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Modeling Complex Systems by Functional Subsystems Representation and Thermostatted-KTAP Methods

Carlo Bianca[1]

Dipartimento di Scienze Matematiche, Politecnico, Corso Duca Degli Abruzzi 24, 10129 Torino, ITALY

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Abstract: In the last two decades the mathematical modeling of real-world complex systems has received much attention. These systems are composed by a high number of interacting entities which are able to express a specific strategy. In order to reduce complexity, the whole system is decomposed in different subsystems that are sets of heterogeneous entities having the ability of expressing the same function. The microscopic interactions among the functional subsystems generate the emerging behaviors that are typical of the complex systems. This paper is concerned with suitable developments of the methods of mathematical kinetic theory for active particles for the modeling of complex systems splitted in functional subsystems and constrained to maintain constant some macroscopic quantities.

Keywords: Nonlinearity, distribution function, thermostats, interactions, active particles, existence, kinetic theory.

1. Introduction

The understanding and simulation of the behavior of most complex systems in life and applies sciences is a new challenge of this century. Complex systems consist of a large number of inhomogeneous agents (or particles) that interact each other in a nonlinear manner and with the outside environment. The collective behavior cannot be simply inferred from the behavior of its agents and the alteration of only one agent or one interaction reverberates on the whole system. An emergent behavior of a complex system is a property of the system as a whole which does not exist at the individual agent level [1,2].

Different tools and methods have been developed in order to model complex systems. Mathematicians, physicists and bio-informatics agree that the complexity of the system is primarily related to the high number of agents that makes unfeasible the analysis of the system at the individual level. Indeed complex systems contain from millions to a few copies of each of thousands of different elements. Therefore reducing the complexity of the system is the first step that has to be pursued. Moreover a remarkable conceptual difficulty arising from dealing with complex living system is the lack of fundamental paradigms (first principles) about equilibrium and conservation rules, see [3–5].

The mathematical methods of the kinetic theory for active particles, in brief KTAP, allow to reduce the complexity by introducing a system approach, namely all the particles expressing the same strategy are grouped in subsystems. The particles, called active particles, are able to perform strategies and have different abilities (functions) that distinguish them from the particles of the inert matter. These abilities are modeled by introducing a scalar variable, called activity, on the microscopic state of the particles. According to this theory the overall system is divided into different subsystems of particles, called functional subsystems. The evolution of a functional subsystem is depicted by a distribution function over the microscopic state of the active particles. The equation which models the evolution is derived by a conservation balance in the elementary volume of the space of the microscopic states, where the inlet and outlet flows are determined by interactions among active particles. Interactions modify both the mechanical state (generally position and velocity) and the activity; those related to mechanical variables do not necessarily obey the laws of classical mechanics, considering that these may turn out to be themselves modified by what we have called a collective behavior. Interactions at the microscopic level are modeled by stochastic games between pairs of active particles that modify their micro-

* Corresponding author: e-mail: carlo.bianca@polito.it

scopic state according to complex rules which attempt to describe some behavior of the living matter. The interested reader in a deeper understanding of this theory is referred to book [6].

The KTAP has been specifically applied for modeling the immune competition and cancer growth, the formation of keloid, traffic, crowds, genetic mutations, social systems, see the review paper [7]. However the kinetic theory for active particles does not ensure the conservation of the energy of the system (in contrast to classical kinetic theory) especially if the system is subjected to external fields at the macroscopic scale. Moreover reaching non equilibrium stationary states remain elusive. Recently these issues have been taken into account in [8–10] for complex systems composed by a functional subsystem only. The goal has been obtained modifying the classical framework of KTAP by introducing a damping term (simulating a Gaussian thermostat [11]) that removes the energy introduced by the external field during the motion (thermostatted kinetic theory for active particles, in brief TKTAP).

The present paper deals with the definition of a new mathematical framework of the kinetic theory for active particles for the modeling of complex systems constituted by different functional subsystems. Specifically, the mathematical structure refers to systems where the global activation energy must be preserved during the motion, e.g., in the formation and the shape of tumors and for finding new therapies [12], in the pedestrian movement for improving the construction of bridges [13], in the formation of school of fish and swarms of insects [14].

