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On the modeling of nonlinear interactions in large complex systems☆

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ABSTRACT

This work deals with the modeling of large systems of interacting entities in the framework of the mathematical kinetic theory for active particles. The contents are specifically focused on the modeling of nonlinear interactions which is one of the most important issues in the mathematical approach to modeling and simulating complex systems, and which includes a learning–hiding dynamics. Applications are focused on the modeling of complex biological systems and on immune competition.

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1. Introduction

Recent developments of mathematical sciences have been devoted to the modeling of complex living systems. An account of the literature in the field is offered by paper [1], which reports on the mathematical approach of the so-called kinetic theory for active particles, for short KTAP theory, that has been specifically developed for modeling complex systems. This method has been applied in several fields of natural and applied sciences such as immune competition (see [2,3], which refer to [4]), epidemics [5], wound healing and diseases [6], social dynamics [7,8], and psychological interactions [9].

The state of the art witnesses several different mathematical approaches in competition toward a common aim—among others, derivation of master equations for agents [10] and suitable developments of spin glass theory [11]. A deeper understanding of this topic could contribute to refinement of the present state of the art in various modeling approaches such as those concerning criminality [12–15], social dynamics [16–18], crowd modeling [19,20], and animal behaviors [21–23], which are treated by approaches technically different from that presented in this work.

The aim of this work is the modeling of nonlinear interactions which is one of the most important issues in the mathematical approach to modeling and simulating complex systems. The contents are related to the mathematical structure derived in [24], which was proposed as a general paradigm for modeling hiding and learning processes in a large system of interacting entities, called *active particles*. Active particles are grouped into subsystems, called *functional subsystems*, consisting of entities which collectively express the same function, called the *activity*, described by the scalar variable $u \in D_u \subseteq \mathbb{R}$, where D_u is a bounded domain that can be taken, after appropriate normalization, equal to $[-1, 1]$. In some cases it is convenient to consider the whole real line $D_u = (-\infty, \infty)$.

This work specifically deals with systems such that space and velocity variables have no relevant physical meaning. This happens if the behavior of the system is uniform in space and the velocity distribution is constant in time, or even when

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both space and velocity do not have a relevant meaning in the modeling approach. That, for instance, is the case for several systems in social sciences when particles interact via devices, such as media, where the localization does not play a relevant role in the interactions.

We assume that there are only interactions which modify the microscopic state of the particles. *Interactions* involve three kinds of particles: *candidate*, *test*, and *field*. The interaction rule is as follows: *candidate* particles can acquire, in probability, the state of the *test* particles, after an interaction with *field* particles, while test particles lose that state after interactions. Moreover, the overall state of the ith functional subsystem is described by the probability distribution

$$f_i = f_i(t, u) : [0, T] \times D_u \to \mathbb{R}^+, \quad \text{for } i \in \{1, 2, \ldots, n\}, \tag{1.1}$$

where n is the number of functional subsystems, while the time evolution of the distribution function f_i is obtained by the balance of particles in the elementary interval $[u, u + \mathrm{d}u]$ of the microscopic state, as follows:

$$\begin{aligned}\partial_t f_i(t, u) &= J_i[\mathbf{f}](t, u) = \sum_{j=1}^{n} J_{ij}[f_i, f_j](t, u)\\ &= \sum_{j=1}^{n} \int_{D_u \times D_u} \eta_{ij}(u_*, u^*)\mathscr{B}_{ij}(u_* \to u|u_*, u^*) f_i(t, u_*) f_j(t, u^*)\, \mathrm{d}u_*\, \mathrm{d}u^*\\ &\quad - f_i(t, u) \sum_{j=1}^{n} \int_{D_u} \eta_{ij}(u, u^*) f_j(t, u^*)\, \mathrm{d}u^*,\end{aligned} \tag{1.2}$$

where:

$\mathbf{f} = (f_1, f_2, \ldots, f_n)$ is the vector of the probability distributions;

$\eta_{ij} = \eta_{ij}(u_*, u^*)$ is the rate of encounters between the candidate particle, with state u_*, of the ith functional subsystem and the field particle, with state u^*, of the jth functional subsystem;

$\mathscr{B}_{ij} = \mathscr{B}_{ij}(u_* \to u|u_*, u^*)$ is the probability density for a candidate particle, with state u_*, of the ith functional subsystem ending up in the state u of the test particle of the same functional subsystem after the interaction with the field particle, with state u^*, of the jth functional subsystem; $\mathscr{B}_{ij}$ satisfies, for all $i, j \in \{1, 2, \ldots, n\}$, the following condition:

$$\int_{D_u} \mathscr{B}_{ij}(u_* \to u|u_*, u^*)\, \mathrm{d}u = 1, \quad \forall u_*, u^* \in D_u. \tag{1.3}$$

Interactions, modeled by the terms $\mathscr{B}_{ij}$, are called *stochastic games* since the microscopic state of the active particles is known in probability and the output is identified by a probability density. Moreover, if migrations in the network or proliferative/destructive events do not occur, the probability distributions f_i can be normalized with respect to the number of active particles within each functional subsystem. Therefore

$$\mathbb{P}_i(u \in A \subseteq D_u; t) = \int_A f_i(t, u)\, \mathrm{d}u, \quad \text{with } \int_{D_u} f_i(t, u)\, \mathrm{d}u = 1 \tag{1.4}$$

denotes the probability that u belongs, at time t, to the A subset of D_u.

