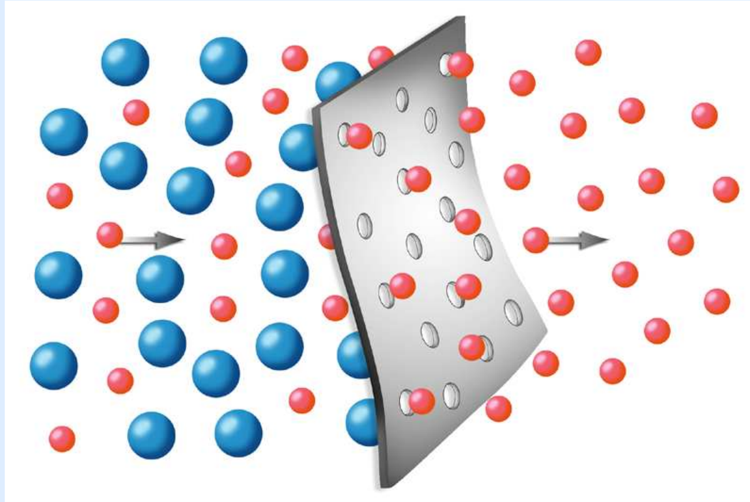

Thermostatted Kinetic Models with Applications to Biological Systems, Crowds and Swarms

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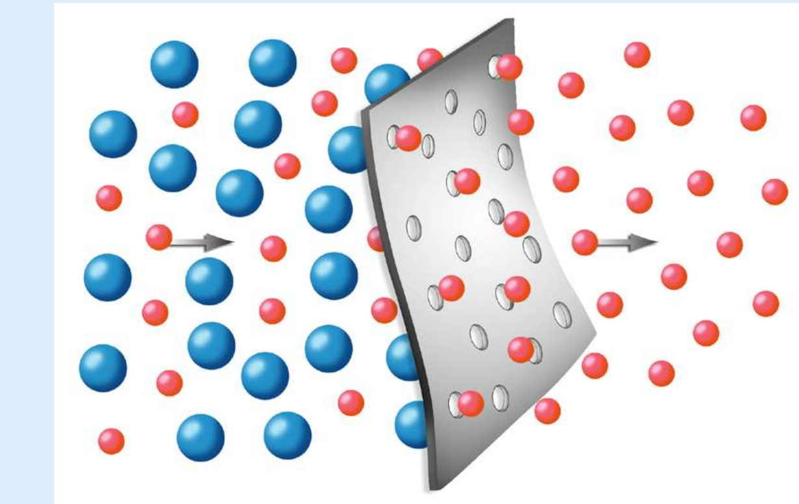

ABSTRACT

This poster is concerned with the derivation of a new discrete general framework of the kinetic theory, suitable for the modelling 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 outlines suitable applications and research perspectives.

1 Introduction

Recently the modelling 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 [15, 22, 35, 40] and [27, 30, 42].
In the context of diluted gas of particles, Gatignol has proposed in [24] 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 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 [15]. In order to take into account these capability, 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 interactions, one derives an integro-differential evolution equation for the distribution function, see the review paper [3]. 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, it is proposed a structure consisting in a system of (ordinary or partial) integro-differential equations, suitable for modelling the evolution of a discrete probability distribution in large complex systems of active particles, see [3] and the references therein.
The DKTAP framework applied to traffic flow or crowds dynamics modelling rests on the assumption that vehicles or pedestrians move with a finite number of velocities only, see [32]. The idea of discretizing the velocity variable in these systems appears worth to be 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 [16] and the analytical investigations contained in [5, 21]. Moreover the discretization of the microscopic variable appears worth 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 [3] and the reference 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 modelling 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 suitable 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 by introducing a damping term into the equations of motion [36, 39] 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*). Gaussian thermostat is based on Gauss' principle of least constrain [25], 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 [10, 12, 14, 18, 19, 20] and the recent review paper [28]. It is worth mentioning the book [31] where it is outlined also an unexpected relationship between deterministic thermostats and active Browian particles modelling biophysical cell motility, and the paper [41] where the author investigates on the analytical properties of a second order nonlinear boundary value problem that models a thermostat.
The present investigation attempts to develop a new general framework within the discrete kinetic theory approach coupled to Gaussian thermostat, we refer in brief to T-DKTAP, to be exploited toward modelling large complex systems of interest in nature and society. Specifically, we take 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 and expressed in the form of systems of partial differential equations or, in particular cases, of ordinary differential equations. The framework here proposed is certainly worth of future research activity concerning both its qualitative analysis and the application to modelling 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 [2, 43, 44] and for the thermostatted kinetic theory for active particles framework when the microscopic state is continuous, see [8, 9]. The interested reader in well-posedness results for classical KTAP models is referred to paper [11] and the references therein.

2 The Gaussian Isokinetic Thermostat

This section briefly outlines the motivation for introducing thermostats in molecular simulation for the studies of nonequilibrium complex system and in particular deals with the isokinetic thermostat, which fixes the kinetic energy of the system. The interested reader in a more specific treatment on general thermostats and applications is referred to the review paper [28] and the main references therein.
The use of computers to simulate molecular systems has grown from humble beginnings to become, in some fields, an indispensable research tool. Molecular simulation allows both qualitative and quantitative investigation of complex systems in nature and society, thanks to the technical and technological progress.
The aim of the earliest thermostats was to provide a means of simulating thermal equilibrium, rather than providing a comprehensive dynamical theory on the subject, see [45]. Thermostatting was performed with recourse to the equipartition theorem: controlling the mean kinetic energy per degree of freedom was equivalent to controlling the system temperature. In this context the following general definition for thermostats can be stated.

