Applied Mathematical Sciences, Vol. 6, 2012, no. 14, 651 - 660

Kinetic Theory for Active Particles Modelling Coupled to Gaussian Thermostats

Carlo Bianca

Dipartimento di Matematica,
Politecnico di Torino
Corso Duca degli Abruzzi 24, 10129, Torino, Italy
carlo.bianca@polito.it

Abstract

This paper deals with the kinetic theory for active particles modelling of complex systems, under the action of a velocity-dependent force field, and constrained to kept constant the total kinetic energy. A further development of the mathematical theory is here proposed, which consists in the external force-Gaussian isokinetic thermostat coupling with the intent to preserve the kinetic energy of the system during the motion. The relative framework constitutes the paradigm for the derivation of specific models in the applied mathematical sciences, e.g., the chemotaxis phenomenon in biological systems.

Mathematics Subject Classification: 35Q20, 82C22, 92B05

Keywords: Complexity, Isokinetic Thermostats, Nonlinearity, PDE, ODE

1 Introduction

The mathematical modelling of complex biological/social systems is one of the major challenges of this century. Complexity arises when large numbers of individuals (cells, bacteria, people) collectively organize into spatial patterns. In these systems the collective organization involves response to spatial/velocity gradients of attractants or repellents, e.g. *chemotaxis* is the movement of cells toward favorable conditions in response to the gradient of a chemical, see the multiscale mathematical models introduced in [1, 14, 19].

The kinetic theory for active particles, hereafter in brief KTAP, has been developed in order to model complex systems constituted by a large number of interacting particles (called *active particles*), whose microscopic state includes, in addition to position and velocity variables, also a scalar variable (called *activity variable*), which is related to the intrinsic biological/social function of

particles. According to KTAP, the overall system is divided into different subsystems each of them composed by particles that collectively express the same biological/social function (*functional subsystems*). The evolution of each functional subsystem is described by a distribution function over the microscopic state of the particles and the time evolution of the subsystem is governed by interactions which can change both the microscopic state (*conservative interactions*) and the number of particles (*nonconservative interactions*). The interested reader on recent developments of this theory is referred to the bibliography section of the recent book [7].

In a complex system composed of a large number of identical individuals, where external effects are neglected, the random interactions among individuals will eventually move the system towards equilibrium. If, on the other hand, an external force field acts on the system, the applied field does work on the system thereby moving it away from equilibrium. The excess energy needs to be removed so as to achieve a steady state. A method, which is common in nonequilibrium molecular dynamics simulations, is the use of deterministic thermostats. This technique has been proposed in statistical mechanics as a means of constructing steady states of relatively simple but still interesting models of far from equilibrium systems.

The use of deterministic thermostats consists by introducing a damping term into the equations of motion. The damping term is adjusted so as to keep the kinetic energy constant. This way of thermostatting nonequilibrium molecular dynamics simulations by modifying the equations of motion was put in a theoretical framework when the connection with Gauss principle of least constraint was established, see [12]. This dynamical principle states that a system subject to constraints will follow trajectories which, in the least-square sense, differ minimally from their unconstrained Newtonian counterparts. In general thermostats are applied in order to achieve equilibration to non equilibrium situation where there is a flux of energy through the system, such as induced by external fields or by imposing temperature or velocity gradients. Gaussian isokinetic thermostats have been used in connection with the Lorentz gas (see [11, 17] and the review paper [4]) and with the nonequilibrium Ehrenfest gas [6, 9]. Related numerical and analytical studies of a system where one or several particles are moving in a two-dimensional array of fixed hard disk scatterer under the influence of an electric field, are also made in [10].

This paper is concerned with further developments of the mathematical framework of the KTAP proposed in [2]. Specifically, the paper takes into account complex systems subjected to external force fields which depend on the velocity variable and whose magnitude exerts an action on the particles. A Gaussian isokinetic thermostat is introduced in order to keep constant the kinetic energy of the system.

The contents of the present paper are organized into four more sections that follow this introduction. In detail, Section 2 and Section 3 highlight the essentials of kinetic theory for active particles and the mathematical settings

of deterministic thermostats in order to motivate our study. Section 4 is concerned with the derivation of the mathematical framework which combines the kinetic theory for active particles and the Gaussian isokinetic thermostat. Finally Section 5 proposes a critical analysis and the research perspective of the mathematical framework developed in Section 4.

