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From the discrete kinetic theory to modelling open systems of active particles

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Abstract

This work deals with a methodological development of the kinetic theory for open systems of active particles with discrete states. It essentially refers to the derivation of mathematical tools which provide the guidelines for modelling open systems in different fields of applied sciences. After a description of closed systems, mathematical frameworks suitable for depicting the evolution of open systems are proposed. Finally, some research perspectives towards modelling are outlined.

Keywords: Kinetic theory; Active particles; Closed and open systems

1. Introduction

A mathematical discrete kinetic theory for describing the collective behavior of large systems of interacting active particles has been developed in [1], where the concept of active particles refers to those interacting entities whose microscopic state includes, in addition to mechanical variables, also additional variables called activities, related to their peculiar functions. Interactions among the active particles modify their individual state and generate proliferating and destructive events.

Paper [1] deals with a kinetic methodological approach where a class of evolution equations are proposed for modelling large systems of interacting individuals such that the microscopic state is a discrete variable; see also [2, 3]. The aim for analyzing such systems is induced by modelling requirements rather than by the intention of reducing computational complexity.

The variety of mathematical tools provided in [1] can be used towards modelling closed systems in applied sciences. Therefore the contents refer to methodological aspects, while a specific application is presented in [4], which deals with the immune competition between tumor and immune cells. The study of methods of the mathematical kinetic theory for modelling multicellular systems with application to the immune competition is documented in several recent papers; see [5,6].

On the other hand, a suitable development of the methods of the kinetic theory for active particles applied to open systems subject to external actions is proposed in [7], which deals with the modelling of degradation phenomena

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for works of art under the action applied by external agents. The model consists in an evolution equation for the probability distribution of the degradation stage. The interpretation of empirical data provides the identification of the parameters of the model and a quantitative prediction of degradation events. The analysis developed in [7] motivates the necessity to define a general framework for open systems of active particles within the discrete kinetic theory approach.

This work is addressed to a deeper and technical analysis of open systems, with the aim of providing a general mathematical framework suitable for modelling a large class of physical open systems. The contents of the work are divided into four sections. Section 1 is this introduction. Section 2 recalls briefly the general structures defined in [1] to illustrate the evolution in time of closed systems of active particles. Section 3 exploits the frameworks reported in the preceding section toward the modelling of open systems of active particles. Some generalizations are proposed in the last part of the section. Finally, in Section 4, the contents of the work are critically analyzed and some perspectives are given.

2. Mathematical frameworks for closed systems

This section provides a brief survey of the mathematical frameworks relating to closed systems of active particles proposed in [1]. Consider the class of systems constituted by a large number of active particles organized into n populations labelled with the subscripts $i = 1, \ldots, n$. The activity of the particles is represented by a discrete variable u belonging to the set $I_u = \{u_1, \ldots, u_h, \ldots, u_H\}$, with components u_h, where $h = 1, \ldots, H$.

Consider the case in which the statistical distributions suitable for describing the overall state of the system depend only on time. They are the set of functions $\mathbf{f} = \{f_i^h\}$, where each element $f_i^h = f_i(t, u = u_h)$ has been called a ‘discrete generalized distribution function’ corresponding to the ith population and the hth activity u_h.

The framework proposed in [1] consists in a set of non-linear differential equations deduced analogously to the Boltzmann equation, by considering the variation of the test particle number of the ith population with microscopic state u_h 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/sink term, leads to a balance equation, which in the spatially homogeneous case takes the form

$$\frac{\mathrm{d}f_i^h}{\mathrm{d}t} = \sum_{j=1}^{n} \left(\sum_{p,q=1}^{H} \eta_{ij} \mathcal{B}_{ij}^{pq}(h) f_i^p f_j^q - f_i^h \sum_{q=1}^{H} \eta_{ij} (1 - \mu_{ij}^{hq}) f_j^q \right). \tag{2.1}$$

The terms modelling the above microscopic interactions are:

- The encounter rate η_{ij}, which denotes the number of encounters per unit of time between two interacting particles of the ith and jth populations respectively.
- The discrete transition density $\mathcal{B}_{ij}^{pq}(h)$, which denotes the probability density for a particle of the ith population with state u_p falling into the state u_h, after an interaction with a particle of the jth population with state u_q.
- The source/sink rate μ_{ij}^{hq}, which denotes, for each encounter between a particle of the ith population in the state u_h and a particle of the jth population with state u_q, the number of particles generated (in the case of proliferating interactions) or destroyed (in the case of destructive ones) with state u_h in the same population. This last term is negative in the case of destructive interactions and positive for proliferating ones. Note that proliferation and/or destruction occurs with the above defined encounter rate.

The mathematical structure of Eq. (2.1) is still relevant for modelling dynamics in which active particles have the ability to generate new particles in a population (and/or a state) different from those of the interacting pair. The expressions for the discrete transition density and the source/sink rate are not still valid. The evolution equations suitable for modelling this kind of phenomenon can be written as follows:

$$\frac{\mathrm{d}f_i^h}{\mathrm{d}t} = \sum_{k,j=1}^{n} \left(\sum_{p,q=1}^{H} [\eta_{ij} \mathcal{B}_{kj}^{pq}(i,h) + \zeta_{kj}^{pq}(i,h)] f_i^p f_j^q - f_i^h \sum_{q=1}^{H} \eta_{ij} [1 + \xi_{ij}^{hq}] f_j^q \right). \tag{2.2}$$

The additional terms $\mathcal{B}_{kj}^{pq}(i,h)$, $\zeta_{kj}^{pq}(i,h)$ and ξ_{ij}^{hq} have been introduced with the following meaning:

- $\mathcal{B}_{kj}^{pq}(i,h)$ denotes the probability density for the candidate particle of the kth population with state u_p falling with state u_h into the ith population, after an interaction with a field particle of the jth population with state u_q.
- $\zeta_{kj}^{pq}(i,h)$ denotes the proliferating encounters between a candidate particle of the kth population in state u_p and a field particle of the jth population in state u_q, in which a particle is created in the ith population with state u_h.
- ξ_{ij}^{hq} denotes the destructive encounters between test particles of the ith population in state u_h and field particles of the jth population with state u_q.

3. Mathematical frameworks for open systems

The contents of this section aim at modelling how an open system of active particles interacts with the 'outer environment'. Specifically, we mean actions addressed to controlling the system, for instance therapeutical actions in the case of biological systems [4], actions devoted to optimizing the flow conditions in the case of traffic flow models [8,9], and actions devoted to controlling economic systems [3]. Consider the specific actions expressed by the following terms:

- $g^{(c)}(t) = \{g_k^{(c)}(t)\}$, which is a set of conservative stochastic actions labelled with the subscripts $k = 1, \ldots, n$. They are known functions of time and act over the candidate active particle of the ith population in the state u_p. Conservative actions $g_k^{(c)}(t)$ produce a transition of the particle into the state u_h.
- $g^{(p)}(t) = \{g_k^{(p)}(t)\}$, which is a set of proliferating/destructive stochastic actions labelled with the subscripts $k = 1, \ldots, n$. They are known functions of time and act over the test active particle of the ith population in the state u_h. Proliferating/destructive actions $g_k^{(p)}(t)$ cause a proliferation or destruction in the state u_h of the test particle.

Modelling the interactions between the system and the 'outer environment', composed by the above conservative and proliferating/destructive actions, is preliminary to deriving the evolution equation for the discrete distribution function f_i^h. These external interactions are modelled computing the following terms:

- *The external interaction rate term*, denoted as c_{ik}^e, for the candidate or test particle of the ith population interacting with the kth external conservative or proliferating/destructive action.
- *The external and conservative transition density function*, denoted as $\mathcal{C}_{ik}^p(h)$, which is the probability that a particle of the ith population with state u_p falls into the state u_h, after an interaction with the kth conservative external action $g_k^{(c)}$.
- *The external and proliferating/destructive transition density function*, denoted as $\mathcal{P}_{ik}^h$, which is the proliferating or destructive rate relating to the test particle of the ith population with state u_h, with a birth or death process in its state due to the interaction with the external non-conservative action $g_k^{(p)}$.