Definition 0.1 *Thermostats are mechanisms by which the internal energy of a many particle-system, and thus its temperature, can be tuned onto a specific value. Systems with a thermostat are called thermostatted.*

In the study of nonequilibrium statistical mechanics, if non Hamiltonian force fields are used to achieve nonequilibrium, a thermostat is needed to cool the system. 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 most elegant way of *thermostatting* a complex system composed by a large number of interacting particles and subjected to external driving is given by the famous Gauss' principle of least constraint [25]:

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 curvature defines as follows:*

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

Gauss' principle suffers some disadvantages when compared with the more commonly used extremal principles of variational mechanics (Hamilton's principle): it requires the calculation of accelerations, which are generally more complicated to evaluate numerically; and it is not independent of coordinate transformation and therefore, not as generally applicable as the Lagrangian and Hamiltonian formulations of mechanics. However, it has at least one significant advantage over these other approaches, it applies equally for non-holonomic and holonomic constraints [34]. In the case of holonomic constraints, Gauss' principle is equivalent to the principle of least action, producing Hamiltonian equations of motion. Differently, nonholonomic constraints (such as keeping constant the kinetic energy) lead to non-Hamiltonian equations of motion. The Gaussian thermostat introduced by Hoover and Evans [23] have the great interest of respecting the deterministic character of the equation of motion.
Let $\dot{\mathbf{x}} = F(\mathbf{x})$ be an evolution equation in a phase space, a Gaussian thermostat constrains the evolution to a prescribe hypersurface $\sum$ by projecting $F(\mathbf{x})$, for $\mathbf{x} \in \sum$, to the tangent plane to $\sum$ at $\mathbf{x}$. We denote the phase space of the system under consideration by $\Gamma = (\mathbf{x}, \mathbf{v})$, where $\mathbf{x}$ is the position and $\mathbf{v}$ the velocity of a particle. Consider the following equations of motion for a system constituted by interacting particles with unity mass:

$$\begin{cases} \dot{\mathbf{x}} = \mathbf{v}, \\ \dot{\mathbf{v}} = \mathbf{F}_1 + \mathbf{F} - \alpha(\Gamma)\mathbf{v}, \end{cases} \tag{1}$$

where $\mathbf{F}_1$ is a conservative force field (then there exist a scalar potential V such that $\partial_{\mathbf{x}} V = -\mathbf{F}_1$) and $\mathbf{F}$ a non gradient vector field. The term $\mathbf{F}$ maintains the system outside of the equilibrium, the term $-\alpha\mathbf{v}$ is the thermostat and makes the dynamics dissipative, allowing the system to reach a steady state in the long time limit. Without the term $\mathbf{F} - \alpha\mathbf{v}$ the dynamics would be Hamiltonian. The Gaussian isokinetic thermostat is obtained by choosing α such that the kinetic energy $\frac{\mathbf{v}^2}{2}$ of the system is constant. Accordingly we have:

$$0 = \frac{d}{dt}\left(\frac{\mathbf{v}^2}{2}\right) = \mathbf{v} \cdot (-\partial_{\mathbf{x}} V + \mathbf{F} - \alpha(\Gamma)\mathbf{v}) = -\partial_{\mathbf{x}} V \cdot \mathbf{v} + \mathbf{F} \cdot \mathbf{v} - \alpha(\Gamma)\mathbf{v}^2,$$

namely

$$\alpha(\Gamma) = \frac{\mathbf{v} \cdot (-\partial_{\mathbf{x}} V + \mathbf{F})}{\mathbf{v}^2}.$$

The force field $\mathbf{F}_1 + \mathbf{F} - \frac{\mathbf{v}\cdot(-\partial_{\mathbf{x}} V + \mathbf{F})}{\mathbf{v}^2}\mathbf{v}$ is called the *Gaussian isokinetic force*. The term α in Eq. (1) is just the Lagrange multiplier which implements Gauss' principle of least constraint.
The isoenergetic problem can be also briefly treated. This problem consists in keeping constant the energy function

$$H(t) = \frac{\mathbf{v}^2}{2} + V(\mathbf{x}).$$

The Gaussian isoenergetic thermostat associated again with the force $-\partial_{\mathbf{x}} V + \mathbf{F}$ implies that

$$0 = \dot{H}(t) = \mathbf{v} \cdot (-\partial_{\mathbf{x}} V + \mathbf{F} - \alpha(\Gamma)\mathbf{v}) + \partial_{\mathbf{x}} V \cdot \mathbf{v}.$$

Therefore

$$\alpha(\Gamma) = \frac{\mathbf{F} \cdot \mathbf{v}}{\mathbf{v}^2}.$$

It is worth stressing that the isokinetic 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, see [28, 45].

3 Partially or Totally Discrete Kinetic Setting

This section deals with a concise description of different discrete kinetic frameworks, some of them already existing in the literature. These mathematical structures consist of a system of nonlinear, with quadratic nonlinearity, autonomous ordinary or partial integro-differential equations. The presentation will be outlined at a formal and tutorial level with the aim to better understanding the introducing of the thermostatted model.
Let $\mathscr{S}$ be a complex system constituted by a large number of active particles whose microscopic state includes the space x, velocity v and activity variables v. As known, see [3], the overall distribution of the system in the mathematical kinetic theory for active particles is described by the following continuous distribution function over the microscopic state:

$$f(t,x,v,u) : [0,\infty[\times D_x \times D_v \times D_u \to \mathbb{R}^+, \tag{2}$$

where $(x,v) \in D_x \times D_v$ is the mechanical microscopic state (here including only the position and velocity variables), and $u \in D_u$ is the biological or social microscopic state. The elementary product $f(t,x,v,u)\,dx\,dv\,du$ is the number of active particles which at the time t are in the elementary volume of the microscopic states $[x,x+dx] \times [v,v+dv] \times [u,u+du]$. Macroscopic observable quantities of the system, such as mass and kinetic energy, are obtained, under suitable integrability assumptions of f, as momenta of the distribution f.
Various systems in nature and society, in general in life sciences, are characterized by the fact that the microscopic state of particles is partially or totally identified by discrete variables rather that continuous ones, e.g. vehicular traffic flow, crowds dynamics, social systems, opinion formation, cancer-immune system competition. Assuming that the discrete variables of the microscopic state can attain only finite values, we define the following subsets:

$$I_x = \{x_1, x_2, \ldots, x_n\}, \quad I_v = \{v_1, v_2, \ldots, v_m\}, \quad I_u = \{u_1, u_2, \ldots, u_l\},$$

which denote the finite sets of the admissible values for the space, velocity and activity variable respectively. If $x_i \in I_x$, $v_j \in I_v$, and $u_k \in I_u$ then

$$f_{ij}^k(t) = f(t, x_i, v_j, u_k) : [0,\infty[\to \mathbb{R}^+,$$

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 $\mathscr{S}$ is written as a sum of Dirac distributions as follows:

$$f(t,x,v,u) = \sum_{i=1}^{n}\sum_{j=1}^{m}\sum_{k=1}^{l} f_{ij}^k(t)\,\delta(x-x_i)\,\delta(v-v_j)\,\delta(u-u_k). \tag{3}$$

Moments of the discrete distribution f are obtained still according to the method of the continuous distribution function, simply replacing integration over the velocity variable by finite sums. We will write the moments casewise.
The microscopic state of particles is modified, at the time t, by *localized binary interactions*, which occur at the microscopic level and refer to the mutual actions between the test and the field individuals, when the test individual enters into the action domain of the field one. The domain is relatively small and the local density is sufficiently small so that only binary encounters are relevant. Accordingly *candidate particle* is the particle, whose microscopic state is indicated by (x_h, v_h, u_h), which wants to change its current microscopic state in that of a *test particle*, whose microscopic state is indicated by (x_i, v_i, u_i); the possibility of this change is conditioned by the presence of the other particle (*field particle*), whose microscopic state is indicated by (x_k, v_k, u_k), with which the candidate particles interacts. Moreover, we consider just *conservative interactions* which modify the microscopic state but not the number of the interacting particles.
The derivation of the different discrete mathematical frameworks in totally or partially discretization of the microscopic state is the object of the next subsections.

