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On Entropy Dynamics for Active "Living" Particles

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Abstract: This paper presents a modeling approach, followed by entropy calculations of the dynamics of large systems of interacting active particles viewed as living—hence, complex—systems. Active particles are partitioned into functional subsystems, while their state is modeled by a discrete scalar variable, while the state of the overall system is defined by a probability distribution function over the state of the particles. The aim of this paper consists of contributing to a further development of the mathematical kinetic theory of active particles.

Keywords: living systems; entropy; statistical dynamics; active particles; kinetic theory

1. Introduction

Let us consider large systems of very many interacting living entities whose dynamics can be modeled by methods of statistical dynamics, and specifically by the so-called "kinetic theory for active particles". A vast body of literature has been developed in the past decade, focusing both on theoretical aspects and on a variety of applications in different scientific fields.

The dynamics of these systems depends on individual behaviors and on interactions of the said entities viewed as *active particles* [1], which can be subdivided into *functional subsystems*—namely, sub-populations whose active particles develop their social functions and interactions following the same rules, but with rules different with respect to those of the other sub-populations. This theory leads to models which describe the dynamics of the probability distribution function over the microscopic state of the interacting active particles. Technical developments are known; for instance, a recent paper [2] proposed a class of hybrid systems where deterministic and stochastic features can coexist, thus limiting stochastic behaviors only to some components of the system and thus reducing the overall uncertainty and the related computational effort.

The interested reader is referred to the book [3] for theoretical aspects and for the rationale to develop specific applications which have been produced to model, for instance, the dynamics of collective learning [4], the immune competition [5], vehicular traffic [6–8], the dynamics of crowds [9–11], and the collective motion of swarms [12].

Mathematical problems in unbounded domains with space homogeneity lead to the initial value problem for systems of nonlinear integro-differential equations, whose dependent variable is the aforementioned probability distribution over time, which is the only independent variable. In several applications, the qualitative analysis of the initial value problem has generated proofs of the existence of solutions for arbitrarily large time; as an example, see [5]. However, information on the shape of the solution has been achieved only by computational solutions. Therefore, a detailed analysis of the dynamics and asymptotic behavior of an appropriate entropy function can provide additional important information on the overall dynamics. In general, computations can be developed by classical deterministic methods in the case of space homogeneity, while Monte Carlo particle methods appear to be more appropriate in the case of models with space dynamics [13–15].

The concept of entropy is well defined in the case of classical particles (e.g., the celebrated Boltzmann's H-functional [16]). However, the concept of entropy is far less developed in the case of living systems which have the ability to express collective strategies and extract energy from the surrounding environment. In addition, biological systems can aggregate or fragment due to consent versus dissent dynamics [17,18], or even undergo Darwinist-type dynamics [5]. The utility of the information which can be obtained from the dynamics of entropy functional is well recognized. An overview and critical analysis of possible entropy applications are presented in [19], known applications refer, as possible examples, to biological systems [20], social and financial markets [21,22], learning dynamics [23], dispersion or aggregation in human crowds, and vehicular traffic [24].

General reasonings about entropy calculations have been developed in various papers, focusing, for instance, on biological systems [25–27] as well as social and financial markets [28,29]. Some papers show how models at the macroscopic scale can be derived from the underlying description at the microscopic scale delivered by kinetic theory models [25,30]. Hence, it is quite natural to develop calculations analogous to those of the classical kinetic theory as well as to multiscale micro-macro problems. Our paper is specifically focused on the aforementioned entropy calculations, which are here presented as a methodological approach in view of forthcoming developments followed by computational analysis.

The contents are presented as follows: Section 2 defines the mathematical description of a multi-particle system and provides the conceptual reference of the developments proposed in our paper; it is a very concise description extracted from [3] (Chapter 3). Section 3 contains the main results obtained by deriving a new class of models with discrete states of the internal variable and analyzes the related entropy dynamics; this general framework includes further developments, with respect to Section 2, to include the aforementioned Darwinist dynamics and selection. Section 4 shows in a number of case studies how the theoretical approach developed in the preceding section can be applied. These case studies are presented as possible research perspectives.