The derivation of a general mathematical framework for describing such systems is analogous to that of the one delivered by Eq. (2.1). The introduction of expressions taking into account the external interactions is necessary and the evolution equations take the form

$$\frac{\mathrm{d}f_i^h}{\mathrm{d}t} = \sum_{j=1}^{n}\left(\sum_{p,q=1}^{H} c_{ij}\mathcal{B}_{ij}^{pq}(h) f_i^p f_j^q - f_i^h \sum_{q=1}^{H} c_{ij}(1-\mu_{ij}^{hq}) f_j^q\right) + \sum_{p=1}^{H}\sum_{k=1}^{n} c_{ik}^e \mathcal{C}_{ik}^p(h) f_i^p g_k^{(c)} - f_i^h \sum_{k=1}^{n} c_{ik}^e g_k^{(c)} + f_i^h \sum_{k=1}^{n} c_{ik}^e \mathcal{P}_{ik}^h g_k^{(p)}. \tag{3.1}$$

The mathematical framework proposed above is technically generalized in the sequel. Specifically, a mathematical framework, suitable for modelling open systems of active particles including the ability to generate new particles in a population (and/or a state) different from those of the interacting pair, is proposed. In detail, applying to Eq. (3.1) the same technical reasoning as was used in the previous section, the following class of evolution equations is obtained:

$$\frac{\mathrm{d}f_i^h}{\mathrm{d}t} = \sum_{j=1}^{n}\left(\sum_{p,q=1}^{H}\sum_{\alpha=1}^{n}[c_{\alpha j}\mathcal{B}_{\alpha j}^{pq}(i,h) + \zeta_{\alpha j}^{pq}(i,h)] f_\alpha^p f_j^q - f_i^h \sum_{q=1}^{H} c_{ij}[1+\xi_{ij}^{hq}] f_j^q\right)$$

$$+\sum_{k=1}^{n}\left(\sum_{p=1}^{H}\sum_{\alpha=1}^{n} c^e_{\alpha k}\mathcal{C}^p_{\alpha k}(i,h) f^p_\alpha g^{(c)}_k - f^h_i c^e_{ik} g^{(c)}_k\right)$$

$$+\sum_{k=1}^{n}\left(\sum_{p=1}^{H}\sum_{\alpha=1}^{n} c^e_{\alpha k}\zeta^p_{\alpha k}(i,h) f^p_\alpha g^{(p)}_k - f^h_i c^e_{ik}\gamma^h_{ik} g^{(p)}_k\right), \tag{3.2}$$

where the following terms, which refer to changes of population due to encounters with conservative and non-conservative external actions, have been introduced:

- $\mathcal{C}^p_{\alpha k}(i,h)$, which denotes the probability that the candidate particle of the αth population with state u_p falls, with state u_h, into the ith population, after an interaction with the kth conservative external action $g^{(c)}_k$.
- $\zeta^p_{\alpha k}(i,h)$, which denotes the number of particles created in the ith population with state u_h, after an interaction between a candidate particle of the αth population in state u_p and the kth proliferating external action $g^{(p)}_k$.
- γ^h_{ik}, which denotes the number of test particles destroyed after interactions with kth destructive external actions $g^{(p)}_k$.

Guidelines for a further and remarkable generalization of Eq. (3.1) are now developed. Consider the problem of modelling open systems with the assumption that the generalized distribution functions corresponding to the external actions depend not only on time, but also on an additional variable. This variable describes the effect of the 'outer environment' on the active particles. The overall effect of the conservative actions is defined by the discrete generalized distribution functions $g^{m,(c)}_k = g_k(t, v = v_{k_m})$. Similarly, the functions describing the overall effect of the proliferating/destructive actions are $g^{m,(p)}_k = g_k(t, z = z_{k_m})$. We have introduced conservative actions whose level of intensity is described by a variable which can assume the set of values $\{v_{k_m}\}$, for $m = 1, \dots, M$. On the other hand, the set $\{z_{k_m}\}$, for $m = 1, \dots, M$, is devoted to defining proliferating/destructive actions.