Remark 0.2 *In principle, if the system is composed by a number of populations greater than one, the mathematical model can even be a hybrid with continuous distribution for some populations (at least, one population only) and discrete distribution for others, leading to a system mixing ordinary differential, partial differential and integro-differential equations.*

3.1 Discrete Activity in Uniform Mechanical Variables

This subsection deals with a complex system whose microscopic state is uniform over the position and velocity variables, so that the distribution function f is independent of x and v. Moreover the activity variable can attain the finite values of the set $I_u = \{u_1, u_2, \ldots, u_n\}$. Therefore the distribution function f of the system is written as follows:

$$f(t,u) = \sum_{i=1}^{n} f_i(t,u)\,\delta(u-u_i) = \sum_{i=1}^{n} f_i(t)\,\delta(u-u_i).$$

Therefore the mathematical model consists in a set of evolution equation (differential equation) for $f_i(t)$. The modelling of microscopic interactions is based on the assumption that the following three quantities can be computed:
-*Interaction rate*. The number of encounters per unit time between candidate individuals with state u_h and field individuals with state u_k, which depends on the states of the interacting pairs, is modelled by the following function

$$\eta_{hk} = \eta(u_h, u_k) : I_u \times I_u \to \mathbb{R}^+.$$

-*Probability density.* The probability for a candidate individual with state u_h to end up into the state u_i of the test individual after an interaction with a field individual with state u_k is modelled by the following density function

$$\mathscr{A}_{hk}^i = \mathscr{A}(u_h, u_k; u_i) : I_u \times I_u \times I_u \to \mathbb{R}^+.$$

The transition density function $\mathscr{A}_{hk}^i$ has the structure of a probability density with respect to the variable u_i, then it satisfies the following condition:

$$\sum_{i=1}^{n} \mathscr{A}_{hk}^i = 1, \quad \forall h,k \in \{1,2,\ldots,n\}.$$

The evolution equation for $f_i = f_i(t)$ is obtained by considering the elementary volume $[u, u+du]$ and equating the rate of growth of subjects with microscopic state in such a volume to the inflow and outflow of subjects per unit time in the volume due to interactions. This statement can be expressed in mathematical terms by the following nonlinear ordinary differential equations:

$$\frac{df_i}{dt} = J_i[\mathbf{f}] = G_i[\mathbf{f}] - L_i[\mathbf{f}], \quad \forall i \in \{1,2,\ldots,n\}, \tag{4}$$

where $\mathbf{f} = \mathbf{f}(t) = (f_1(t), f_2(t), \ldots, f_n(t)) \in \mathbb{R}^n$ is the vector function, $G_i[\mathbf{f}] = G_i[\mathbf{f}](t)$ and $L_i[\mathbf{f}] = L_i[\mathbf{f}](t)$ represent the gain and loss terms in the nonlinear operator $J_i[\mathbf{f}] = J_i[\mathbf{f}](t)$ relative to the i-th active particle, and respectively read:

$$G_i[\mathbf{f}] = \sum_{h=1}^{n}\sum_{k=1}^{n} \eta_{hk} A_{hk}^i f_h f_k, \quad L_i[\mathbf{f}] = f_i \sum_{k=1}^{n} \eta_{ik} f_k, \qquad i \in \{1,\ldots,n\}. \tag{5}$$

The *pth*-order moment of $\mathbf{f}$ is defined as follows:

$$\mathbb{E}_p[\mathbf{f}](t) = \sum_{i=1}^{n} u_i^p f_i(t), \quad p \in \mathbb{N}. \tag{6}$$

Remark 0.3 *The global in time existence and uniqueness of the solution to the relative Cauchy problem for the model (4) is guaranteed under the assumption that the interaction rate η_{hk} is uniformly bounded and the zero-order moment of the nonnegative initial data $f_i(t,0) = f_i^0$ is equal to 1.*

Remark 0.4 *Further nonlinearity can be introduced in the framework (4) by imposing the dependence of the density function by distribution functions and moments, namely $A_{hk}^i = A_{hk}^i[\mathbf{f}, \mathbb{E}_p[\mathbf{f}]]$, see [4].*

It is worth stressing that the framework (4) has been used as paradigm for the derivation of specific models in biology and opinions formation, see the main references listed in the review paper [3].

3.2 Discrete Velocity, Continuous Space in Uniform Activity Systems

This subsection is concerned with complex system where the evolution in the space variable $x \in D_x$ cannot be neglected, so that the discrete distribution function depends also on the velocity variable that can attain the finite values of the set $I_v = \{v_1, v_2, \ldots, v_n\}$. The activity variable does not modify the dynamics. Accordingly the corresponding discrete representation is obtained by computing the distribution function $f(t,x,v)$ in $v_i \in I_v$. Corresponding to the discretized velocity we have a set of n distribution functions $f_i(t,x)$. Therefore the distribution function of the system reads:

$$f(t,x,v) = \sum_{i=1}^{n} f(t,x,v_i)\,\delta(v-v_i) = \sum_{i=1}^{n} f_i(t,x)\,\delta(v-v_i).$$

Note that time and space are left continuous, hence each function f_i, is defined over the set $[0,\infty[\times D_x$ and takes values in $\mathbb{R}^+$. Accordingly if the microscopic state of the candidate particles is (x_*, v_h), the microscopic state of the field particles is (x^*, v_k) and the microscopic state of the test particles is (x, v_i) then
-$\eta_{hk} = \eta_{hk}(x_*, x^*)$ is the interaction rate between the candidate particles (x_*, v_h) and the field particles (x^*, v_k). This rate depends on the position of the candidate and field particles.
-$\mathscr{A}_{hk}^i = \mathscr{A}_{hk}^i(x_*, v_h, x^*, v_k; x, v_i)$ is the probability density that the candidate particle with state (x_*, v_h), interacting with the field particle with state (x^*, v_k) falls into the test particle with state (x, v_i). Moreover in order to ensure conservation in the number of particles, the following condition holds true:

$$\sum_{i=1}^{n} \int_{D_x} \mathscr{A}_{hk}^i\,dx = 1, \quad \forall h,k \in \{1,2,\ldots,n\}, \forall x_*, x^* \in D_x.$$