The pth-order moment is computed as follows:

$$\mathbb{E}^p[f_i](t) = \int_{D_u} u^p f_i(t, u)\, \mathrm{d}u. \tag{1.5}$$

The physical meaning is related to the specific real system under consideration. The main interest is focused on the first-order and second-order moments, namely the mean activation and activation energy, that correspond in mechanics to linear momentum and kinetic energy.

The contents are organized as follows: Section 2 presents the main result of this work, namely the modeling of multiple interactions and the derivation of the evolution equation. Section 3 shows how the approach of the preceding section can be further developed and applied in a number of case studies.

2. Modeling nonlinear interactions

This section deals with various modeling aspects related to the class of equations proposed in the preceding section. The analysis is focused on the modeling of the terms η_{ij} and $\mathscr{B}_{ij}$ that define in Eq. (1.2) the interactions involving active particles.

• *On the concept of the functional subsystem:* The systems under consideration have been subdivided into functional subsystems, which are constituted by active particles that collectively express a certain strategy, called the activity, identified by the scalar variable u. If the particles are distributed on the nodes of a network, these nodes contribute to identifying the functional subsystems through a specific characterization. Namely, several different functional subsystems can be localized at the same node as long as each of them develops a different activity. On the other hand, the same function can be expressed via different functional subsystems if they are localized at different nodes. Therefore, the characterization is due to both localization and the activity which is expressed.

An important concept that is useful to the analysis developed in what follows is the definition of a distance α_{ij} between the active particles of the ith and the jth functional subsystems. The following hierarchy, that corresponds to increasing level of sophistication, is proposed:

(i) $\alpha_{ij} = \eta^0_{ij} \in \mathbb{R}$ is simply a real constant that depends on the interacting functional subsystems.
(ii) $\alpha_{ij} = \alpha_{ij}(u_{*_i}, u^*_j)$ depends on the difference among the microscopic states of the interacting particles:

$$\alpha_{ij}(u_{*_i}, u^*_j) = |u_{*_i} - u^*_j|.$$

(iii) $\alpha_{ij} = \alpha_{ij}[f_i, f_j](t)$ depends on the distance among the overall states of the interacting functional subsystems:

$$\alpha_{ij}[f_i, f_j](t) = \sqrt{\int_{D_u} [f_i - f_j]^2(t, u)\, \mathrm{d}u}.$$

Of course additional examples can be selected according to the specific characteristics of the system under consideration. However, the analysis is restricted, with tutorial aims, to the three simple examples given above, where the difference is that the distance, respectively, is a constant, depends on the state of the interacting pairs, and is a functional of the probability distributions that characterize the two interacting functional subsystems.

• *The encounter rate:* The modeling of the encounter rate introduced by Eq. (1.2) can be achieved in such a fashion that increasing values of the distance α_{ij} correspond to decreasing values of the encounter rate η_{ij}. According to the previous hierarchy we define the encounter rate as follows:

(i) The encounter rate is a constant simply given by

$$\eta_{ij} = \eta^0_{ij}. \tag{2.1}$$

(ii) The encounter rate is related to the difference among the microscopic states of the interacting particles as follows:

$$\eta_{ij} = \eta_{ij}(u_{*_i}, u^*_j) = \eta^0_{ij} \mathrm{e}^{-c\alpha^2_{ij}(u_{*_i}, u^*_j)}, \tag{2.2}$$

where c is a positive real constant.
(iii) The encounter rate is related to the distribution functions of the interacting functional subsystems:

$$\eta_{ij} = \eta_{ij}(t|f_i, f_j) = \eta^0_{ij} \mathrm{e}^{-c\alpha^2_{ij}[f_i, f_j](t)} = \eta^0_{ij} \mathrm{e}^{-c\left(\int_{D_u} [f_i - f_j]^2(t,u)\, \mathrm{d}u\right)}. \tag{2.3}$$

Remark 2.1. The simple model given by (2.1) can be regarded as a particular case of (2.2) obtained by taking $c = 0$, while the model given by (2.2) is obtained with (2.3) approximating the distributions f_i by delta functions over the states of the interacting pairs.