Moreover, the terms $\mathcal{C}^p_{ik}(h)$ and $\mathcal{P}^h_{ik}$ need to be substituted, respectively, by the following ones:

- $\mathcal{C}^{pm}_{ik}(h)$, which denotes the probability that a particle of the ith population with state u_p falls into the state u_h, after an interaction with the kth conservative external action $g^{m,(c)}_k$ with effect v_{k_m}.
- $\mathcal{P}^{hm}_{ik}$, which denotes the proliferating or destructive rate relating to the test particle of the ith population in the state u_h with a birth or death process in its state due to the interaction with the external non-conservative action $g^{m,(p)}_k$ with effect z_{k_m}.

On the basis of the above considerations and still referring to Eq. (3.1), a mathematical framework suitable for describing the evolution of the system is

$$\frac{\mathrm{d}f^h_i}{\mathrm{d}t} = \sum_{j=1}^{n}\left(\sum_{p,q=1}^{H} c_{ij}\mathcal{B}^{pq}_{ij}(h) f^p_i f^q_j - f^h_i\sum_{q=1}^{H} c_{ij}(1-\mu^{hq}_{ij}) f^q_j\right)$$

$$+\sum_{p=1}^{H}\sum_{k=1}^{n}\sum_{m=1}^{M} c^e_{ik}\mathcal{C}^{pm}_{ik}(h) f^p_i g^{m,(c)}_k - f^h_i\sum_{k=1}^{n}\sum_{m=1}^{M} c^e_{ik} g^{m,(c)}_k$$

$$+ f^h_i\sum_{k=1}^{n}\sum_{m=1}^{M} c^e_{ik}\mathcal{P}^{hm}_{ik} g^{m,(p)}_k. \tag{3.3}$$

This last equation can be generalized considering also the case where interactions with changes of population are taken into account. Technical calculations analogous to those performed in Section 2 to obtain Eq. (2.2) yield

$$\frac{\mathrm{d}f^h_i}{\mathrm{d}t} = \sum_{j=1}^{n}\left(\sum_{p,q=1}^{H}\sum_{\alpha=1}^{n}[c_{\alpha j}\mathcal{B}^{pq}_{\alpha j}(i,h) + \zeta^{pq}_{\alpha j}(i,h)] f^p_\alpha f^q_j - f^h_i\sum_{q=1}^{H} c_{ij}[1+\xi^{hq}_{ij}] f^q_j\right)$$

$$+\sum_{k=1}^{n}\left(\sum_{p=1}^{H}\sum_{\alpha=1}^{n}\sum_{m=1}^{M} c^e_{\alpha k}\mathcal{C}^{pm}_{\alpha k}(i,h) f^p_\alpha g^{m,(c)}_k - f^h_i\sum_{m=1}^{M} c^e_{ik} g^{m,(c)}_k\right)$$

$$+\sum_{k=1}^{n}\left(\sum_{p=1}^{H}\sum_{\alpha=1}^{n}\sum_{m=1}^{M} c^{e}_{\alpha k}\zeta^{pm}_{\alpha k}(i,h)f^{p}_{\alpha}g^{m,(p)}_{k} - f^{h}_{i}\sum_{m=1}^{M} c^{e}_{ik}\gamma^{h}_{ik}g^{m,(p)}_{k}\right), \tag{3.4}$$

where:

- $\mathcal{C}^{pm}_{\alpha k}(i,h)$ denotes the probability that the candidate particle of the αth population with state u_p falls, with state u_h, into the ith population, after an interaction with the kth conservative external action $g^{m,(c)}_{k}$ with effect v_{k_m}.
- $\zeta^{pm}_{\alpha k}(i,h)$ denotes the number of particles created in the ith population with state u_h, after an interaction between a candidate particle of the αth population in state u_p and the kth proliferating external action $g^{m,(p)}_{k}$ with effect z_{k_m}.
- γ^{h}_{ik} denotes the number of test particles destroyed after interactions with kth destructive external actions $g^{m,(p)}_{k}$ with effect z_{k_m}.