The evolution equation in time and space of the one-particle distribution function f is obtained via a suitable balance law within any volume element of the state space. The resulting mathematical structure consists in partial integro-differential equations incorporating an advection part and a gain-loss term, written under the main assumption of binary localized interactions:

$$\begin{aligned} \frac{\partial f_i}{\partial t} + v_i \frac{\partial f_i}{\partial x} &= \sum_{h=1}^{n}\sum_{k=1}^{n} \int_{D_x \times D_x} \eta_{hk}(x_*, x^*)\mathscr{A}_{hk}^i(x_* \to x|x^*) f_h(t,x_*) f_k(t,x^*)\,dx_*\,dx^* \\ &- f_i(t,x) \sum_{k=1}^{n} \int_{D_x} \eta_{ik}(x,x^*) f_k(t,x^*)\,dx^* \end{aligned} \tag{7}$$

If the interactions do not modify the space variable, the above framework can be further specialized as follows:

$$\frac{\partial f_i}{\partial t} + v_i \frac{\partial f_i}{\partial x} = \sum_{h=1}^{n}\sum_{k=1}^{n} \eta_{hk} \mathscr{A}_{hk}^i f_h(t,x) f_k(t,x) - f_i(t,x) \sum_{k=1}^{n} \eta_{ik} f_k(t,x) \tag{8}$$

The depicted discrete-velocity framework is quite general, and can be specialized to originate particular models by acting on the specific forms of the interaction rate, the table of games $\mathscr{A}_{hk}^i$, and the grid velocity I_v, see the traffic models [3] and [16].

Remark 0.5 *In the modelling of vehicular traffic flow with framework (8), moments of f define the macroscopic observable quantities. Specifically the local density $\rho[\mathbf{f}](t,x)$ (the number of vehicles, at time t and position x, for unit length), the flux of vehicles $q[\mathbf{f}](t,x)$, and the mean velocity $\bar{v}[\mathbf{f}](t,x)$, where the dimensionless position $x \in D_x = [0,1]$, are computed as follows:*

$$\rho[\mathbf{f}](t,x) = \sum_{i=1}^{n} f_i(t,x), \quad q[\mathbf{f}](t,x) = \sum_{i=1}^{n} v_i f_i(t,x), \quad \bar{v}[\mathbf{f}](t,x) = \frac{q(t,x)}{\rho(t,x)}.$$

3.3 Discrete Velocity and Activity in Continuous Space Systems

This section is concerned with the modelling of complex systems where the velocity variable can attain discrete values of the set $I_v = \{v_1, v_2, \ldots, v_n\}$, the activity variable can attain discrete values of the set $I_u = \{u_1, u_2, \ldots, u_m\}$, and the space variable is continuous $x \in D_x$. Therefore if we denote $f_{ij}(t,x) = f(t,x,v_i,u_j)$, the distribution function f can be written as follows:

$$f(t,x,v,u) = \sum_{i=1}^{n}\sum_{j=1}^{m} f_{ij}(t,x)\,\delta(v-v_i)\,\delta(u-u_j).$$

Accordingly if the microscopic state of the candidate particles is (x_*, v_h, u_k), the microscopic state of the field particles is (x^*, v_r, u_s) and the microscopic state of the test particles is (x, v_i, u_j) then
-$\eta_{hk}^{rs} = \eta_{hk}^{rs}(x_*, x^*)$ is the interaction rate between the candidate particles (x_*, v_h, u_k) and the field particles (x^*, v_r, u_s).
-$\mathscr{A}_{hk,rs}^{ij} = \mathscr{A}_{hk,rs}^{ij}(x_*, x^*; x)$ is the probability density that the candidate particle with state (x_*, v_h, u_k), interacting with the field particle with state (x^*, v_r, u_s) falls into the test particle with state (x, v_i, u_j). Moreover

$$\sum_{i=1}^{n}\sum_{j=1}^{m} \int_{D_x} \mathscr{A}_{hk,rs}^{ij}(x_* \to x|x^*)\,dx = 1,$$

for all $h,k \in \{1,2,\ldots,n\}$, $r,s \in \{1,2,\ldots,m\}$ and $u_*, u^* \in D_u$. The mathematical framework consists in partial integro-differential equations incorporating an advection part and a gain-loss term, and thus reads:

$$\frac{\partial f_{ij}}{\partial t} + v_i \frac{\partial f_{ij}}{\partial x} = \sum_{h,r=1}^{n}\sum_{k,s=1}^{m} G[f_{hk}, f_{rs}](t,x) - \sum_{r=1}^{n}\sum_{s=1}^{m} L[f_{ij}, f_{rs}], \tag{9}$$

where

$$G[f_{hk}, f_{rs}] = \int_{D_x \times D_x} \eta_{hk}^{rs}(x_*, x^*)\mathscr{A}_{hk,rs}^{ij}(x_* \to x|x^*) f_{hk}(t,x_*) f_{rs}(t,x^*)\,dx_*\,dx^* \tag{10}$$

$$L[f_{ij}, f_{rs}] = f_{ij}(t,x) \int_{D_x} \eta_{ij}^{rs}(x,x^*) f_{rs}(t,x^*)\,dx^*. \tag{11}$$

It is worth stressing that, to the best of our knowledge, there are not mathematical models in the literature with the above framework yet. Therefore this framework has to be full explored in order to derive specific models for complex phenomena in nature and society.

Remark 0.6 *The above framework can be further specialized if we assume that the probability density $\mathscr{A}_{hk,rs}^{ij}$ is the product of the probability densities related to independent interactions of the activity and mechanical variables:*

$$\mathscr{A}_{hk,rs}^{ij} = \mathscr{B}_{h,r}^{i} \times \mathscr{C}_{k,s}^{j}.$$

Remark 0.7 *A further specialization of the above framework occurs when the distribution over the activity state (or over the mechanical state) is constant in time, while interactions over the mechanical state (or over the activity state) are also dependent on the activity state (or on the mechanical state) of the interacting pair.*

3.4 Discrete Velocity and Continuous Activity in Uniform Space Systems

This subsection deals with the modelling of complex systems uniform in space and such that the velocity variable v can attain discrete values of the set $I_v = \{v_1, v_2, \ldots, v_n\}$ and the activity variable is continuous $u \in D_u$. Accordingly the distribution function f of the system reads:

$$f(t,v,u) = \sum_{i=1}^{n} f(t,v_i,u)\,\delta(v-v_i) = \sum_{i=1}^{n} f_i(t,u)\,\delta(v-v_i).$$

