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On the discrete kinetic theory for active particles. Mathematical tools☆

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Abstract

This paper deals with the development of a mathematical discrete kinetic theory to model the dynamics of large systems of interacting active particles whose microscopic state includes not only geometrical and mechanical variables (typically position and velocity), but also peculiar functions, called activities, which are able to modify laws of classical mechanics. The number of the above particles is sufficiently large to describe the overall state of the system by a suitable probability distribution over the microscopic state, while the microscopic state is discrete. This paper deals with a methodological approach suitable to derive the mathematical tools and structures which can be properly used to model a variety of models in different fields of applied sciences. The last part of the paper outlines some research perspectives towards modelling.

Keywords: Kinetic theory; Active particles; Discrete microscopic variable

1. Introduction and guiding lines

An interesting research field of applied mathematics is the modelling of large systems of interacting entities whose microscopic state includes, in addition to mechanical variables, also additional variables related to their somehow organized and even "intelligent" behavior. These entities interact among themselves – individual based interactions – thus exchanging information which modify their individual state.

Mathematical methods can be developed to describe by equations the collective behavior starting from a description of microscopic interactions. Methods of the mathematical kinetic theory can be properly developed towards the above target. It is a quite natural approach considering that classical models of the kinetic theory, e.g. the Boltzmann and Vlasov equations, lead to models which describe the collective behavior of classical particles which cannot be individually identified in a large system, while individual interactions are modelled within the framework of classical mechanics.

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On the other hand, systems dealt with in this paper are characterized by the additional difficulty that interactions do not follow rules of classical mechanics. Moreover the identification of the microscopic state itself needs a deep analysis of physical systems characterized by a high level of complexity.

The application of methods of the mathematical kinetic theory to the modelling and simulation of complex systems in applied sciences is documented in several papers related, for instance, to traffic flow modelling [1,2], social systems [3–5], evolution of personal feelings [6,7] and modelling multicellular systems with application to the immune competition [8–11].

Additional bibliographies can be recovered in papers [12,13], devoted to the methodological aspects on the derivation of kinetic equations, as well as in [14,15] concerning the mathematical description of living fluids and tissues.

Some pioneering papers have proposed suitable generalizations and developments of the above mathematical approach to model large complex systems in different fields of applied sciences. Among others, Prigogine and Herman proposed a mathematical theory of traffic flow by Boltzmann type equations [16]. The same approach has been applied to model the social behavior of colonies of insects by Jager and Segel [17], or cell populations with special attention to the immune competition [18].

This paper is motivated by the mathematical approach proposed in [5], where a class of evolution equations was proposed to deal with large systems of interacting individuals such that the microscopic state is a **discrete variable**. Remark that the hint to analyze this type of systems is motivated by modelling requirements rather than by the aim of reducing computational complexity.

The contents refer to the modelling of large complex systems by mathematical methods of the kinetic theory. These systems are mathematically characterized by the fact that the number of variables to describe the evolution of the system is greater than the number of evolution equations. As a matter of fact, microscopic interactions between the entities – called **active particles** – make them change their microscopic state, which is not only characterized by mechanical properties, but also by a social or biological discrete variable called **activity**. Thus we have to define the activity of the entities, which cannot generally be described by the standard evolution equations.

This paper deals with the above mentioned topics with the aim of providing a variety of mathematical tools to be used towards modelling in applied sciences. Therefore the contents refer to methodological aspects, while specific applications will be dealt with in the forthcoming papers as anticipated in the last section.

The contents are organized into four more sections which follow this introduction. Specifically:

Section 2 deals with a relatively more detailed description of the physical systems which have been briefly outlined above. Some technical definitions are introduced first to identify the terminology used in the following. Secondly, the statistical description of the system by means of discrete generalized distribution functions is introduced. This means defining the microscopic state of the interacting entities and the probability distribution over such a state. Macroscopic quantities are obtained by suitable averaged moments of the above distribution functions.

Section 3 develops the derivation of a mathematical framework suitable to model the class of physical systems we are dealing with. The framework consists in a suitable set of nonlinear integro-differential or partial differential equations, which can be particularized into mathematical models once the description of microscopic interactions has been properly modelled. One particular case is given.

Section 4 deals with some additional generalizations. The first part is devoted to the discretization of the velocity variable, and, in general, to the discretization of the whole microscopic state. The second part deals with the modelling of systems of active particles which have the ability to produce particles in a new population.

Section 5 develops a critical analysis on the applicability of the tools derived in this paper. Then some applications are indicated as conceivable research perspectives.

2. Some definitions and statistical representation

Consider the class of physical systems briefly described in Section 1, e.g. a system constituted by a large number of active particles organized into n populations labelled by the subscript $i = 1, \ldots, n$. In this system, each population is characterized by a different way of organizing their peculiar activities as well as interactions with the other populations. Some notations and definitions have to be stated to define precisely the microscopic state of each particle and the statistical description of the system.

Definition 2.1. The variable in charge to describe the state of any active particle is denoted by the variable $\mathbf{w}$ and is called the microscopic state. This microscopic state is split into the geometrical microscopic state, the mechanical microscopic state and the social or biological microscopic state called activity. In our relatively simple case, we consider the microscopic variable

$$\mathbf{w} = \{\mathbf{x}, \mathbf{v}, \mathbf{u}\} \in D_{\mathbf{w}} = D_{\mathbf{x}} \times D_{\mathbf{v}} \times D_{\mathbf{u}}, \tag{2.1}$$

where $\mathbf{x}$ is the position of the active particle, $\mathbf{v}$ is its linear velocity, and $\mathbf{u}$ its activity.