The rest of the paper is organized as follows. After this introduction, Section 2 reviews the functional subsystems decomposition of complex systems according to the kinetic theory for active particles. The mathematical framework for the modeling of complex systems constrained to keep constant the activation energy is proposed in Section 3. The existence and uniqueness result of the solution for the relative Cauchy problem is summarized in Section 4. Finally the paper outlines some possible future directions and applications in Section 5.

2. The Functional Subsystems Decomposition

This section is concerned with the various concepts concerning the decomposition of complex systems into functional subsystems and their representation that can be related to specific applications already available in the literature, see the review paper [7]. Note that the term functional subsystem has been used as an alternative to the term module of the so-called theory of module by Hartwell [3].

The entities that compose complex systems are called *active particles* due to their ability to express a certain strategy, called *activity*, which is heterogeneously distributed, with different intensity, among them. The different activity expressed by the particles allows to decompose the overall system into *functional subsystems*, which are a collection of active particles that have the ability to express collectively the same activity regarded as a scalar variable. Therefore the whole system is constituted by several interacting functional subsystems.

The decomposition into functional subsystems is a flexible approach to be adapted at each particular investigation. More precisely, the identification of each functional subsystem is related to the activity they express as well as to the specificity of the investigation that is developed. Namely, given the same system, different decompositions can be developed. The active particles of the same functional subsystem may, however, differ for specific characteristics. For instance in a multicellular system, cells with a different genotype may however collectively express, with other cells, the same function. Moreover, if the subsystems composing the overall system are linked by networks, the modeling approach needs treating both interactions among nodes and those that occur within the nodes. In some cases nodes of the network may identify different subsystems. Last but not least, dealing with interactions among subsystems may need, in some cases, use of different scales.

Bearing all above in mind we assume that the complex system is composed by n functional subsystems of active particles whose microscopic state includes the activity variable u belonging to a subset D_u of the real line. The description of each functional subsystem is delivered by the probability distribution function $f_i(t,u)$, where $t \in [0,T]$ with $T > 0$. The function $f_i(t,u)\,du$ represents the number of particles whose state, at time t, is in the elementary volume $[u, u+du]$ and consequently the local density number of the ith functional subsystem, with $i \in \{1,2,\ldots,n\}$, is defined as follows:

$$\mathbb{E}_0[f_i](t) = \int_{D_u} f_i(t,u)\,du.$$

Moveover, under suitable integrability assumptions on the distribution function f_i, we can define the pth-order moment of f_i as follows:

$$\mathbb{E}_p[f_i](t) = \int_{D_u} u^p\, f_i(t,u)\,du, \quad \forall p \in \mathbb{N}, \tag{1}$$

and the global pth-order moment of $\mathbf{f} = \{f_1, f_2 \ldots, f_n\}$ as follows:

$$\mathbb{E}_p[\mathbf{f}](t) = \sum_{i=1}^{n} \int_{D_u} u^p\, f_i(t,u)\,du = \int_{D_u} u^p\, \widetilde{f}(t,u)\,du, \tag{2}$$

where $\widetilde{f}(t,u) = \sum_{i=1}^{n} f_i(t,u)$.

The physical meaning of $\mathbb{E}_p[\mathbf{f}]$ depends on the specific real-world system under consideration. The main interest is focused on the zero-order ($p = 0$), first-order ($p = 1$) and second-order ($p = 2$) moments, namely the *density*, *mean activation* and *activation energy*, that correspond in mechanics to mass, linear momentum and kinetic energy.

It is worth stressing that a functional subsystem of a complex system can be itself a complex system and then

can be decomposed in subsystems. Moreover the link between a functional subsystem and its activity depends also on the specific phenomenon that aims at being analyzed. Therefore, the representation of the system by a distribution function appears consistent with the real behavior of the system under consideration.

Finally, the dynamics within each functional subsystem needs to be related to that at the lower scales. This dynamics can be contrasted or favored by the presence of external actions either from the environment or therapeutical actions in the case of cancer modeling.