2 Kinetic Theory for Active Particles: Background

Let $\mathcal{F}$ be a functional subsystem constituted by a large number of interacting active particles whose microscopic state $\mathcal{S} = (\mathbf{x}, \mathbf{v}, u) \in D_{\mathbf{x}} \times D_{\mathbf{v}} \times D_u \subseteq \mathbb{R}^3 \times \mathbb{R}^3 \times \mathbb{R}$ includes, in addition to the usual mechanical variables position $\mathbf{x} \in \mathbb{R}^3$ and velocity $\mathbf{v} \in \mathbb{R}^3$, a scalar variable $u \in \mathbb{R}$ (called *activity variable*) related to the intrinsic biological/social function of particles.

According to KTAP, the overall state of $\mathcal{F}$, at time t, is described by the distribution function $f = f(t, \mathbf{x}, \mathbf{v}, u) : [0, T] \times D_{\mathbf{x}} \times D_{\mathbf{v}} \times D_u \to \mathbb{R}^+$, over the microscopic state $\mathcal{S}$ of the active particles. Under suitable integrability assumptions, $f(t, \mathbf{x}, \mathbf{v}, u)\, d\mathbf{x}\, d\mathbf{v}\, du$ denotes, for all $t \geq 0$, the number of active particles whose state, at time t, is in the elementary volume $d\mathcal{V} = [\mathbf{x}, \mathbf{x} + d\mathbf{x}] \times [\mathbf{v}, \mathbf{v} + d\mathbf{v}] \times [u, u + du]$. Moreover the knowledge of the distribution function f leads to the calculations of macroscopic quantities for $\mathcal{F}$, see [7].

The microscopic state $\mathcal{S}$ of particles is modified, at the time t, by localized *interactions*, which involve three kind of particles: Test particles with microscopic state, at the time t, defined by the variable $(\mathbf{x}, \mathbf{v}, u)$, whose distribution function is $f = f(t, \mathbf{x}, \mathbf{v}, u)$; Field particles with microscopic state, at the time t, defined by the variable $(\mathbf{x}^*, \mathbf{v}^*, u^*)$, whose distribution function is $f^* = f(t, \mathbf{x}^*, \mathbf{v}^*, u^*)$; Candidate particles with microscopic state, at the time t, defined by the variable $(\mathbf{x}_*, \mathbf{v}_*, u_*)$, whose distribution function is $f_* = f(t, \mathbf{x}_*, \mathbf{v}_*, u_*)$. According to KTAP, candidate particles can acquire, in probability, the microscopic state of the test particles, after an interaction with field particles, while test particles loose their microscopic state after interactions.

In what follows we consider interactions that do not modify the active particles number (*conservative interactions*) therefore the distribution function f is a probability function. The presentation of mathematical framework requires the following assumptions:

Assumption 1. The candidate and/or test particles in $\mathbf{x}$, with velocity $\mathbf{v}_*$ and/or $\mathbf{v}$, and activity u_* and/or u, interact with the field particle in $\mathbf{x}^*$, with velocity $\mathbf{v}^*$ and activity u^*, located in the *interaction domain* Ω, namely $\mathbf{x}^* \in \Omega = \Omega(\mathbf{x})$.

Assumption 2. The conservative interactions are weighted by a suitable term $\eta = \eta(\mathbf{x}, \mathbf{x}^*, u_*, u^*)$ that can be interpreted as an *interaction rate*, which

depends on the position and activity variables of the candidate and field particles. The intensity of the topological distribution of the interactions is taken into account by the $(\mathbf{x}, \mathbf{x}^*)$ dependence in η.

