Applied Mathematics & Information Sciences
An International Journal

http://dx.doi.org/10.18576/amis/110623

On the Coupling of the Thermostatted Kinetic Theory with the Information Theory

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Received: 15 Sep. 2017, Revised: 25 Oct. 2017, Accepted: 29 Oct. 2017
Published online: 1 Nov. 2017

Abstract: This paper deals with a further generalization of the continuous thermostatted kinetic theory for active particles. Specifically the interest focuses on the linking between the macroscopic data and the statistical evolution of the system. The connection between measurements and sources is established by defining an inverse problem based on the distribution vector function solution of the thermostatted kinetic framework. The inverse problem belongs to the class of ill-posed Volterra equations of the first kind considering that the number of sources can be greater of the number of measurements. The uniqueness of the solution is obtained by coupling the thermostatted kinetic theory with the information theory and more precisely with the maximum entropy principle of Jayne. Applications, which are discussed into the last section of the paper, refer to biological systems, vehicular traffic, crowds dynamics, and finance.

Keywords: Thermostats, Nonlinearity, Integro-differential Equation, Inverse problem, Shannon entropy

1 Introduction

The modeling of complex systems [1] has increased the need of defining inverse problems for determining the causes of the system evolution. Accordingly the interest in inverse problems has undergone a tremendous growth within the last two decades with special attention to the nonlinear problems. Different classes of inverse problems have been investigated, e.g. tomography [2], inverse scattering [3], inverse heat conduction problems [4], geophysical inverse problems [5]. In this context the inverse theory can be considered a well established approach [6,7]. However the mathematical formulation of inverse problems can lead to models that typically are ill-posed (the solution does not exist, the solution is not unique, the solution is unstable to perturbations).

The present paper deals with the possibility to link the macroscopic data with the mesoscopic (kinetic) description of a complex system which is modeled within the framework of the thermostatted kinetic theory for active particles. The thermostatted kinetic theory has been recently proposed in [8,9] as a general paradigm for the derivation of specific model for nonequilibrium complex systems. According to the theory, the overall system is divided into different subsystems, called functional subsystems, characterized by particles that are able to express the same function (active particles). The microscopic state of the particles consists of a scalar variable, called activity, which models the strategy of the particles. The activity can be a discrete or a continuous real variable. The time evolution of a functional subsystem depends on the interactions among the particles. The interactions yield modification in the magnitude of the active variable (conservative events) and proliferation, destruction, mutation events (nonconservative interactions). The overall description of a functional subsystem is based on the definition of a distribution function (statistical description). The existence of a nonequilibrium stationary is ensured by the introduction of a dissipative term, called thermostat because its analogy with the gaussian thermostat proposed in nonequilibrium statistical mechanics [10,11,12]. Different complex systems have been modeled within this framework, see [9,13,14]. In particular the continuous framework has been also investigated for the derivation of macroscopic equations [15].
As already mentioned, the main aim of this paper is to link a source problem with the macroscopic data. Specifically an inverse problem is proposed where the kernel depends on the distribution function vector

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solution of the continuous thermostatted kinetic framework. The inverse problem belongs to the class of Volterra integral equations of the first kind [16] which can be an ill-posed problem if the number of sources is greater than the number of measurements. In order to ensure the uniqueness of the solution the methods of the information theory are employed and specifically the Jayne principle [17]. The principle of Jayne is a new type of subjective statistic inference based on the Shannon entropy [18,19] which is a measure of the uncertainty associated to a discrete variable. According to the Jayne principle, the probability distribution that maximizes the Shannon entropy is the best candidate to represent the current state of knowledge. The principle of maximum Shannon entropy makes entropy a concept independent from thermodynamics and statistical mechanics where the Clausius entropy [20] and the Boltzmann/Gibbs entropy [21] fulfill an important role, respectively. The interested reader is addressed to the recent review papers [22,23,24, 25] and therein references for further details. It is worth stressing that the concept of entropy has been employed in different research fields, see, among others, papers [26, 27,28].