If the microscopic state of the candidate particles is (v_h, u_*), the microscopic state of the field particles is (v_k, u^*) and the microscopic state of the test particles is (v_i, u) then
-$\eta_{hk} = \eta_{hk}(u_*, u^*)$ is the interaction rate between the candidate particles (v_h, u_*) and the field particles (v_k, u^*).
-$\mathscr{A}_{hk}^i = \mathscr{A}_{hk}^i(u_*, u^*; u)$ is the probability density that the candidate particle with state (v_h, u_*), interacting with a the field particle with state (v_k, u^*) falls into the test particle with state (v_i, u). Moreover

$$\sum_{i=1}^{n} \int_{D_u} \mathscr{A}_{hk}^i(u_* \to u|u^*)\,du = 1, \quad \forall h,k \in \{1,2,\ldots,n\}, \forall u_*, u^* \in D_u.$$

The mathematical framework, which consists in nonlinear partial integro-differential equations, thus reads:

$$\begin{aligned} \frac{\partial f_i}{\partial t} &= \sum_{h=1}^{n}\sum_{k=1}^{n} \int_{D_u \times D_u} \eta_{hk}(u_*, u^*)\mathscr{A}_{hk}^i(u_* \to u|u^*) f_h(t,u_*) f_k(t,u^*)\,du_*\,du^* \\ &- f_i(t,u) \sum_{k=1}^{n} \int_{D_u} \eta_{ik}(u,u^*) f_k(t,u^*)\,du^*. \end{aligned} \tag{12}$$

It is worth stressing that, to the best of our knowledge, there are not mathematical models in the literature with the above framework yet. A mathematical model for vehicular traffic has been developed considering a simplified version of this framework in [26]. Specifically the author analyzes the role of the activity variable in the vehicular traffic system, in the simplest assumption of constant probability distribution over such a variable. The distribution is only modified by interactions among vehicles and depends on local density conditions.
It is worth precising that the framework developed above recovers also the discrete activity and continuous velocity case in uniform space. Finally, further non linearities can be introduced by considering the moments dependence in the terms $\mathscr{A}_{hk}^i$ and η_{hk}.

3.5 Discrete Space, Velocity and Activity

This subsection introduces a mathematical framework for complex system characterized by a full discrete microscopic state. Accordingly to the introduction of this section, we assume that the space variable can attain discrete values of the set I_x, the velocity variable can attain discrete values of the set I_v and the activity variable can attain discrete values of the set I_u. Therefore the distribution function is written as follows:

$$f(t,x,v,u) = \sum_{i_s=1}^{n}\sum_{j_s=1}^{m}\sum_{k_s=1}^{l} f_{i_s j_s k_s}(t)\,\delta(x-x_{i_s})\,\delta(v-v_{j_s})\,\delta(u-u_{k_s}).$$

where $f_{i_s j_s k_s}(t) = f(t, x_{i_s}, v_{j_s}, u_{k_s})$. The mathematical framework refers to the evolution equation for $f_{i_s j_s k_s}(t)$. Accordingly if the microscopic state of the candidate particles is $(x_{i_1}, v_{j_1}, u_{k_1})$, the microscopic state of the field particles is $(x_{i_2}, v_{j_2}, u_{k_2})$ and the microscopic state of the test particles is $(x_{i_3}, v_{j_3}, u_{k_3})$ then
-$\eta_{i_1 j_1 k_1}^{i_2 j_2 k_2} = \eta(x_{i_1}, v_{j_1}, u_{k_1}; x_{i_2}, v_{j_2}, u_{k_2})$ is the interaction rate between the candidate particles with microscopic state $(x_{i_1}, v_{j_1}, u_{k_1})$ and the field particles $(x_{i_2}, v_{j_2}, u_{k_2})$.
-$\mathscr{A}_{i_1 j_1 k_1, i_2 j_2 k_2}^{i_3 j_3 k_3} = \mathscr{A}(x_{i_1}, v_{j_1}, u_{k_1}, x_{i_2}, v_{j_2}, u_{k_2}; x_{i_3}, v_{j_3}, u_{k_3})$ is the probability density that the candidate particle with state $(x_{i_1}, v_{j_1}, u_{k_1})$, interacting with the field particle with state $(x_{i_2}, v_{j_2}, u_{k_2})$ falls into the test particle with state $(x_{i_3}, v_{j_3}, u_{k_3})$.
Moreover

$$\sum_{i_3=1}^{n}\sum_{j_3=1}^{m}\sum_{k_3=1}^{l} \mathscr{A}_{i_1 j_1 k_1, i_2 j_2 k_2}^{i_3 j_3 k_3} = 1, \quad \forall i_1, j_1, k_1, i_2, j_2, k_2.$$

Setting $\alpha = i_1 j_1 k_1$, $\beta = i_2 j_2 k_2$, and $\gamma = i_3 j_3 k_3$, the mathematical framework in the totally discrete microscopic state consists in nonlinear ordinary differential equation and thus reads:

$$\frac{df_\gamma}{dt} + v_{j_s} \mathrm{T}_{i_s j_s k_s}(\mathbf{x}, \mathbf{f}) = \sum_{i_1, i_2=1}^{n}\sum_{j_1, j_2=1}^{m}\sum_{k_1, k_2=1}^{l} \eta_\alpha^\beta \mathscr{A}_{\alpha,\beta}^\gamma f_\alpha f_\beta - f_\gamma \sum_{i_2=1}^{n}\sum_{j_2=1}^{m}\sum_{k_2=1}^{l} \eta_\gamma^\beta f_\alpha, \tag{13}$$

where $v_{j_s}\mathrm{T}_{i_s j_s k_s}(\mathbf{x}, \mathbf{f})$ approximates the transport term. More in detail $\mathrm{T}_{i_s j_s k_s}(\mathbf{x}, \mathbf{f})$ approximates the space derivative of the distribution function for instance by using a first-order upwind points finite collocation. Further details of this framework are explained in [9].

Remark 0.8 *The above framework can be further specialized if we assume that the probability density $\mathscr{A}_{i_1 j_1 k_1, i_2 j_2 k_2}^{i_3 j_3 k_3}$ is the product of the probability densities related to independent interactions of the activity and mechanical variables:*

$$\mathscr{A}_{i_1 j_1 k_1, i_2 j_2 k_2}^{i_3 j_3 k_3} = \mathscr{B}_{i_1, i_2}^{i_3} \times \mathscr{C}_{j_1, j_2}^{j_3} \times \mathscr{D}_{k_1, k_2}^{k_3}.$$

It is worth precising that mathematical models with this framework can be derived for applications in semiconductor devices and nano-sciences.