Assumption 3. The candidate particle modifies its velocity $\mathbf{v}_*$ and activity u_* according to the probability density $\mathcal{A} = \mathcal{A}(\mathbf{v}_* \to \mathbf{v},\, u_* \to u | \mathbf{v}_*, \mathbf{v}^*, u_*, u^*)$, which represents the probability density that a candidate particles with state $(\mathbf{v}_*, u_*)$ reaches the state $(\mathbf{v}, u)$ of the test particle after an interaction with the field particles with state $(\mathbf{v}^*, u^*)$, while the test particle looses its state $(\mathbf{v}, u)$ after interactions with field particles, with state $(\mathbf{v}^*, u^*)$. Moreover the density $\mathcal{A}$ satisfies, $\forall\, \mathbf{v}_*, \mathbf{v}^* \in D_{\mathbf{v}}$ and $\forall\, u_*, u^* \in D_u$, the following property:

$$\int_{D_{\mathbf{v}} \times D_u} \mathcal{A}(\mathbf{v}_* \to \mathbf{v},\, u_* \to u | \mathbf{v}_*, \mathbf{v}^*, u_*, u^*)\, d\mathbf{v}\, du = 1. \tag{1}$$

The time evolution of f is derived by a balance equation of the inlet and outlet flows in the elementary volume $d\mathcal{V}$ of the space of the microscopic states $\mathcal{S}$. Therefore, equating the total variation of $f = f(t, \mathbf{x}, \mathbf{v}, u)$ in the volume $\mathcal{V}$, yields:

$$\Big(\partial_t + \psi(\mathbf{v}) \cdot \nabla_{\mathbf{x}}\Big)\, f + \nabla_{\mathbf{v}} \cdot (\mathbf{F} f) = G[f] - L[f]\,, \tag{2}$$

where:

- The dot stands for the usual Euclidean inner product in $\mathbb{R}^3$.
- $\nabla_{\mathbf{x}}$ and $\nabla_{\mathbf{x}}$ denote the gradient of f with respect to $\mathbf{x}$ and $\mathbf{v}$ respectively.
- The vector field $\psi(\mathbf{v}) = (\psi_1(\mathbf{v}), \psi_2(\mathbf{v}), \psi_3(\mathbf{v})) : D_{\mathbf{v}} \to \mathbb{R}^3$ models the transport in position, which is assumed depending on the velocity variable only (usually the linear transport is assumed, i.e. $\psi(\mathbf{v}) = \mathbf{v}$).
- $\mathbf{F} = \mathbf{F}(\mathbf{v}) = (\mathbf{F}_1(\mathbf{v}), \mathbf{F}_2(\mathbf{v}), \mathbf{F}_3(\mathbf{v})) : D_{\mathbf{v}} \to \mathbb{R}^3$ denotes the external force field acting on the particles, which is assumed depending on the velocity variable only.
- $G[f] = G[f](t, \mathbf{x}, \mathbf{v}, u)$ denotes the *gain* of candidate particles into the state $(\mathbf{x}, \mathbf{v}, u)$ and $L[f] = L[f](t, \mathbf{x}, \mathbf{v}, u)$ models the *loss* of test particles with state $(\mathbf{x}, \mathbf{v}, u)$. These terms read:

$$\begin{aligned} G[f] \;&=\; \int_{\Lambda \times D_u \times D_u} \eta(\mathbf{x}, \mathbf{x}^*, u_*, u^*)\, \mathcal{A}(\mathbf{v}_* \to \mathbf{v},\, u_* \to u | \mathbf{v}_*, \mathbf{v}^*, u_*, u^*) \\ &\times\; f(t, \mathbf{x}, \mathbf{v}_*, u_*) f(t, \mathbf{x}^*, \mathbf{v}^*, u^*)\, d\mathbf{x}^*\, d\mathbf{v}_*\, d\mathbf{v}^*\, du_*\, du^*\,, \end{aligned} \tag{3}$$

and

$$L[f] = f(t, \mathbf{x}, \mathbf{v}, u) \int_{\Gamma \times D_u} \eta(\mathbf{x}, \mathbf{x}^*, u_*, u^*)\, f(t, \mathbf{x}^*, \mathbf{v}^*, u^*)\, d\mathbf{x}^*\, d\mathbf{v}^*\, du^*\,, \tag{4}$$

where $\Lambda = \Omega \times D_{\mathbf{v}} \times D_{\mathbf{v}}$ and $\Gamma = \Omega \times D_{\mathbf{v}}$.

