics. Indeed the literature in the field shows that complexity features of living systems can be taken into account by suitable developments of evolutionary game theory as in Refs. 24, 39 and 43, and of mean field games.[33] Recent developments involve games on graphs,[2] and interactions between probability distributions.[16]

However, modeling the dynamics of the behavioral and complexity features needs the design of a differential framework. For instance, suitable developments of methods of statistical mechanics,[27,42] kinetic theory[40] and the so-called kinetic theory of active particles,[16] which combines methods of the classical kinetic theory and the aforementioned theoretical tools of game theory. These somehow different approaches should possibly be unified into a common framework.

Moreover, it is worth stressing that game theory can contribute to detect early signals of sudden changes[44] looking for the "black swan"[15] (where the expression "black swan" was coined by Taleb,[47] who used it as a metaphor for highly improbable events). The extreme rareness of these events makes them difficult to incorporate into a scientific theory, yet they can have a very large impact.

3. Contents and Critical Analysis

The papers published in this special issue cover a variety of topics mainly focused, with two exceptions, on modeling and qualitative analysis of swarming phenomena. In more detail, the first of the six papers shows how diffusion can occur over networks, while the second paper deals with the derivation of macroscopic models from a description given by the kinetic theory approach, while the other four papers are focused on different aspects of swarming dynamics.

Paper[5] proposes a macroscopic model which describes a meta-population consisting of several sub-populations connected through a network. These sub-populations interact with each other, and the rules of interactions are given by a system of ordinary differential equations. Each sub-population has its own structure and dynamics and occupies an edge of a graph. Its dynamics is driven, according to different cases, by diffusion or by transport along the edge. The analytic properties of these multiscale models are studied in detail and referred to a "systems biology" approach.

The derivation of macroscopic equations from the underlying description at the microscopic scale is treated in Ref. 17. The authors focus on fractional Keller–Segel's-type models. A new class of models, with respect to those reviewed in Secs. 5–7 of Ref. 11, is proposed and brought to the attention of applied mathematicians for further studies concerning both analytic problems and applications. Indeed, fractional models appear to be of special interest in biology. Recently, the micro–macro general approach has been also applied to derive hydrodynamics for multi-agent systems.[9,10]

Paper[20] proposes an individual-based model for fiber elements having the ability to cross-link or unlink each other and to align with each other at the cross links. The authors first formally derive a kinetic model for the fiber and for the cross-links distribution functions, and subsequently consider the fast linking/unlinking regime in which the model can be reduced to the fiber distribution function only, and investigate its diffusion limit. The authors then discuss the use of this model in various applications.

A two-species system of nonlocal interaction PDEs modeling the swarming dynamics of predators and prey is presented in Ref. 21. All agents interact through attractive/repulsive forces of gradient type. The model has a particle-based discrete (ODE) version and a continuum PDE version. The authors investigate the structure of the particle stationary solution and their stability in the ODE system.

Paper[34] presents a detailed study of emerging behaviors delivered by the Kuramoto model under the effect of frustration and inertia corresponding to some possible initial configurations. The authors prove a variety of stability and synchronization properties, which definitely contribute to a deeper understanding of the model.

Social dynamics and collective migration of animals in a cohesive group are studied in Ref. 41. The authors consider a group of agents able to align their velocities to a global target velocity, or to follow the group via interaction with the other agents. The balance between these two attractive forces is the control acting on each agent to drive the group to consensus at the target velocity. It is shown that the optimal control strategies in the case of final and integral costs consist in controlling the agents whose velocities are the furthest from the target one: these agents sense only the target velocity and become leaders, while the uncontrolled ones sense only the group, and become followers.

Papers[5] and Ref. 17 lead to the idea that the study of living systems always needs a *multiscale approach*, where the first step is the selection of the observation scale and of the related representation by mathematical variables and equations, while the second step is the search of the mathematical links between the various scales used to construct the model. For instance, macroscopic equations should not be postulated *a priori*, but related to the underlying scale of individuals. When this approach is applied, the result generally leads to a variety of models at the macroscopic scale which were not foreseen by the purely phenomenological derivation.

The other papers definitely improve the knowledge of the mathematics of swarming phenomena, where applied mathematicians are hunting for a general theory suitable to support the derivation of specific models. Control theory applied to swarming dynamics was already treated in special issues,[18,19] where an interesting interaction appears between swarming models and economics.[1]

Finally, let us stress that several concepts discussed in the previous section can be extended to social and economical systems as well. In fact, this is connected to a radical philosophical change that is taking place in social and economic disciplines, characterizing the interplay among Economics, Psychology, and Sociology in a new framework, where the traditional assumption of "rational socio-economic behavior" is abandoned. The new viewpoint, that looks at these disciplines as highly affected by individual (rational or irrational) behaviors, reactions, and interactions, is becoming more and more widely accepted, see for instance Refs. 4, 7, 8, 32 and 46. Although this topic is not directly treated in the present special issue, we believe it to be a very important direction of research, where a milestone in the modeling approach would consist in understanding the complexity features of living systems and of their social interactions, and then in developing mathematical methods suitable to capture, as well as possible, all these features.

Mathematicians are chasing a unified modeling approach, and possibly for a new mathematical theory. However, the literature in the field, as well as this special issue, indicate that, despite valuable efforts, this challenging objective has not yet been achieved. Waiting for it, we can observe that the consensus toward some common computational tools is still growing. We refer in particular to Monte Carlo particle methods, either semi-regular[3] or stochastic.[22,40] The basic idea of stochastic methods consists in representing the distribution functions by a number of computational particles which move in the computational domain and collide according to stochastic rules which can be directly related to the dynamics of interaction of the specific model under consideration. Macroscopic flow properties are usually obtained by time averaging particle properties, see also the recent applications in Refs. 6, 14 and 23, as well as the various applications in social dynamics treated in Ref. 40.

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