Remark 2.2. The terms η^0_{ij}, for $i, j \in \{1, 2, \ldots, n\}$, depend on the kinds of interacting functional subsystems and can be modeled by taking into account also their localization on the network.

• *The transition probability density:* As already mentioned, $\mathscr{B}_{ij}$ represents the probability density for a candidate particle, with state u_*, of the ith functional subsystem ending up in the state u of the test particle of the same functional subsystem after interaction with the field particle, with state u^*, of the jth functional subsystem.

A high level of nonlinearity is introduced in systems where the encounter rates and also the transition probability density are conditioned by the distribution functions of the interacting functional subsystems. Accordingly, Eq. (1.2) is rewritten as follows:

$$\begin{aligned}
\partial_t f_i(t, u) &= J_i[\mathbf{f}](t, u) = \sum_{j=1}^{n} J_{ij}[f_i, f_j](t, u) \\
&= \sum_{j=1}^{n} \int_{D_u \times D_u} \eta_{ij}(t|f_i, f_j) \mathscr{B}_{ij}(u_* \to u|u_*, u^*, \mathbb{E}^p[f_i], \mathbb{E}^p[f_j]) f_i(t, u_*) f_j(t, u^*)\, \mathrm{d}u_*\, \mathrm{d}u^* \\
&\quad - f_i(t, u) \sum_{j=1}^{n} \int_{D_u} \eta_{ij}(t|f_i, f_j) f_j(t, u^*)\, \mathrm{d}u^*.
\end{aligned} \tag{2.4}$$

A phenomenon which has to be taken into account is that, generally, the interaction domain of the candidate particle with state u_* is not the whole domain D_u but a subset $\Omega_{u_*} \subseteq D_u$, which contains the field particles $u^* \in \Omega_{u_*}$ that are able to interact with the candidate particle. Thus interactions only occur if the distances, in the space of microscopic states of the interacting particles, are sufficiently small.

Therefore a positive function $\omega(u_*, u^*)$, normalized with respect to integration over u^*, is introduced to take into account such dynamics. This function, which weights the interactions among the active particles, is assumed to have a compact support in the domain of influence $\Omega_{u_*} \subseteq D_u$ of the interactions. Moreover,

$$\int_{D_u} \omega(u_*, u^*)\, \mathrm{d}u^* = \int_{\Omega_{u_*}} \omega(u_*, u^*)\, \mathrm{d}u^* = 1. \tag{2.5}$$

Accordingly we define the pth-order weighted moment as follows:

$$\mathbb{E}_w^p[f_i](t, u_*) = \int_{D_u} (u^*)^p \omega(u_*, u^*) f_i(t, u^*)\, \mathrm{d}u^* = \int_{\Omega_{u_*}} (u^*)^p \omega(u_*, u^*) f_i(t, u^*)\, \mathrm{d}u^*. \tag{2.6}$$

Therefore Eq. (2.4) is rewritten as follows:

$$\begin{aligned}
\partial_t f_i(t, u) &= J_i[\mathbf{f}](t, u) = \sum_{j=1}^{n} J_{ij}[f_i, f_j](t, u) \\
&= \sum_{j=1}^{n} \int_{D_u \times D_u} \eta_{ij}(t|f_i, f_j) \mathscr{B}_{ij}(u_* \to u|u_*, u^*, \mathbb{E}_w^p[f_i], \mathbb{E}_w^p[f_j]) f_i(t, u_*) f_j(t, u^*)\, \mathrm{d}u_*\, \mathrm{d}u^* \\
&\quad - f_i(t, u) \sum_{j=1}^{n} \int_{D_u} \eta_{ij}(t|f_i, f_j) f_j(t, u^*) \mathrm{d}u^*.
\end{aligned} \tag{2.7}$$

Remark 2.3. The specific characterization of the terms η_{ij}, which appear in (2.7), is obtained by selecting one of the three cases (2.1)–(2.3), or additional ones, while specific models are obtained by characterization of the term $\mathscr{B}_{ij}$. This matter is discussed in the next section.

Remark 2.4. The modeling of the terms $\mathscr{B}_{ij}$, for $i, j \in \{1, 2, \ldots, n\}$, is based on the idea that the candidate particle interacts with the field particles within its interaction domain, defined by Ω_{u^*}, in the space of the activity variables and feels an action identified by the low order moments of the field of active particles. The action can be also related, whether or not it is consistent with the specific system under consideration, by the most probable value.

Remark 2.5. The time evolution of the distribution functions $f_i(t, u)$, for $i \in \{1, 2, \ldots, n\}$, is obtained by solving the initial value problem for Eq. (2.7) obtained by adding the initial conditions $f_i(0, u)$. Subsequently moments weighted by the variable u can be computed to obtain macroscopic information. The qualitative analysis developed in [25] for a relatively simple class of models needs to be further refined to take into account the higher order nonlinearity of (2.7). Bifurcation may appear, as documented in [26,27].