The contents of the paper are outlined as follows. After this introduction, Section 2 deals with a review of the thermostatted kinetic theory for active particles in the case of a continuous active particles. In particular the case of conservative and nonconservative interactions is taken into account. Section 3 is concerned with the linking between a set of measurements and a set of sources by defining an inverse problem which belongs to the class of Volterra integral equations of the first kind. Section 4 is devoted to the resolution of the inverse problem in the under-determined case, namely when the number of measurements is less than the number of sources, by employing the maximum Shannon entropy principle. Finally Section 5 focuses on applications and future research directions.

2 The thermostatted kinetic framework

This section is devoted to the fundamentals of the continuous thermostatted kinetic theory for active particles which constitutes the framework that will be coupled with the information theory.

Let S be an adaptive complex composed of a large number of interacting particles. The system divided into $n \in \mathbb{N}$ subsystems S_i each of them composed of interacting particles which are able to express the same strategy/function (active particles). The system is assumed homogeneous with respect to the space and velocity variables, then the microscopic state of the particles consists of a continuous scalar variable $u \in D_u \subset \mathbb{R}_+$ (called activity) that models the strategy of the particles. The time evolution of the i-th functional subsystem, for $i \in \{1,2,\dots,n\}$, is depicted by employing a distribution function $f_i = f_i(t,u) : [0,+\infty) \times D_u \to \mathbb{R}_+$.

The time evolution of the system occurs because of interactions among the particles with different magnitude of the activity variable. In this context the interaction rate between the particle of the i-th functional subsystem with activity u_* and the particle of the j-th functional subsystem with activity u^* is denoted by $\eta_{ij}(u_*,u^*) : D_u^2 \to \mathbb{R}_+$. The probability density of the particles of the i-th functional subsystem with microscopic state u_* that interacting with the particles of the j-th functional subsystem with microscopic state u^* fall into the microscopic state u is denoted by $\mathscr{A}_{ij} = \mathscr{A}_{ij}(u_*,u^*,u) : D_u^3 \to \mathbb{R}_+$. In particular, the probability density function is such that:

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

The system is assumed out of equilibrium, namely under the action of an external force field $\mathbf{F}(u) = (F_1(u),F_2(u),\dots,F_n(u)) : D_u \to \mathbb{R}_+^n$ acting on each functional subsystem.

The macroscopic variables are defined as momenta of the distribution functions. Specifically, under suitable integrability assumptions on f_i, the p-th order moment of the i-th functional subsystem is defined as follows:

$$\mathbb{E}_p[f_i](t) = \int_{D_u} u^p f_i(t,u)\,du. \tag{2}$$

In particular the local density, the linear activity-momentum, and the activity-energy are obtained for $p = 0$, $p = 1$, and $p = 2$, respectively. Let $\mathbf{f} = \mathbf{f}(t) = (f_1(t),f_2(t),\dots,f_n(t)) \in \mathbb{R}^n$ be the distribution function vector, global moments are defined according to the following relation:

$$\mathbb{E}_p[\mathbf{f}](t) = \sum_{i=1}^{n} \mathbb{E}_p[f_i](t) = \mathbb{E}_p[\widetilde{f}](t), \tag{3}$$

where

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

Bearing all above in mind, the continuous thermostatted kinetic theory for active particles framework reads:

$$\partial_t f_i(t,u) + T_{F_i}[\mathbf{f}](t,u) = J_i[\mathbf{f}](t,u) + M_i[\mathbf{f}](t,u), \tag{4}$$

where:

• The operator $J_i[\mathbf{f}] = J_i[\mathbf{f}](t,u)$ models the events that modify only the magnitude of the activity variable (conservative operator). In particular

$$J_i[\mathbf{f}](t,u) = G_i[\mathbf{f}](t,u) - L_i[\mathbf{f}](t,u),$$

where the gain particle operator $G_i[\mathbf{f}] = G_i[\mathbf{f}](t,u)$ and the loss particle operator $L_i[\mathbf{f}] = L_i[\mathbf{f}](t,u)$, respectively, reads:

$$G_i[\mathbf{f}] = \sum_{j=1}^{n} \int_{D_u^2} \eta_{ij}(u_*,u^*)\,\mathscr{A}_{ij}(u_*,u^*,u) \times f_i(t,u_*)\,f_j(t,u^*)\,du_*\,du^*, \tag{5}$$