4 Thermostatted-DKTAP Framework

The mathematical framework suitable for the modelling of a complex system composed by a population of pairwise interacting individuals in the presence of some external actions F and constrained to keep constant mass and kinetic energy can be constructed starting from the general frameworks discussed in the previous section and adding to it a term as shown below.
Specifically we show the introduction of the Gaussian thermostat for the mathematical framework (12) simply obtained by assuming a discrete velocity variable and continuous activity for a complex system that is uniform in the space variable. Accordingly, under suitable integrability assumptions on the vector function $\mathbf{f} = (f_1(t,u), f_2(t,u), \ldots, f_n(t,u)) \in \mathbb{R}^n$ we can define the (p,q)th-order moment as follows:

$$\mathbb{E}_{p,q}[\mathbf{f}](t) = \sum_{i=1}^{n} v_i^p \int_{D_u} u^q f_i(t,u)\,du, \quad \forall p,q \in \mathbb{N}. \tag{14}$$

In particular when $p = q$ we write $\mathbb{E}_p[\mathbf{f}](t)$ instead of $\mathbb{E}_{p,p}[\mathbf{f}](t)$. The physical meaning of $\mathbb{E}_{p,q}[\mathbf{f}](t)$ is related to the specific real system under consideration. The main interest is focused on the zero-order ($p = q = 0$), first-order ($p = q = 1$) and second-order ($p = q = 2$) moments, namely the *density*, *mean activation* and *activation energy*, that correspond in mechanics to mass, linear momentum and kinetic energy.
Bearing in mind the general idea of Section 2, we can thermostatted the mathematical framework (12). Accordingly, in the discrete velocity variable, continuous activity and uniform space, the thermostatted-DKTAP framework, for $i \in \{1,2,\ldots,n\}$, thus reads:

$$\partial_t f_i(t,u) + \partial_u \left(F_i(u) \left(1 - u \sum_{i=1}^{n} v_i \int_{D_u} u f_i(t,u)\,du \right) f_i(t,u) \right) = G_i[\mathbf{f}] - L_i[\mathbf{f}], \tag{15}$$

where the gain term $G_i[\mathbf{f}] = G_i[\mathbf{f}](t,u)$ and the loss term $L_i[\mathbf{f}] = L_i[\mathbf{f}](t,u)$ can be written as follows:

$$G_i[\mathbf{f}] = \sum_{h=1}^{n}\sum_{k=1}^{n} \int_{D_u \times D_u} \eta_{hk}(u_*, u^*)\mathscr{A}_{hk}^i(u_* \to u|u^*) f_h(t,u_*) f_k(t,u^*)\,du_*\,du^*, \tag{16}$$

and

$$L_i[\mathbf{f}] = f_i(t,u) \sum_{k=1}^{n} \int_{D_u} \eta_{ik}(u,u^*) f_k(t,u^*)\,du^*. \tag{17}$$

The meaning of each parameter in the above terms can be recovered by the previous Sections. It is worth stressing that the damping term induced by the thermostat adds nonlinearity in the system and complicates the analysis, see [4].
The mathematical framework (15) can be rewritten in compact way as follows:

$$\partial_t \mathbf{f}(t,u) + \partial_u \left(\mathbf{F}(u) \left(1 - u\,\mathbb{E}_1[\mathbf{f}](t) \right) \mathbf{f}(t,u) \right) = \mathbf{G}[\mathbf{f}](t,u) - \mathbf{L}[\mathbf{f}](t,u), \tag{18}$$

where

$$\mathbf{F}(u) = \begin{pmatrix} F_1(u) \\ F_2(u) \\ \vdots \\ F_n(u) \end{pmatrix} \qquad \mathbf{G}(t,u) = \begin{pmatrix} G_1[\mathbf{f}](t,u) \\ G_2[\mathbf{f}](t,u) \\ \vdots \\ G_n[\mathbf{f}](t,u) \end{pmatrix} \qquad \mathbf{L}(t,u) = \begin{pmatrix} L_1[\mathbf{f}](t,u) \\ L_2[\mathbf{f}](t,u) \\ \vdots \\ L_n[\mathbf{f}](t,u) \end{pmatrix}$$

and

$$\mathbf{f}^0(u) = \begin{pmatrix} f_1(0,u) \\ f_2(0,u) \\ \vdots \\ f_n(0,u) \end{pmatrix} = \begin{pmatrix} f_1^0(u) \\ f_2^0(u) \\ \vdots \\ f_n^0(u) \end{pmatrix}$$

being $\mathbf{f}^0(u)$ the relative initial data.
It is worth stressing that the mathematical framework (15) constitutes the paradigm for the derivation of specific models. Therefore a specific model is derived when the encounter rate η_{hk}, the probability density $\mathscr{A}_{hk}^i$ and the force field $\mathbf{F}$ are assessed.

Remark 0.9 *The introduction of the Gaussian thermostat allows to reach a non equilibrium stationary state. The relative stationary problem associated with the thermostatted-DKTAP framework (15) reads:*

$$\partial_u \left(F_i(u) \left(1 - u \sum_{i=1}^{n} v_i \int_{D_u} u f_i(u)\,du \right) f_i(u) \right) = G_i[\mathbf{f}](u) - L_i[\mathbf{f}](u). \tag{19}$$

The next section deals with the existence and uniqueness of the solution to the Cauchy problem for the mathematical framework (15). The proof takes advantage of the techniques developed in papers [1] and [44].

5 On the Cauchy Problem

This section deals with the analysis of the Cauchy problem for the thermostatted-DKTAP framework (15) modelling complex systems constituted by a large number of interacting active particles, homogeneously distributed in space, whose microscopic state is $u \in D_u \subseteq \mathbb{R}$ (activity variable) and subjected to a costant external force field $\mathbf{F} = (F, F, \ldots, F) \in \mathbb{R}^n$.