As mentioned in Section 1, we are interested in active particles characterized by a discrete activity:

$$\mathbf{u} \in I_{\mathbf{u}} = \{\mathbf{u}_1, \ldots, \mathbf{u}_h, \ldots, \mathbf{u}_H\}. \tag{2.2}$$

Therefore we introduce a mixed continuous/discrete microscopic variable

$$\mathbf{w}^h = \{\mathbf{x}, \mathbf{v}, \mathbf{u} = \mathbf{u}_h\} \in D_{\mathbf{w}}^H = D_{\mathbf{x}} \times D_{\mathbf{v}} \times I_{\mathbf{u}}, \tag{2.3}$$

in view of the mathematical framework which will be derived in the sections that follow. Remark that also the variables $\mathbf{x}$ and $\mathbf{v}$ can be considered discrete according to modelling requirements as will be shown in Section 4.

Definition 2.2. The description of the overall state of the system is given by the set of functions

$$\mathbf{f} = \{f_i^h\}, \tag{2.4}$$

where each element $f_i^h = f_i(t, \mathbf{w}^h) = f_i^h(t, \mathbf{x}, \mathbf{v})$, for $i = 1, \ldots, n$ and $h = 1, \ldots, H$, will be called the discrete generalized distribution function corresponding to the i-th population and the h-th activity $\mathbf{u}_h$.

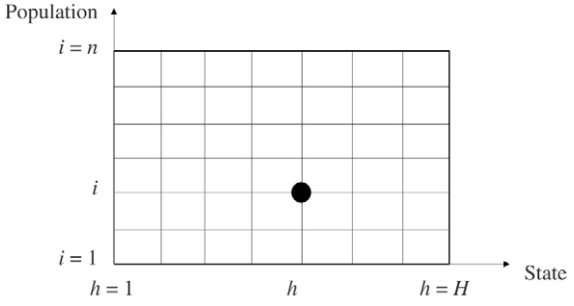

Fig. 1. Representation of the discrete states.

Each element of the system can be viewed as a node of a grid which schematically represents the whole system, as shown in Fig. 1. The distribution function f_i related to the i-th population is then formally given by

$$f_i(t, \mathbf{w}) = f_i(t, \mathbf{x}, \mathbf{v}, \mathbf{u}) = \sum_{h=1}^{H} f_i^h(t, \mathbf{x}, \mathbf{v})\delta(\mathbf{u} - \mathbf{u}_h), \tag{2.5}$$

where δ is the Dirac's delta function.

If each f_i^h is known, then macroscopic variables can be computed, under suitable integrability properties, as moments weighted by the above distribution functions. For instance, the zero-th order moments of the functions f_i^h provide information on the number density for each population:

Definition 2.3. The number density n_i^h is the number density of active particles of the i-th population with activity $\mathbf{u}_h$ at time t and position $\mathbf{x}$. n_i^h is also called the local size and is defined by

$$n_i^h(t, \mathbf{x}) = \int_{D_{\mathbf{v}}} f_i^h(t, \mathbf{x}, \mathbf{v})\mathrm{d}\mathbf{v}. \tag{2.6}$$

The sum over all the activities $\mathbf{u}_h$ provides the number density $n_i(t, \mathbf{x})$ for the i-th population. Then the total number density $n(t, \mathbf{x})$ at the time t at position $\mathbf{x}$, is given by

$$n(t, \mathbf{x}) = \sum_{i=1}^{n} n_i(t, \mathbf{x}) = \sum_{i=1}^{n} \sum_{h=1}^{H} n_i^h(t, \mathbf{x}). \tag{2.7}$$

Integration over the volume $D_{\mathbf{x}}$ containing the particles gives the *total size* $N(t)$ of all populations:

$$N(t) = \int_{D_{\mathbf{x}}} n(t, \mathbf{x}) \mathrm{d}\mathbf{x}, \tag{2.8}$$

which can also be calculated by the sum of all the populations i whose total size will be denoted $N_i(t)$.

Consider now first order moments of the functions f_i^h. They provide either linear mechanical macroscopic quantities, or linear activity macroscopic quantities. For instance, the *local flux of the quantity of movement* of the i-th population with activity $\mathbf{u}_h$ is given by

$$\mathbf{Q}_i^h(t, \mathbf{x}) = \int_{D_{\mathbf{v}}} \mathbf{v} f_i^h(t, \mathbf{x}, \mathbf{v}) \mathrm{d}\mathbf{v}. \tag{2.9}$$

As for the number density, the *local flux* (denoted $\mathbf{Q}_i$) of the quantity of movement for the i-th population, is obtained by summing over all the activities, so that

$$\mathbf{Q}_i(t, \mathbf{x}) = \sum_{h=1}^{H} \mathbf{Q}_i^h(t, \mathbf{x}), \tag{2.10}$$

while local mean flow linked to $\mathbf{Q}_i$ is

$$\mathbf{q}_i(t, \mathbf{x}) = \frac{\mathbf{Q}_i(t, \mathbf{x})}{n_i(t, \mathbf{x})}. \tag{2.11}$$

Focusing on activity terms, linear moments of the activity $\mathbf{u}_h$ related to the i- th population can be called *h-th local activations*, and are computed as follows:

$$\mathcal{A}_i^h(t, \mathbf{x}) = \mathbf{u}_h \int_{D_{\mathbf{v}}} f_i^h(t, \mathbf{x}, \mathbf{v}) \mathrm{d}\mathbf{v}. \tag{2.12}$$

The *local activation* for the i-th population is thus given by

$$\mathcal{A}_i(t, \mathbf{x}) = \sum_{h=1}^{H} \mathcal{A}_i^h(t, \mathbf{x}), \tag{2.13}$$

while *h-th local activation densities* and *local activation density* related to the i-th population are respectively defined by

$$\mathbf{a}_i^h(t, \mathbf{x}) = \frac{\mathcal{A}_i^h(t, \mathbf{x})}{n_i(t, \mathbf{x})}, \quad \text{and} \quad \mathbf{a}_i(t, \mathbf{x}) = \sum_{h=1}^{H} \mathbf{a}_i^h(t, \mathbf{x}). \tag{2.14}$$