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

• The nonconservative operator $M_i[\mathbf{f}] = M_i[\mathbf{f}](t,u)$ models the active particles that are able to change the subsystem (jumping subsystem process) and it reads:

$$M_i[\mathbf{f}] = \sum_{h=1}^{n}\sum_{k=1}^{n}\int_{D_u\times D_u} \eta_{hk}\,\varphi_{hk}^{i}\, f_h(t,u_*)\, f_k(t,u^*)\, du_*\, du^*, \tag{7}$$

where φ_{hk}^{i} is the jumping rate into the i-th subsystem, due to interactions between particles with activity u_* of the h-th subsystem and particles with activity u^* of the k-th subsystem.

• The operator $T_{F_i}[\mathbf{f}] = T_{F_i}[\mathbf{f}](t,u)$ is the dumping term that makes the dynamic dissipative thus avoiding the unbounded increase of the p-th order moment. The term T_{F_i}, called the thermostat operator [10,11,12], allows the system to reach a nonequilibrium stationary state in the long-time limit, and it reads:

$$T_{F_i}[\mathbf{f}] = \partial_u\left(\left(F_i(u) - u\int_{D_u} F_i(u)u\,\widetilde{f}(t,u)\,du\right) f_i(t,u)\right). \tag{8}$$

It is worth to mention that the thermostatted kinetic framework (4) can be considered as a general paradigm for the derivation of a mathematical model for a complex system out of equilibrium. In particular the framework (4) is called a continuous thermostatted kinetic theory framework for distinguishing it from the case where the activity variable can attain discrete values.

3 On the inverse problem

This section is devoted to the coupling of the continuous thermostatted kinetic theory framework (4) with an inverse problem. Specifically the paper focuses on the reconstruction of a time-dependent source through the knowledge of a priori data vector (measurements). The linking between the source and the measurements is conjectured by introducing an operator called kernel of the inverse problem. Accordingly let $\mathscr{S}$ be the space of the source s, $\mathscr{M}$ the measurements space (observed data), and $\mathscr{K} : \mathscr{M} \to \mathscr{S}$ the data kernel operator. Let $\mu \in \mathscr{M}$, the source problem considered in the present paper consists in constructing a solution $s \in \mathscr{S}$ of the following problem:

$$\mu(t) = \int_0^t \mathscr{K}[\mathbf{f},s](t,u)\,du, \tag{9}$$

where $\mu(t) = (\mu_1(t), \mu_2(t), \ldots, \mu_m(t)) : [0,+\infty) \to \mathbb{R}^{m,1}$ is the m-dimensional data vector, $m \in \mathbb{N}^*$, and $\mathbf{f}$ is solution of the framework (4).

The inverse problem (9) is well-posed in the Hadamard sense if for any $\mu \in \mathscr{M}$ exists and is unique the solution $s \in \mathscr{S}$ of (9), and if the solution depends continuously on the measurements (the inverse mapping $\mu \mapsto s$ is continuous). The inverse problem is said ill-posed if one of the Hadamard conditions is violated. In particular the non-uniqueness is sometimes of advantage because it allows to choose among several strategies for obtaining a desired effect.

