Applied Mathematics & Information Sciences
An International Journal

http://dx.doi.org/10.18576/amis/160503

A Nonconservative-Thermostat Kinetic Theory Framework: Density and Linear-Momentum Evolution

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Received: 7 Jun. 2022, Revised: 25 Jul. 2022, Accepted: 6 Aug. 2022
Published online: 1 Sep. 2022

Abstract: This paper is firstly devoted to the derivation of a new mathematical framework of the thermostatted kinetic theory for active particles with continuous activity variable. Specifically the thermostat operator is modified in order to take into account the role of the nonconservative interactions occuring among the particles of a complex biological system. The time evolution of the density of the system and of the linear-momentum are afterwards derived by employing the method of separation of variables. The new framework opens to further research perspectives and applications from the theoretical and modeling viewpoints.

Keywords: Kinetic theory, Thermostas, Nonlinearity, Macroscopic equations, Complex systems

1 Introduction

The aim of the applied mathematics is the proposition of theoretical tools coming from mathematics for the modeling and simulation of systems of the applied sciences. In particular an important research field of the applied mathematics is the modeling and the subsequently analysis and simulation of complex systems [1]. A complex system is usually composed by a large number of particles or elements, called active particles, which are able to carry out a specific job (function). The active particles are able to interact each others and with the outer environment and the result of the interactions is the emerging of a collective behaviour (emerging phenomena) which cannot be explained as a result of the single-particle strategies [2,3].
Scholars of the applied sciences have been attracted by the modeling of complex living systems and have been involved in the development of new mathematical theories [4,5,6,7] and models [8,9,10,11]. Different mathematical frameworks have been proposed and employed in the attempt of understanding the complex mechanics of the living systems [12,13,14]. Differently from the inner matter, a living system is composed of particles which are also able to proliferate and mutate; in particular the modeling and analysis of complex biological systems are the target of the present paper.
Recently, a new mathematical theory has been proposed for the modeling of complex biological systems, called the thermostatted kinetic theory for active particles [15]. According to this theory, the system is modeled by introducing a distribution function which models the time evolution of the system; the microscopic state of the particles is composed by the space, velocity and the activity variables. The activity variable models the role of the particles in the system and this internal variable can attain discrete or continuous values. The thermostatted kinetic theory for active particles is considered as a generalized kinetic theory with respect to the classical kinetic theory [16] and other thermostatted kinetic frameworks proposed in the pertinent literature, see [17, 18].
This paper is firstly devoted to the derivation of a new mathematical framework of the thermostatted kinetic theory for active particles. In particular in a complex biological system the role of the nonconservative interactions needs to be taken into account; a particle in a biological system can proliferate (human cells) or mutate

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[19,20,21,22]. From the mathematical point of view, these events have been already modeled in the generalized thermostatted kinetic theory of the active particles by introducing two specific functional operators [23,24,25]; however the novelty of this paper is the derivation of a new termostat operator which includes the conservative and nonconservative interaction tems for preventing the uncontrolled energy of the system (the activation energy). Specifically the thermostat operator is modified in order to take into account the role of the nonconservative interactions occuring among the particles of a complex biological system. The time evolution of the macroscopic quantities such as the density of the system and the linear-momentum, are investigated and the related evolution equations are derived.
The present paper is organized as follows: After this brief introduction, the new mathematical framework of the thermostatted kinetic theory for active particles is derived in Section 2; the new thermostat term is computed and the main assumptions are summarized within the section. Section 3 deals with the derivation of the evolution equations for the density and the linear-momentum; in particular the derivation of the macroscopic equations is based on the factorization assumption of the distribution function (separation of variables method). The Section 4 contains conclusions and discussions on future research perspectives and possible applications.

2 The nonconservative-thermostat kinetic theory framework

This section is devoted to the derivation of a new mathematical framework of the thermostatted kinetic theory. Specifically the role of nonconservative interactions (proliferation and destruction of active particles) is introduced and a new thermostat operator is proposed which takes into account the new term.
According to the thermostatted kinetic theory [26], the time evolution of the system is modeled by introducing a distribution fonction f defined on the microscopic state of the particles. In particular

$$f = f(t,u) : [0,+\infty[\times D_u \to \mathbb{R}^+,$$

where D_u denotes the domain of the activity variable u introduced to model the strategy of the particles. Let F be a constant external force acting on the system, the *primitive thermostatted framework* writes:

$$\begin{cases} \partial_t f(t,u) + \partial_u\left((F - u\alpha_F[f](t))f(t,u)\right) = \\ = J[f](t,u) + P[f](t,u), \quad u \in D_u \\ \\ f(t,u) = 0, \quad u \in \partial D_u, \end{cases} \tag{1}$$

where:
• $\alpha_F[f](t)$ denotes the primitive thermostat operator which needs to be derived with respect to the selected contraint;
• $J[f](t,u)$ denotes the following conservative interaction operator:

$$\begin{aligned} J[f](t,u) &= G[f](t,u) - L[f](t,u) \\ &= \int_{D_u^2} \eta(u_*,u^*)\mathscr{A}(u,u_*,u^*) f(t,u_*) f(t,u^*)\, du_*\, du^* \\ &- f(t,u)\int_{D_u} \eta(u,u^*) f(t,u^*)\, du^*, \end{aligned} \tag{2}$$

where $\eta(u_*,u^*)$ represents the conservative interaction rate between the particles u_* and u^*, and $\mathscr{A}(u,u_*,u^*)$ denotes the probability function that the particle u_* acquires the state u after the interaction with the particle u^*;
• $P[f](t,u)$ denotes the following nonconservative interaction operator:

$$P[f](t,u) = f(t,u)\int_{D_u} \eta(u,u^*)\,\mu(u,u^*)\, f(t,u^*)\, du^*, \tag{3}$$

where $\mu(u,u^*)$ denotes the nonconservative interaction rate between the particles u and u^*. This operator models the proliferative ($\mu > 0$) and the destructive ($\mu < 0$) events.

The pth-order moment of the distribution function f is defined as follows:

$$\mathbb{E}_p[f](t) = \int_{D_u} u^p f(t,u)\, du, \qquad p \in \mathbb{N}.$$

The thermostat operator α_F is derived by imposing a specific constraint, see [27] for a general understanding of the thermostats in nonequilibrium statistical mechanics. Specifically in this article the thermostatted operator α_F is obtained by requiring the conservation of the 2nd-order moment $\mathbb{E}_2[f](t)$ (the activity energy).
By assuming that $\mathbb{E}_2[f](t) = 1$ for all $t > 0$, we have:

$$\frac{d}{dt}\mathbb{E}_2[f](t) = 0,$$

and then

$$\frac{d}{dt}\mathbb{E}_2[f](t) = \int_{D_u} u^2\, \partial_t f(t,u)\, du = 0. \tag{4}$$

By using the equations (1) and (4) we have:

$$\begin{aligned} -\int_{D_u} u^2\, \partial_u\left((F - \alpha_F u) f(t,u)\right) du + \int_{D_u} u^2 J[f](t,u)\, du \\ + \int_{D_u} u^2 P[f](t,u)\, du = 0, \end{aligned} \tag{5}$$

and by observing that

$$\int_{D_u} u^2 J[f](t,u)\, du = 0,$$

one has:

$$\begin{aligned}\int_{D_u} u^2\,\partial_u\left((F-\alpha_F\,u)f(t,u)\right)du &= \\ &= -2\int_{D_u} u\,(F-\alpha_F\,u)\,f(t,u)\,du \\ &= -2F\,\mathbb{E}_1[f](t)+2\alpha_F.\end{aligned} \tag{6}$$

By using the (5) and the (6), the thermostat term reads:

$$\alpha_F[f,P](t)=F\,\mathbb{E}_1[f](t)+\frac{1}{2}\int_{D_u} u^2\,P[f](t,u)\,du. \tag{7}$$

By using the (7), the *nonconservative-thermostat* framework of the thermostatted kinetic theory for active particles reads:

$$\begin{aligned}&\partial_t f(t,u)\\ &+\partial_u\left(\left(F-\left(\frac{2F\,\mathbb{E}_1[f]+\int_{D_u}u^2\,P[f]\,du}{2}\right)u\right)f(t,u)\right)\\ &=J[f](t,u)+P[f](t,u).\end{aligned} \tag{8}$$

The new framework (8) constitutes a new paradigm for the derivation of specific models for the modeling of complex biologcal systems once the conservative interaction rate η, the nonconservative interaction rate μ and the transition probability function $\mathscr{A}$ are selected. In particular the following main assumptions are required for the function $\mathscr{A}$:

A1: $\int_{D_u}\mathscr{A}(u,u_*,u^*)\,du=1$, for all $u_*,u^*\in D_u$;
A2: $\int_{D_u}u\,\mathscr{A}(u,u_*,u^*)\,du=0$, for all $u_*,u^*\in D_u$;
A3: $\int_{D_u}u^2\mathscr{A}(u,u_*,u^*)\,du=u_*^2$, for all $u_*,u^*\in D_u$.