In summary, this paper introduces and reviews a formulation of ensemble or density dynamics that accommodates a discrete partition of state space. This partition allows for transitions or transformations of particles between (discrete) functional subsystems. Equipped with this formalism, it is then relatively simple to produce measures of entropy production, whose domains of application we briefly survey.

2. On the Dynamics of Active Particles

This section provides a concise presentation of a class of differential systems suitable to model the dynamics of very many interacting active particles. We specifically refer to [3] (Chapter 3) for systems where the interacting entities—viewed as *active particles*—are partitioned into *n functional subsystems* labeled by the subscript $i = 1, \ldots, n$, while the state of each subsystem is defined by the probability distribution functions $f_i = f_i(t,u)$, where $t \in [0,T]$ is the time, $u \in D$ is the activity variable defined in a real domain D, and $dn_i = f_i(t,u)\,du$ represents—under integrability conditions—the elementary number of particles in the domain $[u, u+du]$ which can be normalized with respect to the total number of particles at initial time $N_0 = N\,(t=0)$. If the number of particles in each functional subsystem is constant in time (which occurs when proliferative and/or destructive events do not occur), the f has the properties of a probability density, and in particular the integral over the domain D is equal to one.

Under suitable integrability conditions, the normalized density $n_i(t)$ in each population and for the whole system are given by:

$$n_i(t) = \int_D f_i(t,u)\,du, \quad \text{and} \quad N(t) = \sum_{i=1}^{n} \int_D f_i(t,u)\,du, \tag{1}$$

while r-moments are simply obtained by integrals weighted by u^r.

The collective dynamics is described by the following differential system:

$$\partial_t f_i(t,u) = J_i(f_i, f)(t,u) + P_i(f)(t,u) - D_i(f_i, f)(t,u), \tag{2}$$

which includes number conservative interactions as well as proliferative and destructive interactions which are modeled by the terms J_i, P_i, and D_i, respectively. Their expressions are as follows:

$$\begin{aligned} J_i = \sum_{k=1}^{n} \int_D \int_D \eta_{ik}(u_*, u^*)\, \mathcal{C}_{ik}(u_* \to u | u_*, u^*)\, f_i(t,u_*)\, f_k(t,u^*)\, du_*\, du^* \\ - f_i(t,u) \sum_{k=1}^{n} \int_D \eta_{ik}(u,u^*)\, f_k(t,u^*)\, du^*, \end{aligned} \tag{3}$$

$$P_i = \sum_{h=1}^{n} \sum_{k=1}^{n} \int_D \nu_{hk}(u_*, u^*) \mathcal{P}^i_{hk}(u_* \to u | u_*, u^*)\, f_h(t,u_*)\, f_k(t,u^*)\, du^*, \tag{4}$$

and

$$D_i = \sum_{k=1}^{n} \int_D \mu_{ik}(u,u^*)\, \mathcal{D}^i_{ik} f_i(t,u)\, f_k(t,u^*)\, du^*, \tag{5}$$

where $f = \{f_i\}$.

The various features of the modeling approach leading to this structure are:

1. The *dynamics of interactions* involves *test*, *candidate*, and *field* active particles corresponding to the i-th functional subsystems (FSs), where the state of the particles is denoted respectively by u, u_*, and u^*, while the state of the FSs is delivered by the distribution functions, respectively, $f_i = f_i(t,u)$; $f_k = f_i(t,u_*)$; and $f_k = f_k(t,u^*)$;

2. η, ν and μ model the—positive defined—*encounter rate* of the interactions corresponding, respectively, to conservative, proliferative, and destructive encounters, where the subscripts correspond to the FSs of the interacting pairs;

3. The terms $\mathcal{C}_{ik}$, $\mathcal{P}^i_{hk}$ and $\mathcal{D}^i_{ik}$ model, respectively, the *probability densities* that: A candidate i-particle, with state u_*, ends up into the state u of the same FS after the interaction with a field k-particle with state u^*; A candidate h-particle, with state u_*, proliferates into the state u of the i-FS after the interaction with a field k-particle with state u^*; A test i-particle, with state u_*, is destroyed within the same FS after the interaction with a field k-particle with state u^*.

This structure has been introduced for didactic purposes, as it forms the conceptual basis for the developments proposed in the next section.

