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Nonlinear microscale interactions in the kinetic theory of active particles

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ABSTRACT

The aim of this note is to examine the sources of nonlinearity arising in the kinetic theory of active particles. We show how nonlinearities enter the different terms of the theory, giving rise to possible developments toward the modeling of different types of complex systems, mainly living and social ones, where proliferative–destructive processes must be included. Finally, some research perspectives are discussed.

1. Introduction

The kinetic theory for active particles [1] has shown itself to be useful to the modeling of a large variety of complex systems [2–5]. One of the main issues of the theory, denoted as KTAP in the following, is its ability to reduce the overall complexity of phenomena by partitioning the whole system into a number of functional subsystems, whose elements, called active particles, have the capacity to collectively manifest a common strategy. The latter is expressed in terms of a variable, called activity, that characterizes the microscopic state of particles. The state of each subsystem, and as a consequence of the entire system, is described as a probability distribution, a function of the activity and of time. Active particles are allowed to interact with particles belonging both to the same as well as to other subsystems, with phenomenological rules modeled by theoretical tools borrowed from evolutive and stochastic game theory [6,7].

The aim of the present paper is to analyze the different sources of nonlinearity in KTAP. In particular, we stress the relevance of the non-locality and of the nonlinear additivity of the interaction among active particles in order for the KTAP to be able to model the emergence of collective behaviors typical of complex phenomena. In detail, Section 2 reports the general mathematical structures of KTAP. Section 3 develops the main conceptual issue of the paper, namely a detailed analysis of the structure of nonlinearities concerning interactions among particles that require an appropriate revisiting of tools from game theory. Finally, Section 4 proposes a critical analysis and suggests some research perspectives.

2. Mathematical structures

The KTAP deals with systems made up of a large number of interacting particles. Each particle has the ability of expressing a certain task that depends upon its state and on that of other particles. Such an ability is summarized by a scalar variable u, called activity, ranging in a domain $D_u \subseteq \mathbf{R}$, and consequently the elements of the system are called active particles. The way the KTAP manages to reduce the overall complexity is to subdivide the system into a number of functional subsystems, identified by particles that individually express the same strategy. Let us consider a decomposition of the original system into

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$n > 1$ functional subsystems labeled by an index $i = 1, \ldots, n$. Each subsystem is described by a time-evolving distribution function $f_i(u, t) : D_u \times [0, T] \to \mathbf{R}^+$ over the microscopic activity u, where $0 < T \leq +\infty$. The quantity $f_i(u, t)\, du$ represents the (infinitesimal) number of active particles of the i-th subsystem having at time t an activity comprised in the (infinitesimal) interval $[u,\ u + du]$. Under suitable integrability conditions the quantity $N_i(t) = \int_{D_u} f_i(u, t) du$ represents the number of active particles in the i-th functional subsystem at time t. If this number is constant, then each f_i can be normalized with respect to $N_i(0)$ and understood as a probability density. In this paper, we consider a more general setting of KTAP in which particles' transition among different subsystems and proliferative and/or destructive events are allowed, so that the total number $N(t) = \sum_i N_i(t)$ of particles in the whole system is not constant. Moreover, the mathematical structure of KTAP we present here concerns the particular case in which the spatial variable does not enter the picture as happens, for example, when the functional subsystems are localized in a network. We are here mainly concerned with closed systems, i.e., systems in which the active particles do not interact with agents external to the system, though some remark on open systems will be given in the next section. The evolution in time of the distribution functions $f_i(u, t)$, $i = 1, \ldots, n$ is determined by a system of differential equations obtained from a balance of ingoing and outgoing fluxes in the elementary volume $[u,\ u + du]$ of the space of microscopic states. Interactions involve three types of particles, named test, candidate, and field particles. The test particle, with activity u, is a generic representative entity of the functional subsystem under consideration; candidate particles, with activity u_*, are the particles which can gain the test state u as consequence of the interactions; field particles, with activity u^*, are the particles whose presence triggers the interactions of the candidate particles. Following the lines depicted in [1] we denote by $\mathbf{f} = \{f_1, \ldots, f_n\}$ the set of distribution functions. The structure, to be used as a paradigm for the derivation of specific models, is:

$$\partial_t f_i(u, t) = J_i[\mathbf{f}](u, t) = C_i[\mathbf{f}](u, t) + P_i[\mathbf{f}](u, t) - D_i[\mathbf{f}](u, t), \quad i = 1, \ldots, n, \tag{2.1}$$

where:

$$\begin{aligned} C_i[\mathbf{f}](u, t) \ = \ & \sum_{h,k=1}^{n} \int_{D_u \times D_u} \eta_{hk}[\mathbf{f}](u_*, u^*, t)\, \mathcal{B}^i_{hk}[\mathbf{f}](u_* \to u | u_*, u^*, t) f_h(u_*, t) f_k(u^*, t)\, du_*\, du^* \\ & - f_i(u, t) \sum_{k=1}^{n} \int_{D_u} \eta_{ik}[\mathbf{f}](u, u^*, t) f_k(u^*, t)\, du^*, \end{aligned} \tag{2.2}$$

$$P_i[\mathbf{f}](u, t) = \sum_{h,k=1}^{n} \int_{D_u \times D_u} \eta_{hk}[\mathbf{f}](u_*, u^*, t) \mu^i_{hk}[\mathbf{f}](u_* \to u | u_*, u^*, t) f_h(u_*, t) f_k(u^*, t)\, du_*\, du^*, \tag{2.3}$$

$$D_i[\mathbf{f}](u, t) = f_i(u, t) \sum_{k=1}^{n} \int_{D_u} \eta_{ik}[\mathbf{f}](u, u^*, t) \nu_{ik}[\mathbf{f}](u, u^*, t) f_k(u^*, t)\, du^*. \tag{2.4}$$

The meaning of the terms appearing in the previous relations is the following:

- η_{hk} is the encounter rate between the candidate particle of the h-th functional subsystem and the field particle of the k-th functional subsystem;
- $\mathcal{B}^i_{hk}$ is the probability density that the candidate particle of the h-th subsystem with state u_* falls into the i-th subsystem with state u after an interaction with a field particle with state u^* of the h-th functional subsystem;
- $\eta_{hk}\, \mu^i_{hk}$ models the proliferation rate into the i-th functional subsystem due to interactions between the candidate particle of the h-th subsystem and the field particle of the k-th subsystem;
- $\eta_{ik}\, \nu_{ik}$ models the destruction rate due to interactions between the candidate particle of the i-th subsystem and the field particle the k-th subsystem.

Observe that, generalizing the approach proposed in [1], the encounter rates and the interaction terms are here allowed to depend on the set of distribution function $\mathbf{f} = \{f_1, \ldots, f_n\}$. The same notation u is used for the activity variable in different functional subsystems, the index i assesses the specific feature of such a variable. If the functional subsystems are localized in a network [8], then in general an additional index j, possibly different from i, will identify the node. In order for the corresponding mathematical structure to include interaction between active particles from different nodes, only a technical generalization is needed. The above structure can also be interpreted as a general framework for systems whose dynamics allows for a varying number $n = n(t)$ of subsystems, including either the onset of new ones or the suppression of subsystems existing at $t = 0$.

The time evolution of the distribution functions $f_i(t, u)$, $i = 1, \ldots, n$, is obtained by solving the Cauchy problem for Eq. (2.1) with initial data $f_{i_0} = f_i(u, 0)$. For this issue we refer to [9], where global (in time) existence has been proved for closed systems with linearly additive interactions and open systems with interactions depending also on momenta of the distribution function. In the paper [10] more general nonlinear interactions are introduced, while in [11] the global existence is shown for a modified version of (2.1) in which a linear relaxation term is added on the r.h.s. Moreover, in the paper [12] the role of the nonlinearities is discussed as an analogy of the Enskog approach in kinetic theory in a model of cancer-immune competition. It is worth emphasizing that the mathematical structure (2.1)–(2.4) refers to a situation in which neither the number of particles in each subsystem nor the total number of particles in the whole population is preserved. As

a consequence, it suffers from a lack of an *a priori* estimate both on $\int_{D_u} f_i(u,t)du$ $(i=1,\dots,n)$ and on $\sum_{i=1}^{n}\int_{D_u} f_i(u,t)du$, making the continuation of local solutions a difficult task.