It is worth stressing that the conservative and nonconservative interaction rates η and μ are not assumed constants.
The mathematical analysis (existence and uniqueness of the solution of the related initial-boundary value problem) requires a particular attention considering the nonconservative operator. The results will be presented in due course.
The next section is concerned with the main result of this paper.

3 Density and linear-momentum evolution

This section deals with the derivation of the evolution equations for the *density* ($p=0$) and the *linear-momentum* ($p=1$) of the system, defined as follows:

$$\begin{aligned}\mathbb{E}_0[f](t)&=\int_{D_u}f(t,u)\,du:=\rho(t),\\ \mathbb{E}_1[f](t)&=\int_{D_u}uf(t,u)\,du:=m(t).\end{aligned}$$

Let

$$\Xi[f](t):=u\left(F-\left(\frac{2F\,\mathbb{E}_1[f]+\int_{D_u}u^2\,P[f]\,du}{2}\right)\right),$$

$$\Psi[f](t):=\int_{D_u}u^2\,P[f]\,du.$$

In order to derive the *evolution equations* for the nonconservative-thermostat framework (8), by multipling the equation (8) by a test function $\varphi(u)$ and then by integrating with respect the variable $u\in D_u$, one has:

$$\begin{aligned}&\int_{D_u}\varphi(u)\partial_t f(t,u)\,du\\ &+\int_{D_u}\varphi(u)\partial_u\left(\Xi[f](t)\,f(t,u)\right)du\\ &=\int_{D_u}\varphi(u)J[f](t,u)\,du+\int_{D_u}\varphi(u)P[f](t,u)\,du\\ &=\int_{D_u}\varphi(u)\left(\int_{D_u^2}\eta\,\mathscr{A}\,f(t,u_*)f(t,u^*)\,du_*\,du^*\right)du\\ &-\int_{D_u}\varphi(u)f(t,u)\left(\int_{D_u}\eta f(t,u^*)\,du^*\right)du\\ &+\int_{D_u}\varphi(u)f(t,u)\left(\int_{D_u}\eta\,\mu\,f(t,u^*)\,du^*\right)du.\end{aligned} \tag{9}$$

Since

$$\int_{D_u}\varphi(u)\partial_t f(t,u)\,du=\partial_t\int_{D_u}\varphi(u)f(t,u)\,du,$$

the (9) rewrites:

$$\begin{aligned}&\partial_t\int_{D_u}\varphi(u)f(t,u)\,du\\ &+\int_{D_u}\varphi(u)\partial_u\left(\Xi[f](t)\,f(t,u)\right)du\\ &=\int_{D_u}\int_{D_u^2}\eta\,\varphi(u)\,\mathscr{A}\,f(t,u_*)f(t,u^*)\,du_*\,du^*\,du\\ &-\int_{D_u}\int_{D_u}\eta\,\varphi(u)f(t,u)f(t,u^*)\,du^*\,du\\ &+\int_{D_u}\int_{D_u}\eta\,\mu\,\varphi(u)f(t,u)f(t,u^*)\,du^*\,du.\end{aligned} \tag{10}$$

• Let $\varphi(u)=1$. Then the (10) rewrites:

$$\begin{aligned}&\partial_t\int_{D_u} f(t,u)\,du+\int_{D_u}\partial_u\left(\Xi[f](t)\,f(t,u)\right)du\\&=\int_{D_u^3}\eta\,\mathscr{A}\,f(t,u_*)f(t,u^*)\,du_*\,du^*\,du\\&-\int_{D_u}\left(\int_{D_u}\eta\,f(t,u)f(t,u^*)\,du^*\right)du\\&+\int_{D_u}\left(\int_{D_u}\eta\,\mu\,f(t,u)f(t,u^*)\,du^*\right)du.\end{aligned}\tag{11}$$

The second term on the left hand side of the (11) vanishes since $f(t,u)=0$ on the boundary. Moreover, the property $\mathbf{A_1}$ of the operator $J[f](t,u)$ implies the following identity:

$$\begin{aligned}&\int_{D_u}\int_{D_u^2}\eta\,\mathscr{A}\,f(t,u_*)f(t,u^*)\,du_*\,du^*\,du\\&\qquad-\int_{D_u}\int_{D_u}\eta\,f(t,u)f(t,u^*)\,du^*\,du=0.\end{aligned}$$

Bearing all above in mind, the (11) writes:

$$\partial_t\rho(t)=\int_{D_u^2}\eta(u,u^*)\,\mu(u,u^*)\,f(t,u)f(t,u^*)\,du\,du^*.\tag{12}$$

*Remark.*If the system is subjected to conservative interactions only ($\mu=0$), the (12) reads:

$$\partial_t\rho(t)=0,$$

which means that the density is conserved and $f(t,u)$ acquires the structure of a probability distribution function.