Similar calculations can be developed with higher order moments if required by applications. For instance, *local quadratic energy* and its associated density are defined as follows:

$$E_i(t, \mathbf{x}) = \sum_{h=1}^{H} \int_{D_{\mathbf{v}}} \mathbf{v}^2 f_i^h(t, \mathbf{x}, \mathbf{v}) \mathrm{d}\mathbf{v}, \quad \text{and} \quad e_i(t, \mathbf{x}) = \frac{E_i(t, \mathbf{x})}{n_i(t, \mathbf{x})}. \tag{2.15}$$

Therefore, the *local quadratic activity* and its associated density

$$\mathcal{E}_i(t, \mathbf{x}) = \sum_{h=1}^{H} \mathbf{u}_h^2 \int_{D_{\mathbf{v}}} f_i^h(t, \mathbf{x}, \mathbf{v}) \mathrm{d}\mathbf{v}, \quad \text{and} \quad \varepsilon_i(t, \mathbf{x}) = \frac{\mathcal{E}_i(t, \mathbf{x})}{n_i(t, \mathbf{x})}, \tag{2.16}$$

can be computed as second order moments. The above notations have been used in the case of discretization of the activity variable. Analogous calculations can be developed when the other variables, space and/or velocity, of the microscopic state are also discrete. One has simply to substitute integrations by finite sums over the subscript of the discrete variable.

3. Mathematical framework

This section deals with the derivation of a general framework for the evolution of the discrete distribution functions f_i^h. The modelling of a suitable framework for microscopic interactions is preliminary to the derivation of these evolution equations. The analysis we propose refers to localized interactions. Consider active particles distributed in the domain $D_{\mathbf{x}}$. Interactions between a candidate (or test) particle and a field particle appear when the field one enters into the action domain Λ of the candidate (or test) one, which is relatively small relative to the local density, so that only binary encounters are relevant.

Different kinds of interactions need to be taken into account. Localized interactions can be classified in:

- *Conservative interactions* which modify the state of the interacting particles, but not their number;
- *Proliferating or destructive interactions* which generate the death or birth of active particles due to pair interactions.

A schematic representation of these interactions are proposed in Figs. 2–4.

Consider first the modelling of microscopic conservative interactions. They are based on the knowledge of the following two quantities:

- *The encounter rate*, denoted η_{ij}, which gives the number of encounters per unit of time between two interacting particles of respective populations i and j;
- *The transition density function*, denoted $\varphi_{ij}^{pq}(h)$, which is the probability density that a **candidate** particle of the i-th population with microscopic state $\mathbf{w}_1^p = \{\mathbf{x}_1, \mathbf{v}_1, \mathbf{u}_p\}$ falls into the state $\mathbf{w}^h = \{\mathbf{x}, \mathbf{v}, \mathbf{u}_h\}$, after an interaction with a **field** particle of the j-th population with state $\mathbf{w}_2^q = \{\mathbf{x}_2, \mathbf{v}_2, \mathbf{u}_q\}$.

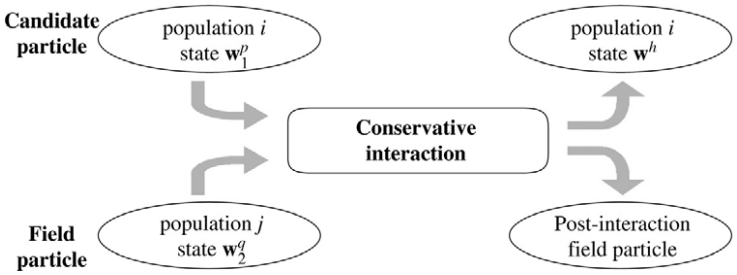

Fig. 2. Representation of conservative encounters.

Consider now the modelling of microscopic non-conservative interactions. Specifically we deal here with the modelling of self-proliferation (or self-destruction) phenomena. They can be modelled by:

- *The source/sink distribution function*, denoted ψ_{ij}^{hq}, which is, for each encounter between a test particle of the i-th population in state $\mathbf{w}^h$ with a field particle of the j-th population with state $\mathbf{w}_2^q$, the number of particles generated (in the case of proliferating interactions) or destroyed (in the case of destructive ones) with population and state of the test particle.

This function is negative in the case of destructive interactions and positive for proliferating ones. In the destructive case, test particles are simply destroyed as represented in Fig. 3. In the proliferating case, particles are assumed to be generated with microscopic state $\mathbf{w}^h$ in the population of the test particle as represented in Fig. 4. Note that proliferation and/or destruction occur with the above defined encounter rate.

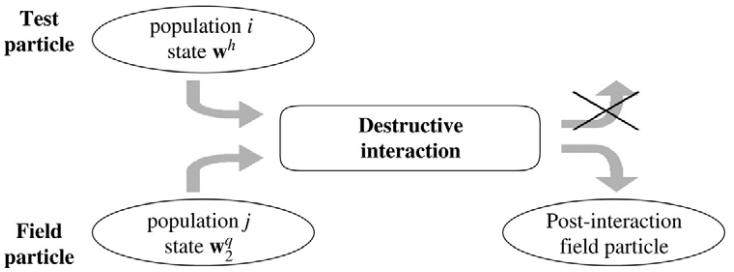

Fig. 3. Representation of destructive encounters.

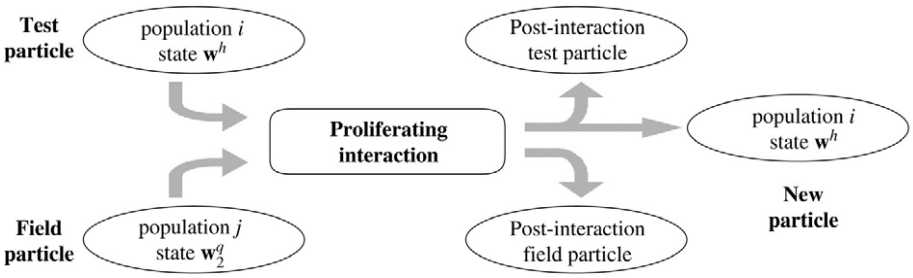

Fig. 4. Representation of proliferating encounters.