3. Thermostatted-KTAP Framework

This section is concerned with the derivation of a mathematical framework of the kinetic theory for active particles for complex systems composed by n functional subsystems under the action of a macroscopic field $\mathbf{F} = \mathbf{F}(u) = (F_1(u), F_2(u), \dots, F_n(u))$, with $u \in D_u$. The overall system is constrained to maintain constant the global activation energy. Interactions among the particles rule the evolution of the system and modify the microscopic state of the particles. Specifically we distinguish three different active particles: The *candidate particles*, whose microscopic state a time t is u_*, that interact with *field particles*, with microscopic state u^* at the same time t, and acquire, with a certain probability, the state of the test particles having a microscopic state u.

Let $f_i = f_i(t,u)$ be the distribution function of the ith functional subsystem, for $i \in \{1,2,\dots,n\}$ and $t > 0$. The evolution equation for f_i is obtain by balancing in the elementary volume of the phase space the inlet and outlet flows of test particles. Setting $\mathbf{f} = \{f_1, f_2, \dots, f_n\}$, the thermostatted KTAP structure thus reads:

$$\partial_t f_i + \partial_u \left(F_i \left(1 - u \int_{D_u} u \, \widetilde{f} \, du \right) f_i \right) = J_i[\mathbf{f}], \qquad (3)$$

with $J_i[\mathbf{f}](t,u) = G_i[\mathbf{f}](t,u) - L_i[\mathbf{f}](t,u)$ where the gain term $G_i[\mathbf{f}] = G_i[\mathbf{f}](t,u)$ and the loss term $L_i[\mathbf{f}] = L_i[\mathbf{f}](t,u)$ of the test particles can be written as follow:

$$G_i[\mathbf{f}] = \sum_{j=1}^{n} \int_{D_u \times D_u} \eta_{ij}(u_*, u^*) \mathscr{A}_{ij}(u_* \to u | u^*) \qquad (4)$$

$$\times \; f_i(t,u_*) f_j(t,u^*) \, du_* \, du^*, \qquad (5)$$

and

$$L_i[\mathbf{f}] = f_i(t,u) \sum_{j=1}^{n} \int_{D_u} \eta_{ij}(u,u^*) f_j(t,u^*) \, du^*, \qquad (6)$$

where η_{ij} is the encounter rate between the candidate particle of the ith functional subsystem and the field particle of the jth functional subsystem; $\mathscr{A}_{ij}$ is the probability density that the candidate particle of the ith functional subsystem with state u_* falls into the state u after an interaction with a field particle of the jth functional subsystem. This density satisfies the following condition:

$$\int_{D_u} \mathscr{A}_{ij}(u_* \to u | u^*) \, du = 1, \quad \forall u_*, u^* \in D_u,$$

that ensures the conservation of the active particles number during the interactions.

The stationary problem associated with the thermostatted-KTAP framework (3) reads:

$$\partial_u \left(F_i(u) \left(1 - u \int_{D_u} u \, \widetilde{f}(u) \, du \right) f_i(u) \right) = J_i[\mathbf{f}](u). \qquad (7)$$

The mathematical framework (3) can be rewritten in compact way as follows:

$$\partial_t \mathbf{f} + \partial_u \left(\mathbf{F} \left(1 - u \, \mathbb{E}_1[\mathbf{f}](t) \right) \mathbf{f} \right) = \mathbf{G}[\mathbf{f}] - \mathbf{L}[\mathbf{f}], \qquad (8)$$

where

$$\mathbf{F} = \mathbf{F}(u) = \begin{pmatrix} F_1(u) \\ F_2(u) \\ \vdots \\ F_n(u) \end{pmatrix} \quad \mathbf{f} = \mathbf{f}(t,u) = \begin{pmatrix} f_1(t,u) \\ f_2(t,u) \\ \vdots \\ f_n(t,u) \end{pmatrix}$$

and

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

It is worth stressing that the mathematical framework (3) constitutes the paradigm for the derivation of specific models. Therefore a specific model is derived when the encounter rate η_{ij}, the probability density $\mathscr{A}_{ij}$ and the force field $\mathbf{F}$ are assessed.

4. On the Cauchy Problem

This section deals with the analysis of the Cauchy problem for the thermostatted-KTAP framework (3).