The present paper focuses on the well-posedness of the following linear problem:

$$\mathscr{K}[\mathbf{f},s](t,u) = \mathbf{K}[\mathbf{f}](t,u)\,s(u),$$

where

$$s(u) = (s_1(u), s_2(u), \ldots, s_n(u)) : D_u \to \mathbb{R}^{n,1}$$

is the unknown n-dimensional sources vector, $n \in \mathbb{N}^*$, and

$$\mathbf{K}[\mathbf{f}](t,u) = [K_{ij}[\mathbf{f}](t,u)] : [0,+\infty) \times D_u \to \mathbb{R}^{m,n}$$

is the data kernel matrix (Green's function), which depends on the distribution functions vector solution of the continuous thermostatted framework (4). Accordingly the inverse problem reads:

$$\mu(t) = \int_0^t \mathbf{K}[\mathbf{f}](t,u)\,s(u)\,du, \tag{10}$$

which is a Volterra equation of the first kind. In particular is not restrictive to assume that:

$$\sum_{i=1}^{n}\int_{D_u} s_i(u)\,du = \int_{D_u} \widetilde{s}(u)\,du = 1, \tag{11}$$

where

$$\widetilde{s}(u) = \sum_{i=1}^{n} s_i(u).$$

Bearing all above in mind the inverse problem reads:

$$\begin{cases} \displaystyle\sum_{i=1}^{n}\int_{D_u} s_i(u)\,du = 1 \\ \displaystyle\mu_j(t) = \int_0^t \sum_{i=1}^{n} K_{ji}[\mathbf{f}](t,u)\,s_i(u)\,du, \; j \in \{1,2,\ldots,m\} \end{cases} \tag{12}$$

The main interest of this paper is the source reconstruction of the inverse problem (12) in the case $m < n$ (under-determined problem). In the latter case the non-uniqueness is not ensured. The uniqueness can be established by introducing an objective function and requiring that the solution maximize/minimize this function.

4 The coupling with the information theory

According to the information theory, the objective function that is chosen in the present paper is the following continuous Shannon entropy:

$$H[s] = -\sum_{i=1}^{n}\int_{D_u} s_i(u)\ln s_i(u)\,du. \tag{13}$$

The principle of maximum entropy of Jayne is a method that can be used to estimate input probabilities more

generally. The result is a probability distribution that is consistent with the known constraints expressed in terms of averages, or expected values, of one or more quantities, but is otherwise as unbiased as possible. Bearing all above in mind, the method consists in finding among the solutions of the inverse problem (9) that, s^H, which maximizes the function (13).
Let $\mu \in \mathscr{M}$, $s = (s_1, s_2, \dots, s_n) \in \mathscr{S}$, $\widetilde{s}(u) = \sum_{i=1}^n s_i(u)$ and $\mathscr{H}_\mu$ the following subset:

$$\mathscr{H}_\mu = \left\{ s \in \mathscr{S} : \begin{cases} \sum_{i=1}^n \int_{D_u} s_i(u)\, du = 1 \\ \mu_j(t) = \int_0^t \sum_{i=1}^n K_{ji}[\mathbf{f}](t,u)\, s_i(u)\, du \\ j \in \{1,2,\dots,m\} \end{cases} \right\}. \tag{14}$$

According to the maximum principle of Jayne, the vector solution $s^H(u) = (s_1^H(u), s_2^H(u), \dots, s_n^H(u))$ of the mathematical framework (9) thus reads:

$$s^H = \underset{s \in \mathscr{H}_\mu}{\operatorname{argmax}} H[s]. \tag{15}$$

Bearing all above in mind, the existence and uniqueness of the solution s of the inverse problem (9) depends on the optimization problem (15). Accordingly the lagrangian function $\mathscr{L}[\mathscr{K}] = \mathscr{L}[\mathscr{K}](s, \lambda_0, \lambda_1, \dots, \lambda_m)$ reads:

$$\begin{aligned} \mathscr{L}[\mathscr{K}] = &-\sum_{i=1}^n \int s_i(u) \ln s_i(u)\, du \\ &-(\lambda_0 - 1)\left(\sum_{i=1}^n \int s_i(u)\, du - 1 \right) \\ &+\sum_{j=1}^m \lambda_j \left(\mu_j' - \sum_{i=1}^n K_{ji}(t,u) s_i(u)\, du \right), \end{aligned} \tag{16}$$