The terms η_{ij}, $\varphi_{ij}^{pq}(h)$ and ψ_{ij}^{hq} have to be particularized according to the phenomenology of the physical problem. However, some technical assumptions are preliminary to the derivation of specific models. In detail, it will be assumed that:

(i) The encounter rate depends on the relative velocity of the interacting particles;
(ii) Interactions which modify the activities are not influenced by mechanical quantities besides the encounter rate;
(iii) Interactions which modify the mechanical state may also be influenced by the activities of the interacting pair.

Moreover, the assumption of short range interactions leads to consider interacting and post-interaction particles localized at the same point. According to these assumptions, the following particularizations are proposed:

- *The encounter rate* is proportional to the relative velocity:

$$\eta_{ij}(\cdot) = c_{ij}|\mathbf{v}_1 - \mathbf{v}_2|\delta(\mathbf{x}_1 - \mathbf{x}_2), \tag{3.1}$$

where c_{ij} is a constant depending on the populations, $\mathbf{x}_1$ and $\mathbf{v}_1$ are the position and velocity of the candidate (or test) particle, whereas the subscript 2 denotes these quantities for the field particle.

The encounter rate could also depend on the states p and q of the interacting pair if required by the modelling, simply considering the constant c_{ij}^{pq} into (3.1).

- *The transition density function* is given by the product of the transition density $\mathcal{M}_{ij}^{pq}$ related to the mechanical variables, with the discrete transition density $\mathcal{B}_{ij}^{pq}(h)$ related to the activity:

$$\varphi_{ij}^{pq}(h)(\cdot) = \mathcal{M}_{ij}^{pq}(\mathbf{v}_1, \mathbf{v}_2; \mathbf{v}|\mathbf{u}_p, \mathbf{u}_q)\mathcal{B}_{ij}^{pq}(h)\delta(\mathbf{x} - \mathbf{x}_1). \tag{3.2}$$

The above transition density functions have the structure of a probability density with respect to their outgoing variables. That leads to the following properties:

$$\begin{aligned} \forall\, i, j, \quad \forall\, p, q: \quad & \sum_{h=1}^{H} \mathcal{B}_{ij}^{pq}(h) = 1, \\ & \int_{D_{\mathbf{v}}} \mathcal{M}_{ij}^{pq}(\mathbf{v}_1, \mathbf{v}_2; \mathbf{v})\mathrm{d}\mathbf{v} = 1 \quad \forall\, \mathbf{v}_1, \mathbf{v}_2. \end{aligned} \tag{3.3}$$

Remark that the output of the mechanical interactions is assumed to depend on velocity and activity, while the output of interactions related to the activity depends on the activity only.

- *The source/sink distribution function* is given by $\psi_{ij}^{hq}(\cdot) = \mu_{ij}^{hq}$, where μ_{ij}^{hq} is a constant depending on populations and activities of the interacting pair.

The knowledge of the above quantities allows us to derive, by methods of the mathematical kinetic theory, a class of evolution equations for the set $\mathbf{f}$ of distribution functions f_i^h. Such a mathematical model can be formally written, within the framework of the discrete kinetic theory, as follows:

$$\mathcal{L} f_i^h = \mathcal{N} f_i^h, \tag{3.4}$$

for $i = 1, \ldots, n$ and $h = 1, \ldots, H$, where $\mathcal{L}$ and $\mathcal{N}$ denote suitable linear and nonlinear operators. In the absence of external forces, $\mathcal{L}$ is the total time derivative

$$\mathcal{L} = \frac{\partial}{\partial t} + \mathbf{v} \cdot \nabla_{\mathbf{x}}. \tag{3.5}$$

On the other hand, the operator $\mathcal{N}$ has to be split into three parts. The first two are related to conservative interactions and correspond to classical inflow and outflow of active particles into the elementary volume of the state space. The third one is the non-conservative term which corresponds to the proliferation and/or destruction of these particles.

The evolution equation, for each f_i^h, is obtained, similarly to the case of the Boltzmann equation, by considering the variation of the test particles number of the i-th population, with microscopic state $\mathbf{w}^h$, again in the elementary state volume. Equating the variation rate of the test particles to the fluxes of particles which reach and leave such a state due to interactions, and the source term, leads to the balance equation:

$$\left(\frac{\partial}{\partial t} + \mathbf{v} \cdot \nabla_{\mathbf{x}}\right) f_i^h = \mathcal{C}_i^{h+}[\mathbf{f}] - \mathcal{C}_i^{h-}[\mathbf{f}] + \mathcal{I}_i^h[\mathbf{f}]. \tag{3.6}$$

We first focus on $\mathcal{C}_i^{h+}[\mathbf{f}]$ which is the number of test particles of the i-th population appearing in the state $\mathbf{w}^h$ – per unit of time and volume – after interactions between candidate particles of the same population with microscopic state $\mathbf{w}_1^p$, and field particles of the j-th population with microscopic state $\mathbf{w}_2^q$. Denoting $D = \Lambda \times D_{\mathbf{v}}$, where Λ is the interaction domain of the candidate particle and $D_{\mathbf{v}}$ is the domain of the velocity, and considering the relations (3.1) and (3.2), one has:

$$\begin{aligned}\mathcal{C}_i^{h+}[\mathbf{f}](t, \mathbf{x}, \mathbf{v}) = \sum_{j=1}^{n} \sum_{p,q=1}^{H} \int_{D\times D} & c_{ij} |\mathbf{v}_1 - \mathbf{v}_2| \mathcal{M}_{ij}^{pq}(\mathbf{v}_1, \mathbf{v}_2; \mathbf{v} | \mathbf{u}_p, \mathbf{u}_q) \mathcal{B}_{ij}^{pq}(h) \\ & \times f_i^p(t, \mathbf{x}_1, \mathbf{v}_1) f_j^q(t, \mathbf{x}_2, \mathbf{v}_2) \delta(\mathbf{x} - \mathbf{x}_1) \delta(\mathbf{x}_1 - \mathbf{x}_2) \mathrm{d}\mathbf{x}_1 \mathrm{d}\mathbf{x}_2 \mathrm{d}\mathbf{v}_1 \mathrm{d}\mathbf{v}_2,\end{aligned} \tag{3.7}$$