• Let $\varphi(u)=u$. The (10) rewrites:

$$\begin{aligned}&\partial_t\int_{D_u} uf(t,u)\,du+\int_{D_u}u\,\partial_u\left(\Xi[f](t)\,f(t,u)\right)du\\&=\int_{D_u^3}\eta\,u\,\mathscr{A}\,f(t,u_*)f(t,u^*)\,du_*\,du^*\,du\\&-\int_{D_u}\int_{D_u}\eta\,u\,f(t,u)f(t,u^*)\,du^*\,du\\&+\int_{D_u}\int_{D_u}\eta\,\mu\,u\,f(t,u)f(t,u^*)\,du^*\,du.\end{aligned}\tag{13}$$

The assumption $\mathbf{A_2}$ on the transition probability function $\mathscr{A}(u,u_*,u^*)$ ensures that the first term on the right hand side of the (13) vanishes. Then straightforward calculations show:

$$\begin{aligned}&\int_{D_u}u\,\partial_u\left(\left(F-\left(\frac{2F\,\mathbb{E}_1[f]+\Psi[f](t)}{2}\right)u\right)f\right)du\\&=-\int_{D_u}\left(\left(F-\left(\frac{2F\,\mathbb{E}_1[f]+\Psi[f](t)}{2}\right)u\right)f\right)du\\&=-\int_{D_u}F\,f\,du+\int_{D_u}\left(\frac{2F\,\mathbb{E}_1[f]+\Psi[f](t)}{2}\right)uf\,du\\&=-F\rho(t)+\int_{D_u}F\,\mathbb{E}_1[f](t)\,uf(t,u)\,du\\&+\frac{1}{2}\left(\int_{D_u}u^2P[f](t,u)\,du\right)\int_{D_u}uf(t,u)\,du\\&=-F\rho(t)+Fm^2(t)+\frac{1}{2}\left(\int_{D_u}u^2P[f]\,du\right)m(t).\end{aligned}\tag{14}$$

The second and the third terms on the right hand side of the (13) writes:

$$\begin{aligned}&-\int_{D_u}\int_{D_u}\eta\,u\,f(t,u)f(t,u^*)\,du^*\,du\\&+\int_{D_u}\int_{D_u}\eta\,\mu\,u\,f(t,u)f(t,u^*)\,du^*\,du\\&=\int_{D_u\times D_u}\eta(\mu-1)\,uf(t,u)f(t,u^*)\,du^*\,du.\end{aligned}\tag{15}$$

By using the (14) and the (15), the (13) furnishes the second equation of the system:

$$\begin{aligned}&\partial_t m=F\rho-Fm^2-\frac{1}{2}\left(\int_{D_u}u^2P[f](t,u)\,du\right)m\\&+\int_{D_u\times D_u}\eta(\mu-1)\,uf(t,u)f(t,u^*)\,du^*\,du.\end{aligned}\tag{16}$$

The system of evolution equations reads:

$$\begin{cases}\partial_t\rho=\displaystyle\int_{D_u^2}\eta\,\mu\,f(t,u)f(t,u^*)\,du^*\,du,\\[2ex]\partial_t m=F\rho-Fm^2-\dfrac{1}{2}\left(\displaystyle\int_{D_u}u^2P[f]\,du\right)m\\+\displaystyle\int_{D_u^2}\eta(\mu-1)\,uf(t,u)f(t,u^*)\,du^*\,du.\end{cases}\tag{17}$$

According to [28], the following assumption of separation of variables on the distribution function f is added:

$$f(t,u)=\rho(t)l(u),$$

where $l(u)$ is a suitable function defined on D_u, e.g. a *Dirac delta* function, such that:

$$\int_{D_u}l(u)\,du=1.$$

Accordingly the integral term in the equation $(17)_1$ rewrites:

$$\begin{aligned}&\int_{D_u}\int_{D_u}\eta\,\mu\,f(t,u)f(t,u^*)\,du^*\,du=\\&=\int_{D_u\times D_u}\eta\,\mu\,\rho^2(t)l(u)l(u^*)\,du^*\,du\\&=\rho^2(t)\left(\int_{D_u\times D_u}\eta\,\mu\,l(u)l(u^*)\,du^*\,du\right)\\&=k\rho^2(t),\end{aligned}\tag{18}$$

