

## Mathematical Models of Self-Propelled Particles

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This note presents the papers published in two special issues devoted to the modeling of large systems of self-propelled particles. The contents of these papers are presented in the general framework of the conceptual analytic difficulties and of the computational problems that are met when dealing with this class of systems. In addition, some perspective ideas on possible objectives of future research are extracted from the contents of this issue and brought to the reader's attention.

*Keywords:* Complexity, active particles, crowds, swarms, nonlinear interactions, nonlocal interactions.

### 1. A General Overview at the State of the Art

The modeling, the qualitative analysis, and the related computational problems of large systems of self-propelled particles have generated a rapidly growing interest of applied mathematicians who are attracted by the conceptual difficulties that these systems have posed to mathematical sciences. Applications refer to vehicular traffic, crowds, swarms, financial markets, and, in general, large social systems.

As a matter of fact, the physics of these systems is still not fully understood, while a unified modeling approach is not yet available, despite various scientific contributions have been produced aiming at this challenging target. This interest has already motivated a sequel of special issues of the journal *M3AS*, appeared in recent years<sup>10,11,24</sup>, where various aspects of the conceptual, analytic, and computational difficulties generated by these systems have been tackled. Still, the amount of open problems is much greater than the amount of those that have been solved.

In parallel, other special issues have been devoted to the modeling of large living systems in different contexts, where individual behaviors play an important role

in the collective and self-organized dynamics. An example is the special issue <sup>45</sup>, devoted to cross diffusion models in biological tissues where qualitative analysis <sup>28,44</sup> of mathematical problems and derivation of different types of models <sup>8</sup> have been presented.

An additional recent example is given by the special issue on behavioral social systems <sup>12</sup>, focusing on different approaches, such as agent based methods <sup>21</sup>, probability theory <sup>4,37</sup>, stochastic differential equations <sup>33</sup>, and kinetic theory methods <sup>20</sup>, looking for a unified approach to a systems sociology <sup>2</sup> where individual behaviors can play an important role in the overall dynamics.

A detailed analysis of the state of the art indicates that different modeling approaches coexist which, however, are still waiting for a unified approach suitable to describe the complex dynamics of large systems of self-propelled particles. Indeed, this challenging search of a unified approach will be indicated, in Section 3, as the most important objective of future research activity in the field..

Our presentation contains two more steps. Section 2 proposes a rationale for the modeling of large systems of self-propelled particles focusing on the conceptual difficulties that this poses to applied mathematicians. Section 3 briefly introduces the contents of the two special issues and, subsequently, brings to the reader's attention some possible research perspectives based also on a direct analysis of the papers presented in these two special issues.

## 2. On the Modeling of Large Systems of Self-propelled Particles

As mentioned already, different modeling approaches have been developed to capture the complex dynamics of self-propelled, hence living, particles. The recent literature shows that behavioral features can be taken into account by suitable developments of several methods coming from different scientific backgrounds: Statistical mechanics <sup>23</sup>, kinetic theory <sup>36</sup>, theoretical tools of evolutionary game theory <sup>3,26,35</sup>, mean field games <sup>29,30,31</sup>, and the so-called kinetic theory of active particles <sup>2</sup>, which combines methods of the classical kinetic theory with theoretical tools of game theory.

Despite several technical differences, all methods are inspired, up to a certain extent, to theoretical tools of non-equilibrium statistical dynamics including suitable developments of kinetic theory methods, where the main difference with respect to the classical kinetic theory is given by modeling interactions. These generally are nonlocal, nonlinearly additive, and irreversible.

Indeed, various difficulties have to be tackled when dealing with self-propelled particles, as these entities often called *active particles*, borrowing this term from theoretical physics of non classical systems <sup>39</sup>, are living entities which have the ability to develop individual strategies based on the interactions with other particles and on their own specific purposes which can be heterogeneously distributed among them. The overall strategy may evolve to a commonly shared consensus <sup>34</sup> which might lead to organized structure, where a collective intelligence appears.

However, in some cases the rupture of consensus can generate large deviations that may end up with non predictable events, occasionally called *a black swan*.

Bearing all the above in mind, let us now report about some technical difficulties, among the various ones, that need to be tackled in the modeling approach.

- (1) Heterogeneous behaviors constitute a common feature of all large living systems, where individual entities belong to different groups, where each group expresses a common strategy. Each individual, in each group, expresses the said strategy by a different level of intensity. Therefore, interactions involve stochastic entities and the output of interactions is also stochastic.
- (2) Interactions are nonlocal and nonlinearly additive and in some cases occur over the so called “topological domains”<sup>6</sup> which depends on the local density. In addition, individuals perceive the presence of walls and obstacles and modify their trajectory to avoid collisions.
- (3) Interactions do not simply follow mechanical rules since psychological behaviors can play an important role on the dynamics. In addition, communications between individuals generate a *social dynamics* that can have an important influence on the whole dynamics. In particular interaction rules can, in various cases, evolve in time. For instance, social dynamics in crowds can generate panic situations which lead to irrational behaviors<sup>9,46</sup> and produce a negative influence on safety during the evacuation processes<sup>13,40,41</sup>.
- (4) The dynamics at the low scale, corresponding to individual based interactions, provides the necessary input to derive kinetic type models at the mesoscopic scale, where the dependent variable is a probability distribution over the microscopic state. Subsequently, models at the macroscopic scale can be derived by asymptotic methods, where the dependent variable is expanded in powers of a small parameter related to the mean distance between particles. The asymptotic is obtained by letting this parameter tend to zero. This approach replaces heuristic methods, where models are obtained by conservation equations at the macroscopic scale closed by phenomenological models of material behaviors.
- (5) Computational methods should take into account the multiscale essence of large systems of self-propelled particles, where the microscopic scale corresponds to individuals, while the overall collective behavior is observed at a macroscopic scale. Simulations in a variety of specific cases indicate that stochastic particle methods<sup>7</sup> appear to be able to capture efficiently the aforementioned heterogeneity. Applied mathematicians are working at deterministic methods to obtain equally efficient results.