which can be written as follows:

$$\begin{aligned}\mathcal{C}_i^{h+}[\mathbf{f}](t, \mathbf{x}, \mathbf{v}) = \sum_{j=1}^{n} \sum_{p,q=1}^{H} \int_{D_{\mathbf{v}}\times D_{\mathbf{v}}} & c_{ij} |\mathbf{v}_1 - \mathbf{v}_2| \mathcal{M}_{ij}^{pq}(\mathbf{v}_1, \mathbf{v}_2; \mathbf{v} | \mathbf{u}_p, \mathbf{u}_q) \mathcal{B}_{ij}^{pq}(h) \\ & \times f_i^p(t, \mathbf{x}, \mathbf{v}_1) f_j^q(t, \mathbf{x}, \mathbf{v}_2) \mathrm{d}\mathbf{v}_1 \mathrm{d}\mathbf{v}_2.\end{aligned} \tag{3.8}$$

The term $\mathcal{C}_i^{h-}[\mathbf{f}]$ is the number of test particles which leave the state $\mathbf{w}^h$, per unit of time and volume, after having interacted with field particles with state $\mathbf{w}_2^q$. It follows, by the same kind of calculations as for the previous term, that

$$\mathcal{C}_i^{h-}[\mathbf{f}](t, \mathbf{x}, \mathbf{v}) = f_i^h(t, \mathbf{x}, \mathbf{v}) \sum_{j=1}^{n} \sum_{q=1}^{H} \int_{D_{\mathbf{v}}} c_{ij} |\mathbf{v} - \mathbf{v}_2| f_j^q(t, \mathbf{x}, \mathbf{v}_2) \mathrm{d}\mathbf{v}_2. \tag{3.9}$$

Analogous calculations for the source term $\mathcal{I}_i^h[\mathbf{f}]$, referring to the proliferating or destructive interactions between test particles in the microscopic state $\mathbf{w}^h$, and field particles with state $\mathbf{w}_2^q$, yields:

$$\mathcal{I}_i^h[\mathbf{f}](t, \mathbf{x}, \mathbf{v}) = f_i^h(t, \mathbf{x}, \mathbf{v}) \sum_{j=1}^{n} \sum_{q=1}^{H} \int_{D_{\mathbf{v}}} c_{ij} |\mathbf{v} - \mathbf{v}_2| \mu_{ij}^{hq} f_j^q(t, \mathbf{x}, \mathbf{v}_2) \mathrm{d}\mathbf{v}_2. \tag{3.10}$$

Substituting into Eq. (3.6) yields finally the following system of $n \times H$ integro-differential equations:

$$\left(\frac{\partial}{\partial t} + \mathbf{v}\cdot\nabla_{\mathbf{x}}\right) f_i^h(t,\mathbf{x},\mathbf{v}) = \sum_{j=1}^{n}\sum_{p,q=1}^{H}\int_{D_{\mathbf{v}}\times D_{\mathbf{v}}} c_{ij}|\mathbf{v}_1-\mathbf{v}_2|\mathcal{B}_{ij}^{pq}(h) \times \mathcal{M}_{ij}^{pq}(\mathbf{v}_1,\mathbf{v}_2;\mathbf{v}|\mathbf{u}_p,\mathbf{u}_q) f_i^p(t,\mathbf{x},\mathbf{v}_1) f_j^q(t,\mathbf{x},\mathbf{v}_2)\mathrm{d}\mathbf{v}_1\mathrm{d}\mathbf{v}_2 - f_i^h(t,\mathbf{x},\mathbf{v})\sum_{j=1}^{n}\sum_{q=1}^{H}\int_{D_{\mathbf{v}}} c_{ij}|\mathbf{v}-\mathbf{v}_2|\left[1-\mu_{ij}^{hq}\right] f_j^q(t,\mathbf{x},\mathbf{v}_2)\mathrm{d}\mathbf{v}_2. \tag{3.11}$$

3.1. Models with dominant activity interactions

The above model can be simplified referring to physical situations where some phenomena can be neglected with respect to some others. Consider the case where particles are homogeneously distributed in space, with uniform or constant in time distribution over the velocity. The evolution equations of such systems are obtained integrating Eqs. (3.11) over the domain of the velocity variable, taking into account the assumption on the distribution function that is written

$$f_i^h(t,\mathbf{v}) = f_i(t,\mathbf{v},\mathbf{u}=\mathbf{u}_h) = f_i^{a,h}(t)P(\mathbf{v}), \qquad \int_{D_{\mathbf{v}}} P(\mathbf{v})\mathrm{d}\mathbf{v} = 1, \tag{3.12}$$

uniform in the space variable.

Using this assumption and the property (3.3) concerning $\mathcal{M}_{ij}^{pq}$, and integrating over the velocity domain $D_{\mathbf{v}}$ yields the following class of ordinary differential equations:

$$\frac{\mathrm{d}}{\mathrm{d}t} f_i^{a,h} = \sum_{j=1}^{n}\sum_{p,q=1}^{H}\eta_{ij}^a\mathcal{B}_{ij}^{pq}(h) f_i^{a,p} f_j^{a,q} - f_i^{a,h}\sum_{j=1}^{n}\sum_{q=1}^{H}\eta_{ij}^a\left[1-\mu_{ij}^{hq}\right] f_j^{a,q}, \tag{3.13}$$

where

$$\eta_{ij}^a = \int_{D_{\mathbf{v}}\times D_{\mathbf{v}}} c_{ij}|\mathbf{v}_1-\mathbf{v}_2|P(\mathbf{v}_1)P(\mathbf{v}_2)\mathrm{d}\mathbf{v}_1\mathrm{d}\mathbf{v}_2, \tag{3.14}$$

while the notation $f_i^{a,h}$ denotes $f_i^{a,h}(t)$. In the static case, the probability $P(\mathbf{v})$ is simply the Dirac's function at the particular value $\mathbf{v} = 0$. In this case, η_{ij} is taken as a constant c_{ij} depending only on populations i and j of the interacting pair, that leads simply to $\eta_{ij}^a = c_{ij}$.

