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Challenges in active particles methods: Theory and applications

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This paper is a brief introduction to the mathematical tools employed in the modeling and simulation of the interactions of a large number of living entities, and provides a presentation of the papers published in a special issue devoted to this topic. In addition, we bring to the reader's attention some perspective ideas on possible objectives of future researches.

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AMS Subject Classification: 35K55, 35Q70, 35Q91, 35Q92

1. Introduction

This paper presents a special issue focused on mathematical tools and applications of the so-called *active particles approach*. This refers to the various analytic and computational tools used in the study, from modeling to simulations, of systems with a large number of interacting living entities, typically called active particles. The term *active particles*, as witnessed in the survey,[38] has been introduced to denote dynamics that go somehow beyond classical deterministic rules, but it is nowadays systematically used just to denote interacting entities in large living systems.

The recent expository paper[34] shows how swarming phenomena, which appear in the natural world (e.g. wheeling flocks of birds, swirling schools of fish, or systems of interacting robots) generate challenging problems in physics and in mathematics, with an immediate interest in technology. This literature is developed from the pioneer paper by Cucker and Smale,[24] which has the great merit of having initiated this research line. Applications are everywhere, as reported for instance in Refs. 4 and 35.

These systems require computational methods suitable to account for the heterogeneity often shown by complex systems. Monte Carlo particle methods and discontinuous Galerkin methods have been recently used for this computational target, see Refs. 6, 27, 35 and 40 as examples of recent developments from the pioneer computational approach of Bird.[17]

The interest of mathematical sciences for this specific research field is rapidly growing due to the joint action of the stimuli exerted by highly challenging problems and by the related interest in various fields: in nature, society, technology, and science in general. Hence mathematicians started to enter a research domain which used to be an almost exclusive field for physicists.

This special issue follows recent other ones in this journal, devoted to closely related topics, specifically self-propelled particles[11,12] and modeling of social systems.[13] Its contents are presented in Sec. 2, which addresses the basic features of the known mathematical approaches to modeling and to related analytical problems. Section 3 is devoted to research perspectives focused on the derivation of models at the higher scale from underlying description at the lower scale. Indeed, this topic pervades all papers proposed in this special issue.

2. Presentation of the Contents, Looking Ahead to Further Developments

A brief description of the contents of this special issue is presented in this section. All papers are devoted to various aspects of the modeling: derivations based on the physical interpretation of interactions, qualitative analyses, and simulations. The interpretation of swarms behavior is broad, as it focuses on organized living entities with the ability to express specific strategies, individual and collective, somehow related to their well-being. This aspect is constantly present in the preceding special issues,[11–13] while new results and research perspectives are proposed in the papers presented here.

In more detail, various topics on control theory applied to alignment dynamics in swarms are presented in Ref. 1. This subject has been introduced in Refs. 2 and 20 and it is now giving rise to various developments. A detailed analysis, starting from modeling and followed by a qualitative analysis of some control actions, is proposed in Ref. 1, where well-focused simulations enlighten the achievements of the theoretical analysis.

Control problems is the key issue treated in Ref. 41, focusing on the description of the dynamics, in time and space, of an ecological model derived from a detailed interpretation of the dynamics at the microscopic scale.

Analytical problems related to swarming models are studied in Ref. 32, where the authors prove a uniform-in-time convergence (from the discrete-time Cucker–Smale model[24] to the continuous-time model) which is valid for the whole time interval, as time-step tends to zero. This improves on classical theory, which yields convergence results valid only in any finite-time interval. This paper belongs to a recent group of several important contributions to the study of analytical properties of swarming models.[15,25,33,37]

Multiscale problems for age structures myxobacteria are dealt with in Ref. 26, where the authors derive an individual-based model by taking into account the information delivered by empirical data. Subsequently, the authors obtain a Kolmogorov–Fokker–Plank kinetic equation by a mean-field approximation, and hence move to the derivation of models at the macroscopic scale. A computational analysis enlightens the descriptive ability of the model.

An additional application in biology is developed in Ref. 23 by a kinetic theory approach focusing on the dynamics of multi-cellular systems. An active particle approach allows to include very special features which characterize biological functions, as shown in Ref. 29 as well as in the micro–macro derivations presented in Ref. 9. The derivation of macroscopic equations from the underlying description by kinetic equations is also developed in Ref. 23 by a first-order perturbation technique. An additional useful reference for higher order approximations can be found in Ref. 18. A class of aggregation–diffusion partial differential equations (PDEs) with nonlinear mobility is derived in Ref. 30 by large particle limit of a suitable nonlocal version of the follow-the-leader scheme. The authors show that the result applies also to strongly degenerate diffusion equations.