Remark 2.1 *When the state of the system is uniform over the activity variable (but interactions modify the mechanical variables), the gain* $G[f] = G[f](t, \mathbf{x}, \mathbf{v})$ *and the loss* $L[f] = L[f](t, \mathbf{x}, \mathbf{v})$ *terms of the mathematical framework (2), which refers to the evolution in time, position and velocity of the test particle distribution function* $f = f(t, \mathbf{x}, \mathbf{v})$*, thus read:*

$$G[f] = \int_{\Lambda} \eta(\mathbf{x}, \mathbf{x}^*)\, \mathcal{A}(\mathbf{v}_* \to \mathbf{v}|\mathbf{v}_*, \mathbf{v}^*) f(t, \mathbf{x}, \mathbf{v}_*) f(t, \mathbf{x}^*, \mathbf{v}^*)\, d\mathbf{x}^*\, d\mathbf{v}_*\, d\mathbf{v}^*\,, \quad (5)$$

and

$$L[f] = f(t, \mathbf{x}, \mathbf{v}) \int_{\Gamma} \eta(\mathbf{x}, \mathbf{x}^*)\, f(t, \mathbf{x}^*, \mathbf{v}^*)\, d\mathbf{x}^*\, d\mathbf{v}^*\,, \quad (6)$$

with $\Lambda = \Omega \times D_{\mathbf{v}} \times D_{\mathbf{v}}$ *and* $\Gamma = \Omega \times D_{\mathbf{v}}$.

Remark 2.2 *When the state of the system is uniform over the position variable, so that the distribution function* f *is independent of* $\mathbf{x}$*, the mathematical framework (2) reduces to the following spatially homogeneous framework:*

$$\partial_t f + \nabla_{\mathbf{v}} \cdot (\mathbf{F} f) = G[f] - L[f]\,, \quad (7)$$

where $G[f] = G[f](t, \mathbf{v}, u)$ *reads:*

$$\begin{aligned} G[f] \;&=\; \int_{D_{\mathbf{v}} \times D_{\mathbf{v}} \times D_u \times D_u} \eta(u_*, u^*)\, \mathcal{A}(\mathbf{v}_* \to \mathbf{v},\, u_* \to u|\mathbf{v}_*, \mathbf{v}^*, u_*, u^*) \\ &\times\; f(t, \mathbf{v}_*, u_*) f(t, \mathbf{v}^*, u^*)\, d\mathbf{v}_*\, d\mathbf{v}^*\, du_*\, du^*\,, \end{aligned} \quad (8)$$

and $L[f] = L[f](t, \mathbf{v}, u)$ *reads:*

$$L[f] = f(t, \mathbf{v}, u) \int_{D_{\mathbf{v}} \times D_u} \eta(u_*, u^*) f(t, \mathbf{v}^*, u^*)\, d\mathbf{v}^*\, du^*. \quad (9)$$

Since the aim of this paper is the modelling of systems where the kinetic energy is a constant of motion, in the remaining part of the paper, only the spatially homogeneous case (7) is considered.

As already mentioned in the introduction, the KTAP models also consider proliferative or destructive events, which modify the number of the active particles in their microscopic state (*nonconservative interactions*) and *transitive* (mutational) interactions, see [5, 7].

3 Gaussian Isokinetic Thermostats (GIT)

As already explained in the introduction, thermostats are mechanisms by which the internal energy of a many particle-system, and thus its temperature, can be tuned onto a specific value but constraints may be imposed onto a system leading, e.g., to constant pressure or constant stress ensemble. Nevertheless any thermostat may be though of being associated with some thermal

reservoir consisting of infinite number of degrees of freedom thus being large enough to absorb any amount of energy pumped into the system. Therefore thermostats are deterministic and time-reversible models of a thermal reservoir that remove energy from a subsystem during the originally free flight of a particle.

Definition 3.1 *A system is called* thermostatted *if the existence of the* non equilibrium steady state *(NSS) is due to the action of the thermal reservoir.*

Twenty years ago Evans and Hoover independently but simultaneously developed time reversible deterministic thermostats to enable convenient and efficient computer simulations of thermostatted dissipative systems [12]. These thermostats do not exist in Nature but nonequilibrium statistical mechanics has been used to prove that under specific circumstances thermodynamic properties and transport coefficients computed from simulations using these thermostats are essentially exact. The development of fictitious mathematical thermostats and algorithms for simulating transport coefficients of nonequilibrium thermodynamic systems has lead to an enormous advancement of nonequilibrium statistical mechanics. These two developments have allowed the mathematical apparatus of dynamical systems theory to be brought to bear on statistical mechanics.