Definition 0.10 *Let $D_u = [-a,a]$ be the domain of the activity variable u, where $a > 0$. We define the function space $\mathscr{K}(D_u)$ of constant density and activation energy vector functions $\mathbf{f}$ as follows:*

$$\mathscr{K}(D_u) = \left\{ \mathbf{f}(t,u) : [0,\infty) \times D_u \to (\mathbb{R}^n)^+ \text{ such that } \mathbb{E}_0[\mathbf{f}](t) = \mathbb{E}_2[\mathbf{f}](t) = 1 \right\}. \tag{20}$$

The Cauchy problem for the thermostatted-KTAP framework (15) thus reads:

$$\begin{cases} \dfrac{\partial \mathbf{f}(t,u)}{\partial t} + \mathbf{F} \dfrac{\partial}{\partial u}\left((1 - u\,\mathbb{E}_0[\mathbf{f}](t))\,\mathbf{f}(t,u) \right) = J[\mathbf{f}, \mathbf{f}](t,u), \\ \mathbf{f}(0,u) = \mathbf{f}^0(u), \end{cases} \tag{21}$$

where $\mathbf{f}^0 \in \mathscr{K}(D_u)$. The analysis of the existence and uniqueness solution of the above Cauchy problem is done under the following assumptions for the terms in $\mathbf{J}[\mathbf{f}, \mathbf{f}](t,u)$:
- The probability density $\mathscr{A}_{hk}^i(u_* \to u|u^*) : D_u \times D_u \times D_u \to \mathbb{R}^+$ is an even nonnegative function on $D_u = [-a,a]$ satisfying the following properties:

$$\sum_{i=1}^{n} \int_{D_u} \mathscr{A}_{hk}^i(u_* \to u|u^*)\,du = 1, \quad \forall u_*, u^* \in D_u \tag{22}$$

$$\int_{D_u} u^2 \mathscr{A}_{hk}^i(u_* \to u|u_*, u^*)\,du = u_*^2, \quad \forall u^* \in D_u. \tag{23}$$

- The encounter rate $\eta_{hk}(u_*, u^*) : D_u \times D_u \to \mathbb{R}^+$ is the constant η.

Definition 0.11 *The vector function $\mathbf{f}$ is said to be a mild solution to the Cauchy problem (21) on the time interval $[0,T]$ if $\mathbf{f}(t,\cdot) \in [L^1(D_u)]^n$ and $\mathbf{f}$ is solution to the integral equation that is obtained by integration along characteristics.*

The notion of mild solutions is weaker than that of strong solutions in the sense of a C^1-function, where all terms in (21) are assumed be well defined in L^1. The main result of this paper is the following.

Theorem 0.12 *Let $\mathbf{f}^0$ be a given nonnegative function such that $\mathbb{E}_0[\mathbf{f}^0] = 1$. Then there exists a unique nonnegative $\mathbf{f} \in C((0,\infty); L^1(D_u)) \cap \mathscr{K}(D_u)$ mild solution to the Cauchy problem (21).*

Remark 0.13 *If p is odd and $\alpha = pF$, simple algebra allows to write the following ordinary differential equation for the time evolution of the moments:*

$$\frac{d}{dt}\mathbb{E}_p[\mathbf{f}](t) = \alpha\,\mathbb{E}_{p-1}[\mathbf{f}](t) - (\alpha\,\mathbb{E}_0[\mathbf{f}](t) + 1)\mathbb{E}_p[\mathbf{f}](t). \tag{24}$$

Therefore if $\mathbb{E}_p[\mathbf{f}](t)$ is initially bounded, it remains bounded for all $t > 0$.

Remark 0.14 *The operator $G_i[\mathbf{f}, \mathbf{f}]$ defined in Eq. (16) satisfies, for all regular vector functions $\mathbf{f}$ and $\mathbf{g}$, the following properties:*

$$G_i[\mathbf{f}, \mathbf{f}] - G_i[\mathbf{g}, \mathbf{g}] = G_i[\mathbf{f} - \mathbf{g}, \mathbf{f}] + G_i[\mathbf{g}, \mathbf{f} - \mathbf{g}], \tag{25}$$

$$\sum_{i=1}^{n} \int_{D_u} G_i[\mathbf{f}, \mathbf{f}](t,u)\,du = \eta\,(\mathbb{E}_0[\mathbf{f}](t))^2, \tag{26}$$

$$\int_{D_u} u\,G_i[\mathbf{f}, \mathbf{f}](t,{}^t u)\,du = 0, \tag{27}$$

$$\sum_{i=1}^{n} v_i^2 \int_{D_u} u^2\,G_i[\mathbf{f}, \mathbf{f}](t,{}^t u)\,du = \eta\,\mathbb{E}_0[\mathbf{f}](t)\,\mathbb{E}_2[\mathbf{f}](t). \tag{28}$$

The proof of Theorem 0.12 is gained by means of the following Lemmas. The first lemma shows that the first-order moment of $\mathbf{f}$ satisfies an ordinary differential equation which can be solved explicitly.

Lemma 0.15 *Let $\mathbf{f}^0$ be the nonnegative initial datum such that $\mathbb{E}_0[\mathbf{f}^0] = 1$. If there exists a nonnegative solution $\mathbf{f}$ of the Cauchy problem (21) such that*

- *$\mathbb{E}_0[\mathbf{f}](t) = \mathbb{E}_{1,0}[\mathbf{f}](t) = 1$,*
- *$f_i(t,u) = 0$ as $u \in \partial D_u$, for $t \geq 0$,*

then the first-order moment $\mathbb{E}_1[\mathbf{f}](t)$ is the following function:

$$\mathbb{E}_1[\mathbf{f}](t) = \frac{\mathbb{E}_1^+(\mathbb{E}_1^- - \mathbb{E}_1^0) - \mathbb{E}_1^-(\mathbb{E}_1^+ - \mathbb{E}_1^0)\,e^{-\frac{\sqrt{\eta^2+4F^2}}{F}t}}{(\mathbb{E}_1^- - \mathbb{E}_1^0) - (\mathbb{E}_1^+ - \mathbb{E}_1^0)\,e^{-\frac{\sqrt{\eta^2+4F^2}}{F}t}}, \tag{29}$$

where

$$\mathbb{E}_1^\pm = \frac{-\eta \pm \sqrt{\eta^2 + 4F^2}}{2F} \quad \text{and} \quad \mathbb{E}_1^0 = \mathbb{E}_1[\mathbf{f}](0) = \sum_{i=1}^{n} v_i \int_{D_u} u f_i^0\,du.$$

Definition 0.16 *Let $D_u = [-a,a]$ be the domain of the activity variable u, where $a > 0$. We define the function space $\mathscr{N}(D_u)$ as follows:*

$$\mathscr{N}(D_u) = \left\{ \mathbf{f} \in \mathscr{K}(D_u) : \mathbb{E}_1[\mathbf{f}](t) = \overline{\mathbb{E}}_1[\mathbf{f}](t) \right\}. \tag{30}$$

Lemma 0.17 *Let $\mathbf{f}^0$ be a nonnegative function such that $\mathbb{E}_0[\mathbf{f}^0](t) = 1$. Then the successive approximations sequence $\{\mathbf{f}^{(n)}(t,\cdot)\}_n$ defined as follows:*

$$\begin{cases} \mathbf{f}^{(1)}(t,u) = 0, \\ \mathbf{f}^{(n)}(t,u) = \Phi_{\mathbf{f}^0}[\mathbf{f}^{(n-1)}](t,u), \quad n > 1 \end{cases} \tag{31}$$

admits a nonnegative limit $\mathbf{f}(t,\cdot) \in [L_1(D_\mathbf{u})]^n$, as $n \to \infty$, such that $\mathbb{E}_0[\mathbf{f}](t) = 1$.