All items in the above list focus on the interpretation and modeling of interactions at the low scale as this is the first step toward the derivation of models at the mesoscopic and, subsequently, macroscopic scale. Therefore attempts toward a unified approach should possibly take into account the possible ways of transferring the individual based dynamics into the collective motion.

### 3. Contributions to the Special Issues and Research Perspectives

Let us now have a more detailed look into the contents of the special issues, where a wide presence is devoted to swarm modeling, while additional topics refer to crowd dynamics and to methodological issues.

Referring to the *first issue*, various aspects of swarm modeling are treated in four papers. In more details, <sup>18</sup> presents a new flocking model based on mechanical coordination, <sup>22</sup>, while <sup>38</sup> enlightens specific properties of the celebrated Cucker and Smale model, and <sup>27</sup> provides a detailed analysis on the blow up of a class of swarm models. The contents of the chapter are completed by <sup>32</sup> devoted to a computational analysis of pedestrian crowds accounting for flux limitation.

Referring to the *second issue*, various topics concerning swarm models have been treated, in particular computational problems <sup>43</sup>, sparse control problems <sup>17</sup>. In addition to warm modeling, crowd dynamics is treated in <sup>25</sup>, where a macroscopic model of pedestrian counter flow is proposed. Analytic problems have been treated in <sup>15</sup>, where an Hilbert type approach has been developed to derive macroscopic equations from the underlying description at the cellular scale delivered by a kinetic theory approach, while multicellular dynamics is studied in <sup>19</sup> also by kinetic type equations focusing on the role of adhesion and proliferation on tumor invasion.

The presentation of the two special issues has shown that a broad variety of topics has been considered, so that the papers of these issues represent an interesting enlargement, with new hints toward open problems, to the already vast literature in the field. Hopefully, mathematicians have now the perspective to develop a number of challenging programs within the environment of mathematical sciences which traditionally attempt, as far as possible, to substitute heuristic tools with rigorous methods that are typical of mathematical sciences.

Bearing all the above in mind, in this section we selected, according to our bias, three possible research perspectives which are brought to the reader's attention.

1. An important, and challenging, topic appears to be the *search of a unified modeling approach* based on a mathematical structure suitable to capture the various complexity features of large systems of self-propelled particles viewed as living systems. This structure should include all types of local and nonlocal interactions. However, its derivation cannot be the end of the story as the main problem still remains the modeling of interactions which characterize each specific system under consideration. This challenging objective needs a deep understanding of the physics of interactions and many empirical data to support and validate the theory. Mathematical sciences look forward to this achievement, which is not yet available in the literature. The search of mathematical structures can interact with the search of physical theories and suggest experiments that might contribute to the validation of the various models.

2. The design of *theoretical tools from game theory* can contribute to the perspective presented in the preceding item. The approach might start from evolutionary game

theory<sup>26,42</sup> accounting for the heterogeneity of players so that their state can be represented by probability distributions. **In addition, space distribution of players could be taken into account, as it plays an important role.** Tools borrowed by mean field games<sup>1,29,30,31</sup> can also contribute to this modeling aspect. Interaction should include the role of collective learning theory<sup>16</sup>. A deep insight into this topic might end up with a new game theory, where players are probability distributions and where the offsprings are not always optimal (as the ones generated by rational behaviors), while irrational, hence non optimal, behaviors should be taken into account at least in some specific circumstances.

**3.** The development of *multiscale methods* is an essential step towards any modeling approach. Individual based models refer to the framework of dynamical systems characterized by a large, but finite, number of degrees of freedom. Models, in general, describe the individual dynamics in space and time of all active particles of the whole systems by large systems of ordinary differential equations. Kinetic type models represent a continuous approximation of models with finite number of degrees of freedom. An open problem consists in the derivation of kinetic type models from the underlying description at the microscopic scale. Indeed, the modeling of interactions at the low scale is a key passage for the derivation of models, as this information is basic in determining the mathematical structures of the kinetic theory approach. The main difficulty consists in showing how kinetic type models can be derived in the limit when the number of particles tends to infinity. An additional problem of interest consists in reversing the process by starting from kinetic type models to understand which type of models at a microscopic scale correspond to a kinetic model. Finally, the classical challenging analytic problem consists in the derivation of models at the macroscopic scale from the underlying description delivered by kinetic type models.

Independently on the aforementioned open problems and scientific contrasts of one approach with respect to the other, our belief is that *modeling* and the development of *computational methods* should march together, without reducing the descriptive ability of models in an attempt to reduce the computational complexity. As a matter of fact, Monte Carlo particle methods<sup>5,7,36</sup> have shown that this computational approach has the ability to transfer into a collective behaviors the dynamics at the low scale. This achievement is obtained without oversimplification of the dynamics of interactions. Hence computational methods obtain at a practical, even though heuristic, level the achievement chased by analytic methods.

The various papers proposed in the two special issues have tackled some of the various problems discussed above. Some of the results are definitely valuable, in particular in connection with the research challenges that were selected here. Therefore, we trust that these special issues can effectively contribute to a significant updating of the state of the art in the field, and hence to the future research activity.

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