The most elegant way of *thermostatting* a particle system subjected to external driving is given by Gauss' principle of least constraint [13]:

Gauss Principle (1829): *Consider N point particles of mass m_i, subjected to frictionless bilateral constraints Φ_i and to external forces $\mathbf{F}_i$. Among all motions allowed by the constraints, the* **natural** *one minimizes the following quantity:*

$$C = \sum_{i=1}^{N} m_i \left(\ddot{\mathbf{x}}_i - \frac{\mathbf{F}_i}{m_i} \right)^2 .$$

According to Gauss, the "Curvature" C is minimized by the accelerations of real motions or, equivalently, real motions minimize the action of the constraints. In the case of holonomic constraints, Gauss' principle is consistent with the principle of least action, and produces Hamiltonian equations of motion.

Differently, nonholonomic constraints lead to non-Hamiltonian equations of motion. In particular, consider the isokinetic (IK) constraint, which fixes the kinetic energy of the system, $2K = \sum_i m_i \mathbf{v}_i^2$. For a N-particle system subjected to an external field, these constraints yield:

$$\begin{cases} \frac{d\mathbf{x}_i}{dt} = \mathbf{v}_i \\ \\ \frac{d\mathbf{v}_i}{dt} = \frac{\mathbf{F}_i}{m_i} - \alpha \mathbf{v}_i \end{cases} \qquad i = 1, \ldots, N \tag{10}$$

where $\mathbf{F}_i$ is the total force, see [15, 16]. The term $-\alpha\mathbf{v}_i$ makes the dynamics dissipative, allowing the system to reach a steady state in the long time limit. Assuming $m_i = 1$, the thermostating multiplier α is determined by the condition that the energy is fixed identically as a consequence of the equations of motion (for the isokinetic thermostat the kinetic energy is fixed) and the term α in Equation (10) is just the Lagrange multiplier which implements Gauss' principle of least constraint. The value of α for the GIK thermostat is given by the following formula:

$$\alpha = \frac{\sum_{i=1}^{N} \mathbf{F}_i \cdot \mathbf{v}_i}{\sum_{i=1}^{N} \mathbf{v}_i \cdot \mathbf{v}_i} \tag{11}$$

The force fields $\frac{\mathbf{F}_i}{m_i} - \alpha\mathbf{v}_i$ are called *Gaussian isokinetic thermostats*. The IK constraint is only one possible option. Depending on the physical property to be described, a wide range of constraints is available, including isobaric, isochoric, isoenthalpic, constant stress constraints, etc.

4 Thermostatted KTAP's Framework

This section deals with the derivation of a framework for the mathematical modelling of a complex system constituted by a large number of active particles and subjected to an external force field $\mathbf{F} = \mathbf{F}(\mathbf{v}) : D_{\mathbf{v}} \to \mathbb{R}^3$. The conservative interactions among the particles and the force field $\mathbf{F}$ guide the time evolution of the distribution function f of the system. The force field $\mathbf{F}$ accelerates, on average, the particles and leads to an indefinite increase in energy in the system. Therefore in order to ensure the reaching of a stationary state, the force field is coupled with the Gaussian isokinetic thermostat (11). We call the resulting model *thermostatted KTAP's framework*. Clearly, a large force field can change the dynamics dramatically, so that the properties of the dynamics will be determined by the character of $\mathbf{F}$ more than by the interactions among the particles. Therefore we restrict ourselves to force fields that will not overcome the conservative interactions.