Interactions are modeled, as we shall see, by suitable developments of tools of game theory. Nonlinearity refers both to the interaction rates and to the games that model the transition densities. Nonlinearity implies, among various aspects of the dynamics, that particles are not simply subject to the superposition of binary actions but are also affected by the global current state of the system.

3. Nonlinearity sources

In this section we examine the source of nonlinearities related to the terms appearing in the mathematical structure of Section 2. Generally speaking, nonlinearity implies that particles are not simply subject to the superposition of binary actions and that the output of the interactions depends on the distribution function over the microscopic states. This explains why the terms η, $\mathcal{B}$, μ and ν in (2.1)–(2.4) are viewed as operators over $\mathbf{f}$. Nonlinearity arises both in the encounter rate and in the transition probability densities. In the following, we refer to the situation in which the interaction rate and the transition probability densities do not depend on the distribution functions as the linear case.

Encounter rate. Concerning the interaction rate η_{hk}, in the linear case its dependence is restricted to the microscopic variables u_* and u^* of the interacting pairs only. Though in the simplest case it can be considered a constant η^0_{hk} independent of the activities, in general we expect a decay with the distance $|u_*-u^*|$ between the states of interacting particles. In the nonlinear case η_{hk} depends also on the distribution functions f_h and f_k. At first glance it seems reasonable assuming that the encounter rate among particles belonging to different subsystems may depend on a gross distance among their functional states. The simplest one we can consider is what we call *hierarchic distance*. Once a suitable numbering criterion, depending on the specific model, has been introduced into the set of functional subsystems, these latter are ordered according to this selection rule. Borrowing a jargon from zoology, we can think of ordering the subsystems starting with, say, the dominant $(i=1)$ up to the most subdued $(i=n)$. In this respect, we expect that the encounter rate decreases with increasing hierarchic distance. A complementary source of nonlinearity arises from the general idea that two subsystems with close distributions are affine and hence interact with higher frequency. Thus, a dependence of η_{hk} on an *affinity distance* between f_h and f_k can be introduced, where many possible norms $\|f_h-f_k\|$ can be considered, according to the physics of the system under consideration. These latter include metrics related to the difference of momenta of the distribution functions that account for the global shape of the distribution functions of interacting particles. Inasmuch as the interactions are triggered by some sort of distance $|u_*-u^*|$, as illustrated in Section 2, it is reasonable to assume that if the distributions $f_h(u_*,t)$, $f_k(u^*,t)$ are both peaked in the same part of the domain D_u of the activity variable, the corresponding encounter frequency is higher than if they show their peaks far away from each other. This corresponds to introducing a dependence of η_{hk} on the skewness difference between the distribution functions $f_h(u_*,t)$, $f_k(u^*,t)$, that is related to their momenta of order three. Whatever the nonlinearity degree we expect, as before, the encounter frequency η_{hk} decays with increasing affinity distance. A possible choice for the encounter rate that meets the aforesaid criteria is:

$$\eta_{hk}=\eta^0\mathcal{E}_{hk},\quad \mathcal{E}_{hk}=\frac{1}{1+|h-k|}e^{-\left(c_1|u_*-u^*|+c_2\|f_h(u_*,t)-f_k(u^*,t)\|\right)},\ h,k=1,\dots,n, \tag{3.1}$$

where c_1 and c_2 are suitable constants and where the denominator $1+|h-k|$ weights the frequency of encounters according to the hierarchic distance between the subsystems.