In order to prove that $\mathbf{f}$ is a mild solution of Eq. (21) it is enough to show that $\mathbb{E}_1[\mathbf{f}](t) = \overline{\mathbb{E}}_1[\mathbf{f}](t)$. Accordingly we consider the following successive approximations sequence:

$$\begin{cases} \mathbf{g}^{(1)}(t,u) = \mathbf{f}^0(u), \\ \mathbf{g}^{(n)}(t,u) = \Phi_{\mathbf{f}^0}[\mathbf{g}^{(n-1)}](t,u), \quad n > 1 \end{cases} \tag{32}$$

or the following equivalent form of (32):

$$e^{\Lambda(t)}\mathbf{g}^{(n)}(t, \varphi_t(u)) = \mathbf{f}^0(u) + \int_0^t e^{\Lambda(\tau)}\mathbf{G}[\mathbf{g}^{(n-1)}, \mathbf{g}^{(n-1)}](\tau, \varphi_\tau(u))\,d\tau. \tag{33}$$

The sequence $\{\mathbf{g}^{(n)}(t,\cdot)\}_n$ is defined in the same way as the sequence $\{\mathbf{f}^{(n)}(t,\cdot)\}_n$ except for the initial term, here replaced by $\mathbf{g}^{(1)}(t,u) = \mathbf{f}^0(u)$. This sequence is not monotonous in general. The advantage of working with $\{\mathbf{g}^{(n)}(t,\cdot)\}_n$ is that the first few moments can be computed explicitly and are independent of n, as stated in the following Lemma.

Lemma 0.18 *If the initial datum $\mathbf{f}^0 \in \mathscr{M}(D_u)$. Then*

a) $\mathbf{g}^{(n)} \in \mathscr{N}(D_u)$,

b) $\mathbf{g}^{(n)} \to \mathbf{f}$ in L^1.

6 Critical Analysis and Research Perspective

This poster contains, as its main contribution, discretization schemes for a class of models describing the evolution of the distribution function over the microscopic state of complex systems composed by a large number of active particles whose microscopic state does not include only the mechanical variables but also a scalar variable related to the intrinsic characteristics of the particles of the system. The proposed mathematical structures are designed to take into account, in addition to the interactions among the individuals of the system, also the effects of external actions that moves out of the equilibrium the system. The frameworks are originated from a generalized discrete kinetic approach and, most of them, are modifications of the structures summarized in [3]. The evolution equations for the discrete distribution functions generates a system of nonlinear ordinary or partial integro-differential equations. In order to ensure the reaching of a nonequilibrium stationary state, the action of the Gaussian isokinetic thermostat is taken into account. The coupling of the discrete kinetic theory for active particles with the mathematical thermostat generates the thermostatted framework. The global in time existence and uniqueness of the solution to the relative Cauchy problem has been examined in Section 4. According to this analysis the thermostatted equations are able to preserve during the motion the mass density and the kinetic or the activation energy of the system. Therefore the proposed mathematical framework (15) can be considered as paradigm for the derivation of specific models for complex systems in nature and society (traffic, crowds, social systems).
The mathematical thermostat can be introduced in each of the discrete frameworks considered here. Technically, the discretization of the microscopic state generates a new class of nonlinear dynamical systems with quadratic type nonlinearities which can be regarded as a useful framework to model complex systems in various fields of applied sciences, as mentioned in the overall paper. To the best of our knowledge, this is the first time that Gaussian thermostats are coupled to the discrete kinetic theory for active particles; a similar framework was proposed in [9] for the continuous KTAP framework and the well-posedness problem was studied in [8].
The mathematical frameworks proposed here can be further generalized in order to include the role of nonconservative and transitive (mutational) interactions taken into account into the mathematical frameworks presented in [11], in the KTAP models of the reference section of book [15] and in the recent kinetic models [13, 17, 29, 37, 38, 46]. When nonconservative interactions (proliferation/destruction) terms are different from zero, e.g. in the competition between the immune system and cancer cells, the dependent variable may blow up or decay to zero in finite time. So, global existence may not occur. In this case investigation may possibly lead to the discovery of bifurcations between different behaviors. Moreover some KTAP models are such that the interaction rate η and the density distribution $\mathscr{A}$ are conditioned by the distribution functions of the candidate and field particles respectively, and low-order moments: linear momentum and kinetic energy (nonlinear interactions). These considerations include further nonlinearities in the mathematical framework proposed in the present paper. However, the analysis of models which include nonlinear interactions is still an open problem. The framework (15) can be also explored for open complex systems, namely systems where external actions are introduced not only at the macroscopic state, as considered in the present paper, but also at the microscopic scale. This is a work in progress and results will be presented due course.
From the mathematical point of view, the qualitative analysis of the initial value problem for the framework proposed in this paper in unbounded domains, or with periodic boundary conditions on a torus, has to be properly developed with reference to specific models. A technical difficulty is related to the quadratic nonlinearity with localized interactions. Hence one has the same difficulty related to the discrete and continuous Boltzmann equation. Moreover the interactions with the boundary (which are mechanical in the case of the Boltzmann equation) may be affected by the activity microscopic state before the interaction with the wall. In principle, this interaction may even modify the above state. These topics are not dealt with in this paper, while it has to be regarded as an interesting research perspective.
A further goal to be pursued seems to be the recovering of the existence and uniqueness proofs of stationary states, and the presence of the activity variable, that may affect also the velocity variable, makes the problem harder and harder. Moreover, an explorative strategy can be adopted, directed to investigate which type of interactions and/or external action lead to a desired or undesired asymptotic behavior. A fundamental perspective is also the multiscale problem that has to be considered, namely the possibility of linking these frameworks to lower and upper scales by means of hydrodynamic limits with the aim to derive macroscopic equations based on the underlying description at the microscopic scale delivered by the discrete kinetic theory models of this paper. The derivation has been pursued for KTAP models with continuous microscopic state, see [6, 7, 33].
Finally, the general idea proposed here (keep constant some moments of the system), can be generalized to quantities of the system that have to be maintained constant (for instance the global wealth of the populations in the social systems). Accordingly the external force fields have to be rewritten 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.

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