Consider the spatially homogeneous framework (7) in the presence of an external force field $\mathbf{F} = \mathbf{F}(\mathbf{v}) \in \mathbb{R}^3$ and a Gaussian thermostat. Assuming that:

$$\int_{D_{\mathbf{v}} \times D_u} f(t, \mathbf{v}, u)\, d\mathbf{v}\, du = 1 \quad \text{and} \quad \int_{D_{\mathbf{v}} \times D_u} \mathbf{v}^2 f(t, \mathbf{v}, u)\, d\mathbf{v}\, du = 1 \tag{12}$$

the thermostatted KTAP framework for $f(t, \mathbf{v}, u)$ thus reads:

$$\partial_t f(t, \mathbf{v}, u) + \nabla_{\mathbf{v}} \cdot \big((\mathbf{F} - \zeta_{\mathbf{F}}(t)\, \mathbf{v}) f(t, \mathbf{v}, u)\big) = G[f](t, \mathbf{v}, u) - L[f](t, \mathbf{v}, u), \tag{13}$$

where

$$\zeta_{\mathbf{F}}(t) = \int_{D_{\mathbf{v}} \times D_u} \mathbf{F} \cdot \mathbf{v}\, f(t, \mathbf{v}, u)\, d\mathbf{v}\, du, \tag{14}$$

denotes the current density and the gain G and the loss L terms are given by formulas (8) and (9), respectively.

It is worth stressing that the mathematical framework (13) constitutes the paradigm for the derivation of specific models. Therefore a specific model is derived when the encounter rate η, the probability density $\mathcal{A}$ and the force field $\mathbf{F}$ are assessed.

Remark 4.1 *The relative stationary problem associated with the thermostatted KTAP framework (13) satisfies the following equation:*

$$\nabla_{\mathbf{v}} \cdot \big((\boldsymbol{F} - \zeta_{\boldsymbol{F}} \mathbf{v}) f(\mathbf{v}, u)\big) = G[f](\mathbf{v}, u) - L[f](\mathbf{v}, u). \tag{15}$$

5 Critical Analysis and Perspective

The main contribution of the present paper consists in the modification of the structures summarized in [7]. The proposed mathematical framework (13) can be considered as paradigm for the derivation of specific models of KTAP for complex systems (biological, traffic, crowds, social systems) where the time evolution of the distribution function of the system is determined not only by the microscopic interactions but also by the action of an external force field. To the best of our knowledge, this is the first time that Gaussian thermostats are coupled to kinetic theory for active particles; a similar problem was studied in [18] where the nonequilibrium stationary states for the thermostatted Kac equation are studied in detail.

The framework given by equation (13) has to be further generalized in order to include the role of nonconservative and transitive (mutational) interactions taken into account into the mathematical model presented in [5] and in the KTAP models of the reference section of book [7]. Moreover some KTAP models are such that the interaction rate η and the density $\mathcal{A}$ are conditioned by the distribution functions f_* and f^* of the candidate and field particles respectively, and low-order moments: linear momentum and kinetic energy (*nonlinear interactions*), see [3]. However, the analysis of models which include nonlinear interactions is still an open problem. Finally the framework (13) has to be explored for open systems, namely systems where external actions are introduced at the microscopic scale.

From the mathematical point of view, a research perspective is to examine the conditions under which exists a non-negative solution f to the following time-dependent thermostatted KTAP's framework:

$$\begin{cases} \partial_t f(t, \mathbf{v}, u) + \nabla_{\mathbf{v}} \cdot \big((\mathbf{F} - \zeta_{\mathbf{F}}(t)\, \mathbf{v}) f(t, \mathbf{v}, u)\big) = G[f](t, \mathbf{v}, u) - L[f](t, \mathbf{v}, u), \\ \\ f(0, \mathbf{v}, u) = f_0(\mathbf{v}, u) \end{cases}$$

where the initial datum $f_0 = f_0(\mathbf{v}, u)$ is a nonnegative function and $\zeta_{\mathbf{F}}$ is given by formula (14). Moveover the analysis of the stationary problem given by equation (15) is an open problem and the presence of the activity variable, that may affect also the velocity variable, makes the problem harder and harder.

It is worth stressing that the introduction of Gaussian thermostats can be also pursued in the mathematical models developed for the immune system and summarized in the recent expository paper [8].

Finally, following the general idea proposed in the present paper (keep constant the kinetic energy of the system), one may define in a system subjected to external force fields, quantities that have to be maintained constant (for instance the *global wealth* of the populations in the social systems, see the review paper [2]) and rewrites the external force fields in order to ensure these constraints. Of course the constraints may pertain to quantities related to the activity variable as well as the velocity variable.