Transition probability densities. Let us now consider the nonlinearities that can characterize the transition probability density $\mathcal{B}^i_{hk}$. The considerations we are going to make hold, to a large extent, also for the terms μ^i_{hk}, ν_{ik} related to the proliferative and destructive events. In the case of linear interactions the transition probability density is conditioned only by the states of the interacting particles for each pair of functional subsystems. The sources of nonlinearity in the interaction terms naturally arise when we consider the general framework KTAP uses to build up those quantities. As we said above, the transition probabilities are obtained by using tools from game theory, for it is essential to distinguish a number of key features corresponding to the possible situations presented in specific models. Basically, interacting subjects conduct themselves (play a game) according to a *cooperative*, *competitive* or *hiding/learning* behavior. In the case of cooperation, the candidate particle either increases its activity u_*, taking advantage of its interaction with a field particle having a higher state $u^*>u_*$, or decreases its activity u_* interacting with a field particle with a lower state $u^*<u_*$, producing a sort of dragging effect in which the candidate "follows the leader". In the competitive behavior, instead, the candidate particle either increases its activity u_* when encounters a field particle with a lower state $u^*<u_*$ or decreases its activity facing a field agent with a higher state $u^*>u_*$, with a resulting driving back effect. Finally, the hiding/learning behavior is characterized by the attempt of the first particle to increase its activity difference with the second one while the latter tries reducing this difference by a learning process [13]. All of these interaction behaviors (games) can possibly occur simultaneously in a general context. However, each of them shows random features, that is, the interaction output is generally known only in probability, due for instance to a variability in the reactions of particles to similar conditions, in some cases related to irrational behaviors. This observation motivates their attribution of stochastic games.

The games the active particles play, whatever they are, are sources of nonlinearity through different possible mechanisms. For example, the occurrence of one type of interaction with respect to another is ruled, in several models (see e.g. [14]), by a

threshold on the distance between the interacting particles. On the other hand, in a recent model on opinion formation [15] it is shown how this type of dynamics depends on that of the overall system through the momenta of the distribution functions f_i, $i = 1, \ldots, n$.

Another relevant source of nonlinearity in the interaction terms arises from the observation that, in many model situations, the candidate particle interacts with the field particles only within a certain domain of influence in the space of microstates. In the simplest case it is fixed [14], while in general it depends on the density of active particles which can be captured in the communication. In [16], where bird swarm modeling is studied, it is conjectured that more effective than the usual metric distance among the interacting "particles" is a kind of topological distance, that is a distance based on a suitable definition of local neighborhoods of particles. In that context, this means that the domain of influence of each agent (bird) is not simply the total amount of individuals that fall into its observational range, rather only a finite number of neighbors enter into the interaction domain, giving rise to the emergence of the observed collective behavior of swarms. Such a conjecture has been reconsidered in the framework of the KTAP approach in [17]. In this latter, the topological domain of influence Ω is suggested to depend on the particles' density ρ through a function β that dynamically relates the above mentioned quantities via a critical density defining the maximum number of particles which can be included in the interaction. When the space variables do not appear, it seems reasonable that the dependence of the domain of influence on the density is related to the shape of the distribution functions of interacting particles, thus introducing a mild source of topological nonlinearity.

Finally, we must include as a source of nonlinearity the possible threshold effect on the processes of proliferation/destruction of active particles. These events, modeled by the terms μ^i_{hk} and ν_{ik} in the structure (2.1)–(2.4), are particularly relevant in situations such as the modeling of immune competition [11]. The onset of a birth/death process is in general triggered not only by the microstate of interacting entities but also by their size and their distribution in time over the activity variable. More generally, in the proliferative/destructive category we should include the processes that lead to the appearance or disappearance of new functional subsystems. These processes are contrasted by a mechanism that shows a nonlinearity in its onset thresholds. Thus, if the size $N_i[f_i]$ of a functional subsystem falls below a critical value $N_{\min}$, then interactions reduce transferring particles from the original one toward an aggregation to another one. Similarly, a large critical size $N_{\max}$ might exist such that if such a threshold is overcome, particles are induced to move into another functional subsystem.