The analysis of the existence and uniqueness of the solution of the above Cauchy problem is pursued assuming that the probability density $\mathscr{A}_{ij}(u_* \to u | u^*) : D_u \times D_u \times D_u \to \mathbb{R}^+$ is an even nonnegative function on $D_u = [-a, a]$ satisfying the following properties:

$$\int_{D_u} \mathscr{A}_{ij}(u_* \to u | u^*) \, du = 1, \quad \forall u_*, u^* \in D_u, \qquad (9)$$

$$\int_{D_u} u^2 \, \mathscr{A}_{ij}(u_* \to u | u^*) \, du = u_*^2, \quad \forall u_*, u^* \in D_u. \qquad (10)$$

Moreover the encounter rate $\eta_{ij}(u_*, u^*)$ and the external field F_i are assumed as constants η and F respectively.

Definition 1.*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 $\mathbf{f} = \mathbf{f}(t,u) : [0,\infty) \times D_u \to (\mathbb{R}^n)^+$ as follows:*

$$\mathscr{K}(D_u) := \{\mathbf{f}(t,u) : \mathbb{E}_0[\mathbf{f}](t) = \mathbb{E}_2[\mathbf{f}](t) = 1\}. \qquad (11)$$

Let $\Xi_{\mathbf{F}}[\mathbf{f}]$ be the following operator:

$$\Xi_{\mathbf{F}}[\mathbf{f}](t,u) = \partial_t \mathbf{f}(t,u) + \mathbf{F}\,\partial_u\left((1 - u\,\mathbb{E}_0[\mathbf{f}](t))\,\mathbf{f}(t,u)\right).$$

The Cauchy problem for the thermostatted-KTAP framework (3) thus reads:

$$\begin{cases} \Xi_{\mathbf{F}}[\mathbf{f}](t,u) = J[\mathbf{f}](t,u), \\ \mathbf{f}(0,u) = \mathbf{f}^0(u), \end{cases} \qquad (12)$$

where $\mathbf{f}^0 \in \mathscr{K}(D_u)$ is the initial data.

Definition 2.*The vector function $\mathbf{f}$ is said to be a mild solution to the Cauchy problem (12) 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 (12) are assumed be well defined in L^1. The following theorem holds true.

Theorem 1.*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 (12).*

The proof of Theorem 1 follows by the following lemma.

Lemma 1([8,10]). *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 (12) such that*

–$\mathbb{E}_0[\mathbf{f}](t) = 1$,
–$\mathbf{f}(t,u) = 0$ 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:

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

where

$$\mathbb{E}_1^{\pm} = \frac{-\eta \pm \sqrt{\eta^2+4F^2}}{2F} \quad \textit{and} \quad \mathbb{E}_1^0 = \int_{D_u} u\,\widetilde{f}^0\,du.$$

*Remark.*As shown in the previous lemma, the time evolution of $\mathbb{E}_1[\mathbf{f}](t)$ depends on the magnitude of the external force F and on the interaction rate η. Further $\mathbb{E}_1[\mathbf{f}](t) \to \mathbb{E}_1^+$, as $t \to \infty$, independently of the initial data $\mathbb{E}_1^0$.

According to Lemma 1, the Cauchy problem (12) can be rewritten as follows:

$$\partial_t \mathbf{f}(t,u) + \mathbf{F}\partial_u\left((1 - u\overline{\mathbb{E}}_1[\mathbf{f}](t))\mathbf{f}(t,u)\right) = \mathbf{J}[\mathbf{f}](t,u), \quad (13)$$

with $\mathbf{f}(0,u) = \mathbf{f}^0(u)$. Therefore we have:

$$\partial_t \mathbf{f} + \mathbf{F}(1 - u\overline{\mathbb{E}}_1[\mathbf{f}](t))\partial_u \mathbf{f} + (\eta - \mathbf{F}\overline{\mathbb{E}}_1[\mathbf{f}](t))\mathbf{f} = \mathbf{G}[\mathbf{f}](t,u),$$

which is a first-order semilinear vector equation that can be solved by the method of characteristics, see [8].

5. Conclusion and Perspective

This paper dealt with further investigations on the methods of the kinetic theory for active particles for modeling and analyzing complex systems in the life and applied sciences that are decomposed in different functional subsystems. The dynamics of the system evolves according to a modified mathematical structure, called thermostatted kinetic theory for active particles, allowing the presence of external fields at the macroscopic scale. For a generic field, we obtain the existence and uniqueness proof of the solution which preserves the global activation energy. The analysis developed in the present paper is of both theoretical and practical interest.

