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Research paper

Qualitative analysis of a discrete thermostatted kinetic framework modeling complex adaptive systems

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A B S T R A C T

This paper deals with the derivation of a new discrete thermostatted kinetic framework for the modeling of complex adaptive systems subjected to external force fields (nonequilibrium system). Specifically, in order to model nonequilibrium stationary states of the system, the external force field is coupled to a dissipative term (thermostat). The well-posedness of the related Cauchy problem is investigated thus allowing the new discrete thermostatted framework to be suitable for the derivation of specific models and the related computational analysis. Applications to crowd dynamics and future research directions are also discussed within the paper.

1. Introduction

The modeling of complex adaptive systems has recently gained the attention of many scholars coming from different fields of the applied sciences. Complex adaptive systems are composed by a large numbers of particles, often called agents, that are able to interact, to adapt and to learn, see [1]. In particular self-similarity, complexity, emergence and self-organization are the main features of a complex adaptive system, see the book [2]. However what became really interesting these systems is the high degree of adaptive capacity, which allows them to face the perturbations. The adaptation is an important issue, considering that, among the characteristics that are typical of the complex systems, the system operates under far from equilibrium conditions thus requiring a constant flow of energy to maintain the organization of the system. The emerging behaviors are consequence of nonlinear interactions among many agents (not only in the immediate neighbors) of the system and, in particular, small changes in the microscopic scale interactions can cause significant changes in the macroscopic scale [3]. Among the complex adaptive systems, the living systems are of great importance and recently much attention has been paid to biological systems (immune system, tumor growth, cell evolution, see [4,5]), social and economic systems (stock market, labor, political parties, communities, terrorist networks, see [6–9]), collective systems (vehicular traffic, crowds and swarms dynamics, see [10–15]).

A complex adaptive systems is usually modeled by means of mathematical (ODE- and PDE-based models) and computational models (agent-based models, complex network-based models), see the review papers [16,17] and the references cited therein. The microscopic (individual) interactions follow the rules of the game theory [18], which appears the most suitable framework for the modeling of the interactions at the microscopic scale. In general each model operates at one of the observation scales (microscopic, mesoscopic or kinetic, macroscopic). However, considering also the multi-levels characteristics

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of the complex adaptive systems, a multiscale framework is required [19]. The multiscale approach aims at envisaging the possibility to obtain information at the macroscopic scale by means of the analysis of the interactions at the microscopic scale.

Recently a kinetic framework for particles with internal structure has been proposed in [20] for the modeling of complex adaptive systems. Specifically the system is composed by a large number of particles that are able to express a strategy (active particles) and whose microscopic state includes the mechanical variables $(x, v) \in D_x \times D_v \subset \mathbb{R}^3 \times \mathbb{R}^3$, where x is the space variable and v the velocity variable, and an internal variable $u \in D_u \subset \mathbb{R}$ (activity), which models the (social or biological) strategy expressed by the particles. The system is described by employing a statistical mechanical approach by means of the continuous distribution over the microscopic state $f(t, x, v, u) : \mathbb{R}_+ \times D_x \times D_v \times D_u \to \mathbb{R}_+$, where $\mathbb{R}_+ = [0, +\infty[$. The elementary product $f(t, x, v, u)dxdvdu$ represents the number of active particles that, at time t, are in the elementary volume of the microscopic states $d\Omega = [x, x + dx] \times [v, v + dv] \times [u, u + du]$. The evolution equation for the distribution function f is obtained by equating in $d\Omega$ the inflow and outflow of particles per unit of time due to internal and external interactions. The corresponding evolution equation for f consists of an integro-differential equation for f. Macroscopic quantities, such as local density, the linear activity-momentum, and the activity-energy can be recovered, under suitable integrability assumptions on f, as momenta of the distribution function f.

The present paper is devoted to the derivation of a new discrete thermostatted kinetic framework for the modeling of complex adaptive systems subjected to external force fields and whose evolution occurs under some constrains (density, energy, momentum conservation). The new thermostatted framework further generalizes the contents of paper [20], considering that here also the activity variable can attain discrete values thus requiring the definition of an appropriate thermostat term. Moreover the constrain is not limited to the energy conservation but it refers to a generic-order moment of f. The new thermostatted framework is proposed for the modeling of out-of-equilibrium complex living systems, e.g. crowd dynamics where the external force field represents in general an event, such as panic condition, that is not consequence of the inner dynamics of the particle (earthquake, fire). The external force field acts on the system moving it out of equilibrium. In order to ensure the existence of a nonequilibrium stationary state, a dissipative term needs to be introduced into the evolution equations to counterbalance the energy injected by the external field. In this context the *Gaussian thermostats* have been proposed as damping terms to be introduced in the equations of motion in order to keep constant the kinetic and total energy of the system [21]. The Gaussian thermostat has been proved in [22] to be equivalent to the *Gauss' principle of least constraint* [23]. The reader interested in a more deeper understanding of thermostats and their recent applications is referred to the review paper [24] and the references cited therein. It is worth stressing that Gaussian thermostats are not the only thermostats that have been proposed in the pertinent literature, see the review paper [25].

The contents of the present paper are organized into four more sections, which follow this introduction. Specifically Section 2 deals with the discrete kinetic theory of active particles proposed in [20] for the modeling of complex systems. In particular this section briefly overviews the discrete setting of the generalized kinetic theory. Section 3 is devoted to the derivation of a new discrete kinetic framework for complex systems subjected to external force fields coupled to thermostats (thermostatted systems). Section 4 is concerned with the statement of the related Cauchy problem and the proof of the existence and uniqueness of solution. Finally Section 5 concludes the paper with a critical analysis which focuses on applications to pedestrian and animal dynamics. This section, unlike the previous ones, highlights also research perspectives from the mathematical and modeling viewpoint.

2. Discrete kinetic setting of the generalized kinetic theory

The physical and life sciences systems are usually characterized by discrete mechanical and/or activity variables, e.g. opinion formation, crowd dynamics, vehicular traffic flow, and biological systems. In order to take into account the discrete characteristics of these systems, the variables composing the microscopic state of the particles is assumed discrete. Accordingly the subsets of admissible discrete values read:

$$I_x = \{x_1, x_2, ..., x_n\}, \quad I_v = \{v_1, v_2, ..., v_n\}, \quad I_u = \{u_1, u_2, ..., u_n\},$$

where I_x, I_v, I_u, denote the domain for the space, the velocity and the activity variable, respectively. If $x \in I_x$, $v \in I_v$ and $u \in I_u$, then $f_{ij}^k(t, x, v, u) = f(t, x_i, v_j, u_k)$, for $i, j, k \in \{1, 2, \dots, n\}$, denotes the discrete distribution function of the active particles located at time t in x_i with velocity v_j and activity u_k. Consequently the distribution function f of the system can be written as sum of Delta functions:

$$f(t, x, v, u) = \sum_{i=1}^{n} \sum_{j=1}^{m} \sum_{k=1}^{l} f_{ij}^k(t) \delta(x - x_i) \delta(v - v_j) \delta(u - u_k). \tag{2.1}$$

The discretization of the microscopic state variables can yield a system of partial differential equation or ordinary differential equations, see [20] for all conceivable cases. Indeed not all variables may be discrete; for instance the microscopic state of the active particles can be characterized by a discrete velocity/space variable and a continuous activity variable.

In this paper the interest focuses on complex systems whose microscopic state is homogeneous with respect to the space variable x and the velocity variable v, and the activity variable u attains discrete values. Accordingly, the distribution function