4. Some generalizations

This section deals with some generalizations of the mathematical framework developed in Section 3. Specifically, and bearing in mind applications, we consider two types of generalizations: (i) a mathematical framework for discrete space and/or velocity variables and (ii) the modelling of generation of particles in a population different from the ones of the interacting pair. These generalizations may be useful in various fields of applied sciences, but specifically in biology [14] where active particles are cells which may be constrained to move along selected directions, and/or cell interactions between pairs of two populations may generate cells in a new population identified by a different genetic characterization.

4.1. Framework for discrete microscopic variables

Consider the general case in which the evolution in space cannot be neglected. As mentioned above, specific modelling may require the use of discrete microscopic variables rather than continuous ones.

As a first approach, let us consider a discrete velocity variable with a left continuous space variable. According to the following discretization of the velocity

$$\mathbf{v} \in I_{\mathbf{v}} = \{\mathbf{v}_1,\ldots,\mathbf{v}_k,\ldots,\mathbf{v}_K\}, \tag{4.1}$$

the distribution function for the i-th population – given by (2.5) – is now formally written as follows:

$$f_i(t, \mathbf{w}) = f_i(t, \mathbf{x}, \mathbf{v}, \mathbf{u}) = \sum_{k=1}^{K} \sum_{h=1}^{H} f_i^{kh}(t, \mathbf{x}) \delta(\mathbf{v} - \mathbf{v}_k) \delta(\mathbf{u} - \mathbf{u}_h). \tag{4.2}$$

A mixed continuous/discrete microscopic variable

$$\mathbf{w}^{kh} = \{\mathbf{x}, \mathbf{v} = \mathbf{v}_k, \mathbf{u} = \mathbf{u}_h\} \in D_{\mathbf{w}}^{KH} = D_{\mathbf{x}} \times I_{\mathbf{v}} \times I_{\mathbf{u}}, \tag{4.3}$$

is introduced as in Section 2.

In this case, the encounter rate η_{ij} and the transition probability density $\varphi_{ij}^{pq}(h)$ are particularized by (3.1) and (3.2), while the source/sink distribution function remains unchanged. Taking into account the discretization of the velocity, the following expressions are obtained:

- *Encounter rate*:

$$\eta_{ij}(\cdot) = c_{ij} |\mathbf{v}_r - \mathbf{v}_s| \delta(\mathbf{x}_1 - \mathbf{x}_2). \tag{4.4}$$

- *Transition probability density*:

$$\varphi_{ij}^{pq}(h)(\cdot) = \mathcal{M}_{ij}^{\sigma}(\mathbf{v}_r, \mathbf{v}_s; \mathbf{v}_k | \mathbf{u}_p, \mathbf{u}_q) \mathcal{B}_{ij}^{pq}(h) \delta(\mathbf{x} - \mathbf{x}_1), \tag{4.5}$$

where $\sigma = \{r, s, p, q\}$ and

$$\forall\, i, j, \quad \forall\, \sigma: \quad \sum_{k=1}^{K} \mathcal{M}_{ij}^{\sigma}(\mathbf{v}_r, \mathbf{v}_s; \mathbf{v}_k) = 1 \quad \text{and} \quad \sum_{h=1}^{H} \mathcal{B}_{ij}^{pq}(h) = 1. \tag{4.6}$$

The balance equation is obtained by following the reasoning of Section 3, considering the variation of the active particles number with state $\mathbf{w}^{kh}$ in the elementary state volume. This equation is characterized by the same structure

$$\left(\frac{\partial}{\partial t} + \mathbf{v}_k \cdot \nabla_{\mathbf{x}} \right) f_i^{kh} = \mathcal{C}_i^{kh+}[\mathbf{f}] - \mathcal{C}_i^{kh-}[\mathbf{f}] + \mathcal{I}_i^{kh}[\mathbf{f}]. \tag{4.7}$$

Therefore performing calculations analogous to those we have seen in Section 3 yields the following system of $n \times K \times H$ partial differential equations:

$$\begin{aligned} \left(\frac{\partial}{\partial t} + \mathbf{v}_k \cdot \nabla_{\mathbf{x}} \right) f_i^{kh} &= \sum_{j=1}^{n} \sum_{\sigma} c_{ij} |\mathbf{v}_r - \mathbf{v}_s| \mathcal{M}_{ij}^{\sigma}(\mathbf{v}_r, \mathbf{v}_s; \mathbf{v}_k | \mathbf{u}_p, \mathbf{u}_q) \mathcal{B}_{ij}^{pq}(h) f_i^{rp} f_j^{sq} \\ &\quad - f_i^{kh} \sum_{j=1}^{n} \sum_{s=1}^{K} \sum_{q=1}^{H} c_{ij} |\mathbf{v}_k - \mathbf{v}_s| \left[1 - \mu_{ij}^{hq} \right] f_j^{sq}, \end{aligned} \tag{4.8}$$

where $f_i^{kh} = f_i^{kh}(t, \mathbf{x})$.