One interesting future direction would be the extension of this mathematical framework to open systems subjected to external actions at the microscopic scale. These actions take into account the role that the outer environment has in the whole dynamics. In fact, living systems receive inputs from the environment and have the ability to learn from past experience, in order to adapt themselves to the changing-in-time external conditions [15]. Perspectives include also the introduction of stochastic terms that model jump processes both in the activity and velocity variable [16] and the role of the spatial variable. Moreover the proof of the existence of solutions to the stationary problem (7) and their convergence to steady state are missing.

It is worth stressing that the mathematical framework proposed in this paper has been obtained under the hypothesis of linearly additive interactions. In fact, the present state of the art essentially refers to linearly additive interactions either localized or distributed in space. Nevertheless in some complex systems, especially in the animal world, the individuals communicate within a fixed number of them rather that within an interaction domain. Moreover, the strategy expressed by these interactions is nonlinearly additive.

It is worth mentioning that the mathematical structure proposed in this paper allows to generalize most of the mathematical models existing in the pertinent literature, among others [17–21]. Finally the mathematical structure proposed in this paper can be coupled to mathematical billiard models contained in papers [22,23] with the aim to derive mathematical models for the movement of cells, pedestrian and insects.

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References

[1] Y. Bar-Yam, Dynamics of Complex Systems (Studies in Nonlinearity) (Westview Press, 2003).
[2] G. Nicolis and C. Nicolis, Foundations of Complex Systems: Nonlinear Dynamics, Statistical Physics, Information and Prediction (World Scientific, New Jersey, 2007).
[3] H.L. Hartwell, J.J. Hopfield, S. Leibner, A.W. Murray, Nature **402**, c47 (1999).
[4] R.M. May, Science **303**, 790 (2004).
[5] R. Reed, Notices Amer. Math. Soc. **51**, 338 (2004).
[6] C. Bianca and N. Bellomo, Towards a Mathematical Theory of Multiscale Complex Biological Systems (World Scientific, Series in Mathematical Biology and Medicine, London and Singapore, 2011).
[7] N. Bellomo, C. Bianca, and M. Delitala, Physics of Life Reviews **6**, 144 (2009).
[8] C. Bianca, Nonlinear Anal Real World Appl doi:10.1016/j.nonrwa.2012.03.005, (2012).
[9] C. Bianca, Applied Mathematical Sciences **6**, 651 (2012).
[10] C. Bianca, Int Journal of Math Analysis **6**, 813 (2012).
[11] D.J. Evans, G.P. Morriss, Statistical Mechanics of Nonequilibrium Fluids (Academic Press, New York, 1990).
[12] T. Deisboeck, M. Berens, A. Kansal, S. Torquato, Cell Prolif **34**, 115 (2001).
[13] D. Helbing, Rev Mod Phys **73**, 1067 (2001).
[14] J.K. Parrish and L.E. Keshet, Science **284**, 99 (1999).
[15] E. Mayr, Science **305**, 46 (2004).
[16] T. Hillen, H.G. Othmer, SIAM J Appl Math **61**, 751 (2000).
[17] C. Bianca, Math Models Methods Appl Sci **21**, 389 (2011).
[18] P. Degond, S. Motsch, J Stat Phys **131**, 989 (2008).
[19] J. Carillo, M. Dorsogna, V. Panferov, Kinet Relat Models **2**, 363 (2009).
[20] H. Maroufy and Z. Taib, Applied Mathematics & Information Sciences **3**, 159 (2009).
[21] Z. Zainuddin and M. M. A. Shuaib, Applied Mathematics & Information Sciences **5**, 53 (2011).
[22] C. Bianca, Nonlinear Analysis: Hybrid Systems **4**, 699 (2010).
[23] C. Bianca, Nonlinear Analysis: Hybrid Systems **5**, 32 (2011).

Carlo Bianca received the PhD degree in Mathematics for Engineering Science at Politecnico of Turin. His research interests are in the areas of applied mathematics and mathematical physics including the mathematical methods and models for complex systems, mathematical billiards, chaos, anomalous transport in microporous media and numerical methods for kinetic equations. He has published research articles in reputed international journals of mathematical and engineering sciences. He is referee and editor of mathematical journals.