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Onset of nonlinearity in thermostatted active particles models for complex systems[☆]

Carlo Bianca[*]

Dipartimento di Scienze Matematiche, Politecnico, Corso Duca degli Abruzzi 24, 10129 Torino, Italy

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ABSTRACT

This paper is concerned with the derivation of a new discrete general framework of the kinetic theory, suitable for the modeling of complex systems under the action of an external force field and constrained to kept constant the mass or density, and the kinetic or activation energy. The resulting model relies on the interactions of single individuals within the population and is expressed by means of nonlinear ordinary or partial integro-differential equations. The global in time existence and uniqueness of the solution to the relative Cauchy problem are proved for which the density and the energy of the solution are preserved. A critical analysis, proposed in the last part of the paper, outlines suitable applications and research perspectives.

1. Introduction

Recently the modeling of complex phenomena in nature and society have been the object of several investigations based on methods originally developed in a physical context. Different approaches inspired to equilibrium or non equilibrium statistical mechanics have been developed, adapted and employed in an attempt to describe collective behaviors and macroscopic features as the result of microscopic (individual) interactions, among others see [1–7].

In the context of diluted gas of particles, Gatignol has proposed in [8] the discrete Boltzmann equation as a model suitable to describe the behavior of this gas which can attain only a finite (discrete) number of velocities. In the discrete approach the original continuous Boltzmann equation, which is an integro-differential equation, is transformed into a suitable set of partial differential equations, each corresponding to a discrete velocity. Therefore the computational complexity of the original Boltzmann equation is reduced.

Differently from the inert matter, complex phenomena occurring in nature and society are a consequence of the ability of individuals to develop strategies. The interested reader in the ability of biological systems to develop strategies is referred to book [1]. In order to take into account these capabilities, methods of the mathematical kinetic theory have been developed, somehow similarly to those for diluted gas. Accordingly, the *kinetic theory for active particles model* is based on the assumption that complex systems under considerations are composed by a large number of (intelligent) individuals, called *active particles*, whose microscopic state is described not only by the classical mechanical variables, but also by a continuous variable, called *activity*, which expresses a biological or social function or purpose. The mathematical theory describes the system under consideration by means of a distribution function over the microscopic state. After modeling the microscopic

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[*] Tel.: +39 0115647538.
E-mail addresses: carlo.bianca@polito.it, bianca.carlo@gmail.com.

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interactions, one derives an integro-differential evolution equation for the distribution function, see the review paper [9]. On the other hand, there are complex systems in which the microscopic state, rather than being naturally representable by continuous variables, can attain only a finite number of values (*discrete kinetic theory for active particles*, in brief DKTAP). Accordingly a structure is proposed consisting in a system of (ordinary or partial) integro-differential equations, suitable for modeling the evolution of a discrete probability distribution in large complex systems of active particles, see [9] and the references therein.

The DKTAP framework applied to traffic flow or crowds dynamics modeling rests on the assumption that vehicles or pedestrians move with a finite number of velocities only, see [10]. The idea of discretizing the velocity variable in these systems appears worthy of being developed, not only because the active particles often move in clusters identified by a discrete set of velocities, but also considering that experiments developed to identify the parameters of the models can be effectively performed looking at groups of vehicles or pedestrians with the same velocity, see the recent mathematical model [11] and the analytical investigations contained in [12,13]. Moreover the discretization of the microscopic variable appears worthy also for biological systems, e.g. in models of the competition between tumor and immune system cells, where the goal is to identify the specific activities of the different cell populations interacting in a vertebrate. This idea was developed by various authors related to specific models in the spatially homogeneous case as documented in [9] and the references therein.

The mathematical frameworks described previously can be called *equilibrium* models, because there is no dissipation of energy. Indeed in complex systems 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. Such situations necessitate the modeling of an infinite dimensional thermal reservoir that is able to continuously absorb energy in order to prevent a subsystem from heating up. The dissipation of energy into a thermal reservoir thus properly counterbalances the pumping of energy into the system by external field and enables the system to evolve into a *nonequilibrium steady state* (NSS), namely the statistical physical parameters describing the system on macroscopic scales are constant in time, despite the fact that the system in no longer in thermal equilibrium. If the existence of a NSS is due to the action of a thermal reservoir the system is called *thermostatted*. The following question now arises: How can we suitably amend the DKTAP framework in order to model an energy dissipation into a thermal reservoir? A popular deterministic and time-reversible modeling of a thermal reservoir is known as the *deterministic thermostat*. The use of deterministic thermostats consists of introducing a damping term into the equations of motion [14,15] and amounts to projecting the force field onto the tangent plane to the energy surface. The damping term is adjusted so as to keep the kinetic energy constant (*Gaussian thermostat*). The Gaussian thermostat is based on the Gauss' principle of least constraint [16], which states that *a system subject to constraints will follow trajectories which, in the least-square sense, differ minimally from their unconstrained Newtonian counterparts*. The characteristic features of thermostatted many-particle systems have been recovered for specific one-particle systems such as the Gaussian thermostatted Lorentz gas and Ehrenfest gas, among others [17–22] and the recent review paper [23]. It is worth mentioning the book [24] where an unexpected relationship is outlined between deterministic thermostats and active Browian particles modeling biophysical cell motility, and the paper [25] where the author investigates the analytical properties of a second order nonlinear boundary value problem that models a thermostat.

The present paper attempts to develop a new general framework within the discrete kinetic theory approach coupled to a Gaussian thermostat. We refer briefly to T-DKTAP, to be exploited toward modeling large complex systems of interest in nature and society. Specifically, the paper takes into account complex systems subjected to external force fields which depend on the velocity or activity variable and whose magnitude exerts an action on the particles. A Gaussian isokinetic thermostat is introduced in order to keep constant the mass and the kinetic energy of the system. This framework led to a new class of dynamical systems contemplating stochastic interactions, expressed in the form of systems of partial differential equations or, in particular cases, of ordinary differential equations. The framework proposed here is certainly worthy of future research concerning both its qualitative analysis and the application to modeling complex systems in applied sciences. The global in time existence and uniqueness proof of a solution for the T-DKTAP framework are here established, for which the zero (density) and second (activation energy) order moments are preserved. The existence result is based on integration along characteristics and successive approximations and is gained under the sole assumptions that the zero and the second order moments of the initial data are finite. To the best of our knowledge, the existence, smoothness and uniqueness of a solution to thermostatted kinetic equations has been investigated for the thermostatted non-cutoff Kac equation [26–28] and for the thermostatted kinetic theory for active particles framework when the microscopic state is continuous, see [29,30]. The interested reader in well-posedness results for classical KTAP models is referred to paper [31] and the references therein.

The contents of the present paper are divided into more four sections which follow this introduction. Section 2 highlights the essential mathematical settings of deterministic thermostats in order to motivate our study. Section 3 briefly deals with particular cases of the discrete kinetic theory for active particles framework, suitable for the description of homogeneous or nonhomogeneous in space systems, i.e. systems for which the distribution function only depends on the biological or social state or can also depend on the space and velocity variables. Section 4 is concerned with the derivation of the mathematical framework which combines the discrete kinetic theory for active particles framework with the Gaussian isokinetic thermostat. Moreover the analysis of the relative Cauchy problem is considered. Specifically the existence and