Consider now the general case with a complete discrete microscopic variable. In addition to the discretization of the velocity variable proposed above, we introduce the following discretization of the space variable:

$$\mathbf{x} \in I_{\mathbf{x}} = \{\mathbf{x}_1, \ldots, \mathbf{x}_\ell, \ldots, \mathbf{x}_L\}. \tag{4.9}$$

The formal expression of the distribution function related to the i-th population is thus:

$$f_i(t, \mathbf{w}) = f_i(t, \mathbf{x}, \mathbf{v}, \mathbf{u}) = \sum_{\ell=1}^{L} \sum_{k=1}^{K} \sum_{h=1}^{H} f_i^{\ell kh}(t) \delta(\mathbf{x} - \mathbf{x}_\ell) \delta(\mathbf{v} - \mathbf{v}_k) \delta(\mathbf{u} - \mathbf{u}_h). \tag{4.10}$$

.

As mentioned in the introduction of this section, specific modelling has to be developed according to the system we are dealing with. As an example, when specific areas are modelled by a discrete space variable, the role of the velocity may be in some special cases not relevant. Then the distribution function is formally written as follows:

$$f_i(t, \mathbf{x}, \mathbf{u}) = \sum_{\ell=1}^{L} \sum_{h=1}^{H} f_i^{\ell h}(t) \delta(\mathbf{x} - \mathbf{x}_\ell) \delta(\mathbf{u} - \mathbf{u}_h). \tag{4.11}$$

Technical calculations leads to a $n \times L \times H$ system of ordinary differential equations.

4.2. Models with change of population

Various complex systems of active particles include the ability to generate new particles in a population (and/or a state) different from the ones of the interacting pair. As an example of greater interest in mathematical modelling, human healthy cells may change their own genetic structure due to mutations caused by a tumoral environment. The mathematical framework proposed in Section 3 is still relevant to model this kind of phenomenon, but the expressions of the transition density and source/sink distribution functions are not still valid.

Consider first the case of conservative encounters. In this case, the candidate particle falls into the population and state of the test particle after an interaction with a field particle:

The transition density function $\varphi_{kj}^{pq}(i,h)$ needs to be introduced. It denotes the probability density that the candidate particle of the k-th population with state $\mathbf{w}_1^p$ falls, with state $\mathbf{w}^h$, into the population i, after an interaction with a field particle of the j-th population with state $\mathbf{w}_2^q$ (see Fig. 5).

Using assumptions analogous to those proposed in Section 3 allows us to write this transition density function as the product of the transition densities related to mechanical and activity variables. Precisely, $\varphi_{kj}^{pq}(i,h)$ is given by the expression (3.2) written for the population k and j, with a new discrete probability density $\mathcal{B}_{kj}^{pq}(i,h)$ which satisfies the probability density relation

$$\forall\, k, j, \quad \forall\, p, q: \qquad \sum_{i=1}^{n}\sum_{h=1}^{H}\mathcal{B}_{kj}^{pq}(i,h) = 1. \tag{4.12}$$

This discrete probability density is the generalization of $\mathcal{B}_{ij}^{pq}(h)$, which can be recovered by taking $\mathcal{B}_{kj}^{pq}(i,h) = 0$ for each $k \neq i$.

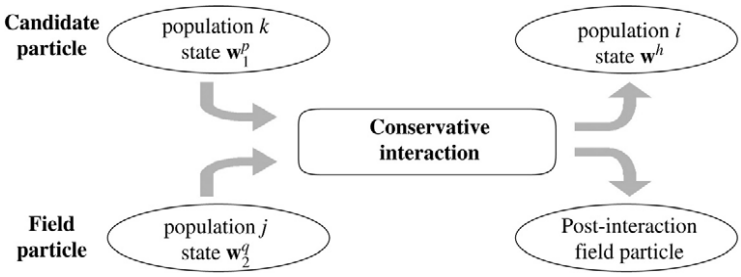

Fig. 5. Representation of conservative encounters.

Consider now non-conservative encounters, related to the source/sink distribution function. It is useful splitting this function into proliferating and destructive terms. As a matter of fact, destructive encounters between test particles of the i-th population in state $\mathbf{w}^h$, with field particles of the j-th population with state $\mathbf{w}_2^q$, still refer to destruction of the test particles as described in Fig. 3. Thus they are modelled in the way proposed in Section 3 by $\psi_{ij}^{hq}(\cdot) = -\xi_{ij}^{hq}$, where ξ_{ij}^{hq} is a positive constant.

Consider now the proliferating encounter between a candidate particle of the k-th population in state $\mathbf{w}_1^p$, with a field particle of the j-th population in state $\mathbf{w}_2^q$, in which a particle is created in the i-th population with state $\mathbf{w}^h$ (see Fig. 6):

As for the transition density function, the following source distribution function

$$\psi_{kj}^{pq}(i,h)(\cdot) = \zeta_{kj}^{pq}(i,h)\delta(\mathbf{x}-\mathbf{x}_1), \tag{4.13}$$

needs to be introduced, where the proliferation function $\zeta_{kj}^{pq}(i,h)$ is positive, and the Dirac's function over the space variable results from the assumption on localized interactions. This expression of the source distribution function also allows us to model proliferation with change of state only. One has simply to take $\zeta_{kj}^{pq}(i,h) = 0$ for each $k \neq i$, e.g. considering the proliferation function $\zeta_{ij}^{pq}(h)$.

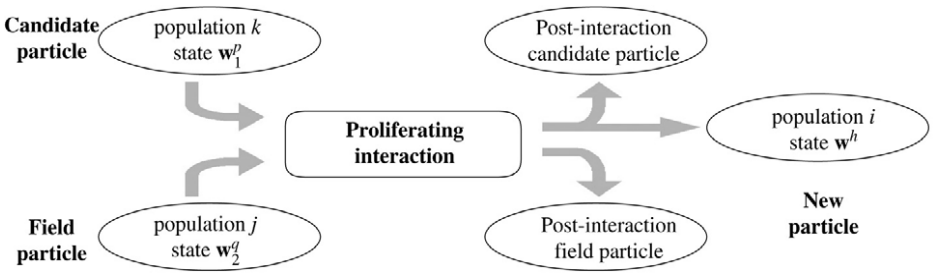

Fig. 6. Representation of proliferating encounters.