where

$$k:=\int_{D_u\times D_u}\eta(u,u^*)\,\mu(u,u^*)\,l(u)l(u^*)\,du^*\,du.$$

The integral term in the equation $(17)_2$ rewrites:

$$\begin{aligned}&\int_{D_u^2}\eta(\mu-1)\,uf(t,u)f(t,u^*)\,du^*\,du=\\&=\int_{D_u^2}\eta(\mu-1)\,u\rho^2(t)l(u)l(u^*)\,du^*\,du\\&=\rho^2(t)\left(\int_{D_u^2}\eta(\mu-1)\,ul(u)l(u^*)\,du^*\,du\right)\\&=h\rho^2(t),\end{aligned}\tag{19}$$

where

$$h:=\int_{D_u\times D_u}\eta(u,u^*)(\mu(u,u^*)-1)\,ul(u)l(u^*)\,du^*\,du.$$

Finally:

$$\begin{aligned}&\int_{D_u}u^2P[f](t,u)\,du=\\&=\int_{D_u}u^2f(t,u)\left(\int_{D_u}\eta\,\mu\,f(t,u^*)\,du^*\right)du\\&=\int_{D_u^2}\eta\,\mu\,u^2\rho^2(t)l(u)l(u^*)\,du^*\,du\\&=\rho^2(t)\left(\int_{D_u^2}\eta\,\mu\,u^2l(u)l(u^*)\,du^*\,du\right)\\&=\theta\rho^2(t),\end{aligned}\tag{20}$$

where

$$\theta:=\int_{D_u\times D_u}\eta(u,u^*)\mu(u,u^*)u^2l(u)l(u^*)\,du^*\,du.$$

By using the (18), (19) and (20), the system (17) rewrites:

$$\begin{cases}\partial_t\rho(t)=k\rho^2(t),\\\partial_t m(t)=-Fm^2(t)-\dfrac{\theta}{2}\rho^2(t)m(t)+h\rho^2(t)+F\rho(t).\end{cases}\tag{21}$$

It is worth stressing that the solutions of the above system will help in the investigation of the existence and uniqueness of the solution of the initial-boundary value problem related to the mathematical framework (8).

4 Conclusions and research perspectives

The new mathematical framework proposed in this paper allows the modeling of complex biological systems and in particular a control is introduced for the time evolution of the activity-energy moment. The control is based on the definition of a new thermostat term (7), which also includes the role of the nonconservative interactions.
The paper has been also devoted to the derivation of the evolution equation for the density of the system and for the linear-momentum. As shown in the last section (see (21)), the evolution equations are ordinary differential equations with quadratic nonlinearities. Specifically the equation for the density of the system is a separable differential equation whereas the equation fulfilled by the linear-momentum is a Riccati differential equation.

The new framework (8) opens to future research perspectives from the theoretical and applied point of views. Firstly the existence and uniqueness of solutions of the related initial boundary value problem needs to be investigated. The main difficulty is the introduction of the nonconservative interactions which can affect the global existence of solutions; a future investigation could be addressed to the question if the conservation of the activity-energy moment could allow the existence of the global solution or if the control of the density evolution needs to be required by further modifing the thermostat term. In this context the topology of the domain D_u is an important step of investigation in particular in the case of the unbounded domain.

The generalization of the framework (8) to the complex systems composed by different functional subsystems is straightforward. Indeed as shown in [26], the modification of the general framework consists in introducing the summation over the number of functional subsystems. In this context, the mutative events can be also taken into account.

New inverse problems based on the information theory could be also investigated as in the paper [29]. The result should be again straightforward but the proof of the existence of solutions could be affected by the new thermostat term and a new technique should be employed.

From the application viewpoint, the target complex living systems are of biological fashion considering the role of proliferation and mutation of the particles composing the system. Some systems can be mentioned: immune system [25], tumor growth [30], cancer immune system competition [31], virus infection [32].

Acknowledgement

The second author acknowledges VALERE: VAnviteLli pEr la RicErca of Università degli Studi della Campania Luigi Vanvitelli, in the project "ANDROIDS", and the support of GNFM (National Group of Mathematical-Physics) of INDAM (National Institute of Advanced Mathematics).
The authors are grateful to the anonymous referee for a careful checking of the details and for helpful comments that improved this paper.

Conflict of Interest

The authors declare that they have no conflict of interest.

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