where $(\lambda_0 - 1)$ and λ_j, for $j \in \{1,2,\dots,m\}$, are the related Lagrangian multipliers. Differentiating the lagrangian function $\mathscr{L}[\mathscr{K}]$ with respect to the variable s_i and setting the result equals to zero yields:

$$s_i^H(t,u) = \exp\left[-\lambda_0 - \sum_{j=1}^m \lambda_j K_{ji}(t,u) \right], \, i \in \{1,2,\dots,n\}, \tag{17}$$

and according to the constraints one has:

$$s_i^H(t,u) = \frac{\exp\left[-\sum_{j=1}^m \lambda_j K_{ji}(t,u) \right]}{\int_{D_u} \exp\left[-\sum_{j=1}^m \lambda_j K_{ji}(t,u) \right] du}, \tag{18}$$

where $i \in \{1,2,\dots,n\}$, and $\lambda = (\lambda_1, \lambda_2, \dots, \lambda_n)$ is solution of the following problem:

$$-\nabla_\lambda \ln \mathrm{Z}(\lambda, t) = \mu, \tag{19}$$

where $\mathrm{Z}(\lambda, t)$, called partition function, reads:

$$\mathrm{Z}(\lambda, t) = \int_{D_u} \exp\left[-\sum_{j=1}^m \lambda_j K_{ji}(t,u) \right] du. \tag{20}$$

According to the above solution, the maximum value of the entropy function reads:

$$H_{\max} = \lambda_0 + \sum_{j=1}^m \lambda_j \mu_j. \tag{21}$$

5 Applications and research perspectives

The present paper has been devoted to the definition of an inverse problem for the continuous thermostatted kinetic theory for active particles framework. Specifically the inverse problem consists in a source problem namely the construction of a signal that triggers the measurements. The inverse problem is analyzed in the under-determined problem case, namely when the number of unknown sources is less than the number of measurements. Accordingly the uniqueness of the solution is not ensured and the criterium for establishing the uniqueness of the solution is based on the information theory and more precisely on the continuous Shannon entropy and the maximum entropy principle of Jayne. In particular the solution is based on a probabilistic approach considering that the unknown source is assumed to be a continuous random variable vector. It is worth stressing that different algorithms can be employed for computing numerically the solution proposed in this paper, see, among others, [29,30,31]. Moreover, as already mentioned, the continuous inverse problem (12) is based on a Volterra integral equation of the first kind [32]. The reader interested to some algorithms of resolution is referred to the book [16], papers [33,34] and the references cited therein.
It is worth stressing that the meaning of the measurements and of the sources depends on the complex system under consideration. Indeed considering that the thermostatted kinetic theory has been employed for the modeling of complex biological systems [13,14,35], vehicular traffic [36], crowds dynamics [9], financial markets [37], the interpretation of the source is that of a signal that triggers the empirical data. Further applications of the thermostatted kinetic theory coupled with the information theory can be in the field of computerized tomography [38], meteorology [39,40,41], imaging [42], finance [43, 44,45].
Future research directions can be also established from the theoretical point of view. Firstly the theory that has been presented in this paper can be considered as a regularization method for linear ill-posed problems. However in the nonlinear case the inverse problem can be cast into the abstract framework of nonlinear operator equations [46]. A research perspective is the possibility to

employ a different entropy; indeed the Shannon entropy presents some limitations related to the case where the events are not independents. In this context a different concept of entropy can be involved. In particular if an *a priori* distribution function of the sources is available then the relative entropy concept can be applied [47, 48, 49, 50]. Specifically if the prior distribution is denoted by $\{q_i(u)\}$, then the information (also known as the discrete Kullback-Leibler divergence) reads:

$$KL[s,q] = \sum_{i=1}^{n} \int s_i(u) \ln\left(\frac{s_i(u)}{q_i(u)}\right) du. \qquad (22)$$

This investigation constitutes the basis of future works.

Acknowledgement

This work was partially supported by La Direction Générale de l'Armement (DGA) under the project: Conception d'un réseau de surveillance de la pollution de l'air d'un site sensible.

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