Using this type of modelling allows us to compute each term in the balance equation (3.6). Specifically, the quantity $\mathcal{C}_i^{h+}[\mathbf{f}]$ related to conservative interactions is now given by the following expression

$$\mathcal{C}_i^{h+}[\mathbf{f}](t,\mathbf{x},\mathbf{v}) = \sum_{k,j=1}^{n}\sum_{p,q=1}^{H}\int_{D_\mathbf{v}\times D_\mathbf{v}} c_{kj}|\mathbf{v}_1-\mathbf{v}_2|\mathcal{M}_{kj}^{pq}(\mathbf{v}_1,\mathbf{v}_2;\mathbf{v}|\mathbf{u}_p,\mathbf{u}_q)\mathcal{B}_{kj}^{pq}(i,h) \times f_k^p(t,\mathbf{x},\mathbf{v}_1)f_j^q(t,\mathbf{x},\mathbf{v}_2)\mathrm{d}\mathbf{v}_1\mathrm{d}\mathbf{v}_2, \tag{4.14}$$

while $\mathcal{C}_i^{h-}[\mathbf{f}]$ remains unchanged. Concerning the quantities related to non-conservative interactions, they are split into proliferating and destructive processes, as follows:

$$\mathcal{I}_i^h[\mathbf{f}] = \mathcal{I}_i^{h+}[\mathbf{f}] - \mathcal{I}_i^{h-}[\mathbf{f}], \tag{4.15}$$

where

$$\mathcal{I}_i^{h-}[\mathbf{f}](t,\mathbf{x},\mathbf{v}) = f_i^h(t,\mathbf{x},\mathbf{v})\sum_{j=1}^{n}\sum_{q=1}^{H}\int_{D_\mathbf{v}} c_{ij}|\mathbf{v}-\mathbf{v}_2|\xi_{ij}^{hq}f_j^q(t,\mathbf{x},\mathbf{v}_2)\mathrm{d}\mathbf{v}_2, \tag{4.16}$$

and

$$\mathcal{I}_i^{h+}[\mathbf{f}](t,\mathbf{x},\mathbf{v}) = \sum_{k,j=1}^{n}\sum_{p,q=1}^{H}\int_{D_\mathbf{v}\times D_\mathbf{v}} c_{kj}|\mathbf{v}_1-\mathbf{v}_2|\zeta_{kj}^{pq}(i,h)f_k^p(t,\mathbf{x},\mathbf{v}_1)f_j^q(t,\mathbf{x},\mathbf{v}_2)\mathrm{d}\mathbf{v}_1\mathrm{d}\mathbf{v}_2. \tag{4.17}$$

Finally, substituting these above expressions into (3.6) yields the evolution equations:

$$\left(\frac{\partial}{\partial t}+\mathbf{v}\cdot\nabla_\mathbf{x}\right)f_i^h(t,\mathbf{x},\mathbf{v}) = \sum_{k,j=1}^{n}\sum_{p,q=1}^{H}\int_{D_\mathbf{v}\times D_\mathbf{v}} c_{kj}|\mathbf{v}_1-\mathbf{v}_2| \times\left[\mathcal{M}_{kj}^{pq}(\mathbf{v}_1,\mathbf{v}_2;\mathbf{v}|\mathbf{u}_p,\mathbf{u}_q)\mathcal{B}_{kj}^{pq}(i,h)+\zeta_{kj}^{pq}(i,h)\right]f_k^p(t,\mathbf{x},\mathbf{v}_1)f_j^q(t,\mathbf{x},\mathbf{v}_2)\mathrm{d}\mathbf{v}_1\mathrm{d}\mathbf{v}_2 - f_i^h(t,\mathbf{x},\mathbf{v})\sum_{j=1}^{n}\sum_{q=1}^{H}\int_{D_\mathbf{v}} c_{ij}|\mathbf{v}-\mathbf{v}_2|\left[1+\xi_{ij}^{hq}\right]f_j^q(t,\mathbf{x},\mathbf{v}_2)\mathrm{d}\mathbf{v}_2, \tag{4.18}$$

which technically differ from the expression delivered by (3.11).

5. Critical analysis and perspectives

This paper has developed a general mathematical framework for systems of interacting active particles such that individual based interactions modify their microscopic state. Such a state includes, in addition to position and velocity, also a specific additional variable, called activity, which models the ability of organizing the dynamics of the particles.

The main characteristic of the above system is that the microscopic state is discrete. The analysis has been first developed when the activity is discrete, while space and velocity are allowed to be continuous. Then the generalization

to the case of fully discrete microscopic variables is performed. Motivations to provide such a framework have been given in Section 1 and in paper [5] which initiated this research line.

The contents have been developed leaving in mind conceivable modelling applications related to complex systems in applied sciences, which can be achieved after a detailed modelling of the various terms which mathematically describe microscopic interactions.

Therefore, this paper is proposed as the first one of a project which exploits the above mentioned framework towards modelling. Specifically the first application is going to be devoted to the modelling of the immune competition with special attention to the interaction between tumor and immune cells. The existing literature in the field can be recovered in the already cited papers [13] and [14]. In the field of biological sciences, motivations can be recovered in the paper by Jager and Segel [17], but also, among others, by Greller et al. [19], who link the discrete state to subsequent states of progressing cells from the normal state to the metastatic one. Additional literature can be found in the special issue [20].

Finally, it is worth stressing that the analysis developed in this paper offers a mathematical framework to be specialized into models derived after the modelling of microscopic interactions. It is not a simple task considering the difficulty in dealing with mathematical models of living matter [21,22]. Various authors [23–25] suggest to develop new mathematical approaches towards a game theory suitable to describe the output of the interaction of active particles. Indeed, this approach defines a relevant guiding line along the above mentioned research perspective.

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