4. Critical analysis

Complexity is a feature shared by a large number of physical, biological, and social systems. These systems are characterized by a huge number of constituents whose overall behavior shows, under certain circumstances, the emergence of collective phenomena that are not deducible in a straightforward manner from the dynamics of their microscopic interactions, though they depend somewhat on it [13,18]. The kinetic theory of active particles has been revealed to be suitable in the modeling of many such systems. However, in order to try to capture the whole picture, the presence of nonlinear and nonlinearly additive interaction, together with the presence of different dynamics, appears to be of crucial importance, especially when looking at the appearance of highly improbable events [19].

In this paper we analyze the conceptual basis relating the sources of nonlinearity arising in the KTAP in contexts where the space variable does not play a relevant role. On the other hand, a dependence on spatial localization even in the absence of the (continuous or discrete) space variable can conceivably be introduced, reformulating the mathematical structure of Section 2 on a network. In this case, the mathematical structure (2.1)–(2.4) needs to be generalized, including the possibility for the candidate active particle to interact with field particles from different nodes. As a consequence, we are led to generalize the encounter rate as η_{ijhk}, where $i, h = 1, \ldots, m$ represent the node indices while $j, k = 1, \ldots, n$ distinguish the functional subsystems, a similar notation holding for the transition probabilities $\mathcal{B}$, μ and ν. The network nature of the topological arrangement naturally introduces a hierarchic distance among different nodes. Thus, for example, we expect the encounter frequency of particles belonging to different nodes is lower than that of individuals from the same node. The encounter rate η_{ijhk} would have an expression similar to (3.1) with $\mathcal{E}_{hk}$ replaced by

$$\mathcal{E}_{ijhk} = \frac{1 + \delta_{ih}(n-1)}{n(1+|j-k|)} e^{-\left(c_1|u_*-u^*|+c_2\|f_{ij}(u_*,t)-f_{hk}(u^*,t)\|\right)}, \quad i, h = 1, \ldots, m;\ j, k = 1, \ldots, n, \tag{4.1}$$

and δ_{ih} is the Kronecker's delta. Observe that in (4.1) the distribution functions are labeled by two indices, denoting respectively the node and the subsystem. The nonlinearity of interactions is then spread out on the whole network, mimicking the spatial aspect of nonlinear additivity which is formally absent in the picture.

A further source of nonlinearity in KTAP arises when the mathematical structure outlined in Section 2 is extended to include open systems. In the latter case, active particles from each functional subsystem can interact with a number of active external agents, collected in $p \geq 1$ functional subsystems whose distribution functions $g_1(w, t), \ldots, g_p(w, t)$, characterized by an activity $w \in D_w \subseteq \mathbf{R}$, are prescribed. The mathematical structure of KTAP is modified, for open systems, to include the encounter rate and the transition probabilities relative to the interaction of particles in the system with external agents. Though in principle these new terms are affected by the same sources of nonlinearity described in Section 3, it is worth observing that the external agents can both interact with every active particle and deal with each subsystems as a whole.

In other words, a nonlinear multiscale interaction can be included in the KTAP picture, with interactions affecting the microstate of individuals as well as the macrostate at the level of functional subsystems. We do not go further on this subject, as it requires not only a generalization of interaction frequencies and transition probabilities in (2.2)–(2.4) but also a structural change in the evolution equation (2.1).

The previous general discussion shows how the issues characterizing complex systems are related to nonlinear aspects. We here limited ourselves to outline how and where these latter may enter the KTAP approach. On the other hand, the general structure introduced in Section 2 and its generalizations briefly described in the present one must be suitably specialized when modeling specific physical, biological or social systems. In this respect, the stochastic games that in this paper have been considered just as a source of nonlinearity must be pointed out in view of building up the transition terms appearing in (2.2)–(2.4). Living and social systems are objects of forthcoming studies, where the nonlinear character of interactions and their nonlinear additivity will hopefully highlight the ability of KTAP to capture even the early stages of emerging collective behaviors and of singular, highly improbable events that characterize complex systems.

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