An immediate technical generalization consists in inserting in Eq. (2.7) the modeling of proliferative and/or destructive events as well as transitions from one functional subsystem to the other. The result is achieved by combining the guidelines of [1] with those of this present work. The following mathematical framework is obtained:

$$\begin{aligned}
\partial_t f_i(t, u) &= Q_i[\mathbf{f}](t, u) = \sum_{h=1}^{n} \sum_{k=1}^{n} Q_{hk}[f_h, f_k](t, u) \\
&= \sum_{h=1}^{n} \sum_{k=1}^{n} \int_{D_u \times D_u} \eta_{hk}^0 \mathrm{e}^{-c\alpha_{hk}^2(t|f_h, f_k)} \mathscr{B}_{hk}^i(u_* \to u|u_*, u^*, \mathbb{E}_w^p[f_h], \mathbb{E}_w^p[f_k]) f_h(t, u_*) f_k(t, u^*)\, \mathrm{d}u_*\, \mathrm{d}u^* \\
&\quad - \sum_{h=1}^{n} \sum_{k=1}^{n} \int_{D_u} \eta_{hk}^0 \mathrm{e}^{-c\alpha_{hk}^2(t|f_h, f_k)} [1 - \mu_{hk}^i(u_*, u^*)] f_h(t, u_*) f_k(t, u^*)\, \mathrm{d}u_*\, \mathrm{d}u^*,
\end{aligned} \tag{2.8}$$

where the number of particles is no longer constant in time due to the term that models proliferative and/or destructive events:

μ_{hk}^i models the proliferative/destructive rate for particles of the hth functional subsystem, with state u_*, going into the state u of the ith functional subsystem due to an encounter with the particle (field) of the kth functional subsystem, with state u^*. In particular, destructive events occur only within the functional subsystem of the field particles.

Moreover, conservative interactions include transitions from one functional subsystem to the other. This dynamics is modeled by the following term:

$\mathscr{B}_{hk}^i$ models the probability density for a candidate particle of the hth functional subsystem, and with state u_*, ending up in the state u of the ith functional subsystem after the interaction with the field particle, with state u^*, of the kth functional subsystem.

3. Perspectives

This section briefly analyzes some further developments of the approach proposed in Section 2, related to methodological issues, with a view to applications. The selection of topics proposed in this section does not claim to be exhaustive, but it is simply a suggestion of future research perspectives proposed according to the authors' bias.

The main contribution of this work consists in the modification of the structures summarized in Section 1, which were based on linear interactions, to include the modeling of nonlinear interactions. Indeed a variety of papers have been proposed, based on Eq. (1.2), for modeling complex systems in the life sciences; see Refs. [2,5–7,9], and many others. An interesting problem consists in analyzing the role of nonlinear interactions, namely how these can modify the output of the overall collective dynamics. An additional research perspective that is worth bringing to the attention of applied mathematicians consists in developing the contribution of papers [28,29] devoted to modeling, respectively, the roles of space dynamics and aggregation/fragmentation phenomena. Moreover, paper [29] shows, following the guidelines of [30], how macroscopic models can be derived from the underlying description delivered by kinetic type models. This topic has been treated recently by several authors, as documented in [31] and the bibliography cited therein. However, the analysis of models which include nonlinear interactions is still an open problem.

Finally, let us remark that the most relevant research perspective consists in modeling the interaction dynamics at the scale of the active particles, from the underlying description at a lower scale, typical of the system under consideration. Some perspective ideas have been given on this challenging topic, mainly focusing on the modeling of biological systems [32–34]. However, also in this case, the approach is limited to the case of binary additive interactions.

Applications are not limited to the case of living systems. Indeed, a variety of systems in technology and physics can be modeled by taking advantage of the theory formulated here. The common feature of these systems is that they are constituted by a large number of interacting entities, whose state includes, in addition to the classical position and velocity variables, an additional specific state that is heterogeneously distributed and that modifies the interaction rules otherwise defined by classical conservation laws. Some examples, selected among several, can be given.

A generalized kinetic model of sedimentation of polydisperse suspensions has been proposed in [35]. A challenging problem, which may be addressed using this theory, is turbulence in superfluids. Indeed, superfluid turbulence is described as a disordered tangle of quantized vortex lines [36]. The vortex lines are either closed loops or open vortex lines pinned on the walls, which interact with each other through breaking and reconnection processes. The approach proposed in this work can contribute to modeling the time evolution of the statistical properties of vortex loops [37,38], and their thermodynamic consequences [39].

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