Acknowledgements

CB was partially supported by the FIRB project-RBID08PP3J-Metodi matematici e relativi strumenti per la modellizzazione e la simulazione della formazione di tumori, competizione con il sistema immunitario, e conseguenti suggerimenti terapeutici. The research was also partially supported by the INDAM-GNFM-Young Researchers Project-prot.n.43-*Mathematical Modelling for the Cancer-Immune System Competition Elicited by a Vaccine*.

References

[1] N. Bellomo, A. Bellouquid, J. Nieto, and J. Soler, Multiscale biological tissue models and flux-limited chemotaxis for multicellular growing systems, Math. Models Methods Appl. Sci., **20** (2010), 1179-1207.

[2] N. Bellomo, C. Bianca, and M. Delitala, Complexity analysis and mathematical tools towards the modelling of living systems, Physics of Life Reviews, **6** (2009), 144-175.

[3] N. Bellomo, C. Bianca, and M.S. Mongiovì, On the modeling of nonlinear interactions in large complex systems, Appl. Math. Lett., **23** (2010), 1372-1377.

[4] C. Bianca, On the mathematical transport theory in microporous media: The billiard approach, Nonlinear Analysis: Hybrid Systems, **4** (2010), 699-735.

[5] C. Bianca, Mathematical modelling for keloid formation triggered by virus: Malignant effects and immune system competition, Math. Models Methods Appl. Sci., **21** (2011), 389-419.

[6] C. Bianca, Weyl-flow and the conformally symplectic structure of thermostatted billiards: The problem of the hyperbolicity, Nonlinear Analysis: Hybrid Systems, **5** (2011), 32-51.

[7] C. Bianca and N. Bellomo, Towards a Mathematical Theory of Multiscale Complex Biological Systems, World Scientific, Series in Mathematical Biology and Medicine, 2011.

[8] C. Bianca and M. Pennisi, Immune system modelling by top-down and bottom-up approaches, Int. Math. Forum, **7** (2012), 109-128.

[9] C. Bianca and L. Rondoni, The nonequilibrium Ehrenfest gas: A chaotic model with flat obstacles?, Chaos, **19** (2009), 013121.

[10] F. Bonetto, D. Daems, J.L. Lebowitz, and V. Ricci, Properties of stationary nonequilibrium states in the thermostatted periodic Lorentz gas: The multiparticle system, Phys. Rev. E, **65** (2002), 051204.

[11] N.I. Chernov, G.L. Eyink, J.L. Lebowitz, and Ya.G. Sinai, Derivation of Ohm's law in a deterministic mechanical model, Phys. Rev. Lett., **70** (1993), 2209-2212.

[12] D.J. Evans, W. G. Hoover, B. H. Failor, B. Moran, and A. J. C. Ladd, Nonequilibrium molecular dynamics via Gauss's principle of least constraint, Phys. Rev. A, **28** (1983), 1016-1021.

[13] K.F. Gauss, Uber ein Neues Allgemeines Grundgesatz der Mechanik (On a New Fundamental Law of Mechanics), J. Reine Angewandte Math., **4** (1829), 232-235.

[14] T. Hillen, Hyperbolic models for chemosensitive movement, Math. Models Methods Appl. Sci., **12** (2002), 1007-1034.

[15] G.P. Morriss and C.P. Dettmann, Thermostats: Analysis and application, Chaos, **8** (1998), 321-336.

[16] L. Rondoni, Deterministic thermostats and fluctuation relations, P. Garbaczewski and R. Olkiewicz Eds., Dynamics of dissipations, Lecture Notes in Physics **597**, Springer, Berlin (2002), 35-61.

[17] D. Ruelle, Smooth dynamics and new theoretical ideas in nonequilibrium statistical mechanics, J. Statist. Phys., **95** (1999), 393-468.

[18] B. Wennberg and Y. Wondmagegne, Stationary states for the Kac equation with a Gaussian thermostat, Nonlinearity, **17** (2004), 633-648.

[19] C. Xue and H.G. Othmer, Multiscale models of taxis-driven patterning in bacterial populations, SIAM J. Appl. Math., **70** (2009), 133-167.

Received: October, 2011