Active particle methods can also be used to model human crowds by macroscopic equations, as shown in Ref. 22, where models at the microscopic scale are used to develop a macroscopic description of the dynamics by which pedestrians select their velocity direction. This delicate matter has also been treated by the kinetic theory approach in Ref. 14. The model is subsequently applied to describe the behaviors of pedestrians in the presence of obstacles.

A model of the diffusion of criminality is proposed in Ref. 21. The authors start from an agent-type model and move to the higher scale by a mean-field continuum model with truncated Lévy flights for residential burglary in one space dimension. The authors show that the continuum model has an excellent agreement with the agent-based simulations. This suggests that local diffusion models are universal for continuum limits of this problem, the important quantity being the diffusion coefficient. A detailed analysis of the diffusion dynamics is supported by the additional aid of computational simulations.

3. From the Contents of the Special Issue to Research Perspectives

The papers of this special issue focus a variety of research perspectives, too many to be treated in a short note like the present one. Indeed, we trust that the hints present in these papers will rapidly motivate future research activity on several challenging frontier problems.

A research perspective refers to a topic which pervades the whole contents of the issue, namely the derivation, by asymptotic methods, of models at the higher macroscopic scale from the underlying description at the lower scale.

As it is known, the physical–biological systems of a large number of interacting individuals can be modeled at three classical scales as follows:

- Microscopic (individual-based) scales, where interacting entities are individually identified, while the state of the whole system is given by their position and velocity (which are variables depending on time) and the dynamics is described by the systems of ordinary differential equations.
- Mesoscopic (kinetic) scales, where position and velocity are still used to identify the microscopic state, but their representation is delivered by a suitable probability distribution function over the microscopic state.
- Macroscopic (hydrodynamic) scales, where the overall state of the system is described by locally averaged quantities, typically density and linear momentum, regarded as dependent variables of time and space. Mathematical models describe the evolution of the macrovariables by systems of PDEs where the acceleration term of the momentum equation, which acts on the particles in the elementary space volume, has to be modeled by suitable heuristic interpretations of the physical reality.

The scientific community agrees that the approach at each scale presents advantages and drawbacks.

For instance, models at the microscopic scale are definitely consistent with physical reality (as the number of entities, say active particles, is always finite), but the computation of local-averaged quantities, as well as the action on each particle from the surrounding ones, is subject to fluctuations that are density dependent.

The kinetic theory approach allows to insert in the individual state additional variables, as for instance emotional states (see Ref. 14) in crowd models, or biological functions (see Ref. 16) in the case of multicellular systems. In addition, macroscopic quantities are simply obtained by weighted moments of the dependent variables, namely by quadrature, but the number of particles is not high enough to justify the continuous approximation of the dependent variables which are statistical distributions over the microscopic state.

The macroscopic approach provides directly the dynamics of the macroscopic quantities which are of interest for the applications and allow the use of deterministic methods for PDEs, but the continuity assumption does not correspond to physical reality, while the averaging process hides the heterogeneous behavior of individuals that is typical of living systems.

These reasoning's motivate the need to develop a unified modeling approach, where interactions at each scale are modeled by the same principles. In more details, each active particle interacts, at the microscale, with all particles in its sensitivity domain by interactions which are nonlocal and nonlinearly additive. Further, the theoretical–empirical approach proposed in Ref. 5 suggests that interactions involve only a fixed number of individuals rather than all individuals in their sensitivity domain. Some pioneering papers have accounted for this specific feature in swarming modeling[15] and in related computational problems.[3] An additional hint is given by the research activity on socio-economical systems,[28] that suggest to take nonsymmetric interactions also into account.

It is rather immediate to observe that these modeling principles have to be accounted in the kinetic theory approach, where it is required that the number of interacting particles is sufficiently high to allow the use of a continuous probability distribution, to be identified as a dependent variable of the differential system.

On the other hand, the modeling approach at the macroscopic scale is less immediate, as in it the aforementioned principles should be referred to the active particles in the elementary volume of the physical space rather than to individuals.

An additional difficulty to be accounted for is that the microscopic state of active particles might include an additional variable, called activity, modeling emotional-social states as shown in vehicular traffic[19] and in crowd modeling.[8,42] This feature is always present in the modeling of social systems, and it becomes an important feature when stress conditions appear in crowd dynamics.[39,43]

The *unified approach* that has been outlined above is a necessary preliminary step for the derivation of models at the macroscopic scale from the underlying models at the lower scale, say from individual-based to macroscopic, and/or from kinetic to macroscopic, being understood that kinetic models should use models of individual-based interactions derived from those at the microscopic scale. Some results can already be found in the literature concerning, for instance, vehicular traffic,[10] crowd dynamics,[8] and swarms.[7,18,37] We might say that such a unified approach is the challenging research perspective that we propose in this paper.

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