4. Critical analysis and perspectives

A class of mathematical structures have been proposed in this work for describing physical systems within the kinetic theory of active particles with discrete states. The analysis has been developed for an open system, i.e. in the presence of external actions generated to control and optimize the evolution of the system.

As already mentioned, the analysis has been motivated by paper [7], which was however limited to the case of conservative interactions, while this work deals with the more general case of proliferating/destructive events which occur in various fields of applied sciences, e.g. in biology [4]. In this case, e.g. for multicellular systems [5], specific therapeutical actions can be possibly addressed to repair or destroy cells that are carriers of pathology in competition with cells of the immune system which, on the other hand, need to be activated in its specific biological functions.

Additional fields of applications have already been mentioned in Section 3; nevertheless it is not worth analyzing them in detail considering that this work aims at providing some general frameworks to be used towards modelling a variety of systems of interest in applied sciences. This objective has been precisely developed in Section 3. Further developments of the mathematical framework may be possibly addressed to include delay terms, if these are required, through a learning dynamics [10].

The mathematical structures derived in the preceding sections look at providing additional frameworks of the kinetic theory for active particles to be used for applications in natural sciences. This work specifically completes the analysis of [1].

Finally, it is worth mentioning that an interesting perspective is the analysis of the link between the classical kinetic theory and that of active particles. This topic has been dealt with in [11] for closed systems, while the case of open systems needs further analysis.

References

[1] A. Chauviere, I. Brazzoli, On the discrete kinetic theory for active particles—mathematical tools, Math. Comput. Modelling 43 (2006) 933–944.

[2] L. Bertotti, M. Delitala, On the qualitative analysis of the solutions of a mathematical model of social dynamics, Appl. Math. Lett. 19 (2006) 1107–1112.

[3] L. Bertotti, M. Delitala, Conservations laws and asymptotic behavior of a model of social dynamics, Nonlinear Anal. Real. World Appl. (2006), in press (doi:10.1016/j.nonrwa.2006.09.012).

[4] I. Brazzoli, A. Chauviere, On the discrete kinetic theory for active particles. Modelling the immune competition, Comput. Math. Methods Med. 7 (2006) 143–157.

[5] N. Bellomo, G. Forni, Looking for new paradigms towards a biological–mathematical theory of complex multicellular systems, Math. Models Methods Appl. Sci. 16 (2006) 1001–1029.

[6] A. Bellouquid, M. Delitala, Mathematical methods and tools of kinetic theory towards modelling complex biological system, Math. Models Methods Appl. Sci. 15 (2005) 1639–1666.

[7] I. Brazzoli, S.P. Corgnati, M. Filippi, S. Viazzo, On a kinetic theory approach to modelling degradation phenomena in conservation sciences, Math. Comput. Modelling 45 (2007) 1201–1213.

[8] M. Delitala, A. Tosin, Mathematical modelling of vehicular traffic: a discrete kinetic approach, Math. Models Methods Appl. Sci. 17 (6) (2007) (in press).

[9] V. Coscia, M. Delitala, P. Frasca, On the mathematical theory of vehicular traffic flow II. Discrete velocity kinetic models, Int. J. Nonlinear Mech. (2007), in press (doi:10.1016/j.ijnonlinmec.2006.02.008).

[10] C. Cattani, A. Ciancio, Hybrid two scales mathematical tools for active particles modelling complex systems with learning hiding dynamics, Math. Models Methods Appl. Sci. 17 (2007) 171–187 (in press).
[11] L. Arlotti, N. Bellomo, E. De Angelis, Generalized kinetic (Boltzmann) models: Mathematical structures and applications, Math. Models Methods Appl. Sci. 12 (2002) 579–604.