3. Models with Discrete Internal Variables and Entropy Dynamics

Generally, models in the literature (with a few exceptions) use continuous activity variables defined over over a compact domain D. However, these models—including those cited in Section 1—refer to systems belonging to the so-called *soft sciences* [31,32]. Therefore, the actual measurement of these variables might be impossible, or at least conceptually very difficult [33].

Therefore, we suggest a modeling strategy where the domain of the variable u is normalized in a finite interval (say $u \in [0,1]$ identified by the minimal and maximal physically admissible values of u), while the activity variable attains a number m of finite values $u = \{u_1 = 0, \ldots, u_m = 1\}$, called m-states, so that the "soft" variables define possible intervals where they can be defined.

The consequence of this approach is that the overall state of the system is described for each FS by the values of the probability distribution over the discrete ij points:

$$f_{ij} = f_{ij}(t), \quad \text{such that} \quad n_i(t) = \sum_{j=1}^{m} f_{ij}(t); \quad N(t) = \sum_{1=1}^{n} n_i(t). \tag{6}$$

The dynamics of the overall system can be described by the following differential system:

$$\begin{aligned}\partial_t f_{ij} &= C_{ij}(f) + P_{ij}(f) - D_{ij}(f) \\ &= \sum_{k=1}^{n} \sum_{p,q=1}^{m} \eta_{ik}^{pq} C_{ik}^{pq}(ip \to ij) f_{ip} f_{kq} - f_{ij} \sum_{k=1}^{n} \sum_{q=1}^{m} \eta_{ik}^{jq} f_{kq} \\ &\quad + \sum_{h,k=1}^{n} \sum_{p,q=1}^{m} \nu_{hk}^{pq} P_{hp}^{pq}(hk \to ij) f_{hp} f_{kq} \\ &\quad - \sum_{k=1}^{n} \sum_{q=1}^{m} \mu_{ij}^{pq} D_{ik}^{jq}(ij) f_{ij} f_{kq},\end{aligned} \tag{7}$$

where $f = \{f_{ij}\}$, while subscripts i correspond—for the interaction pairs—to the FSs, while the superscripts j to the m-states.

The definition of various interacting terms is analogous to that of the preceding section. Namely, η, ν, and μ model the *encounter rates* of interactions corresponding, respectively, to conservative, proliferative, and destructive encounters, while $C_{ik}^{pq}(ij)$, $P_{hk}^{pq}(ij)$, and $D_{ik}^{jq}(ij)$ model the discrete probability transitions of the aforementioned dynamics which end in the FS i with m-state j. These terms are subject to the constraints:

$$\sum_{i=1}^{n} \sum_{j=1}^{m} C_{ik}^{pq}(ip \to ij) = \sum_{i=1}^{n} \sum_{j=1}^{m} P_{hk}^{pq}(hk \to ij) = \sum_{i=1}^{n} \sum_{j=1}^{m} D_{ik}^{jq}(ij) = 1, \tag{8}$$

for all inputs (ik, pq), (hk, pq), and (ik, jq), respectively.

It worth mentioning that proliferation of a candidate particle can occur in a different FS of the particle, while it is assumed that conservative interactions occur within the same functional subsystem.

A discrete Entropy function can be defined for the system (7) as follows:

$$H_i(t) = -\frac{\eta_0}{(m+1)} \sum_{j=1}^{m} \frac{f_{ij}(t)}{n_i(t)} \log \frac{f_{ij}(t)}{(m+1)\, n_i(t)}, \tag{9}$$

where η_0 is a constant, while the total Entropy is given by the sum of H_i for each i-th functional subsystem.

It is useful to derive the direct expression for the time evolution of H_i so that it can be solved jointly with Equation (7). Technical calculations yield:

$$\begin{aligned}\partial_t H_i &= -\frac{\eta_0}{(m+1)} \sum_{j=1}^{m} \frac{n_i\, \partial_t f_{ij} - f_{ij}\, \partial_t n_i}{n_i^2} \left(1 + \log \frac{f_{ij}}{(m+1)\, n_i}\right) \\ &= -\frac{\eta_0}{(m+1) n_i^2} \sum_{j=1}^{m} \left(J_{ij} \sum_{k=1}^{m} f_{ik} - f_{ij} \sum_{k=1}^{m} J_{ik}\right) \left(1 + \log \frac{f_{ij}}{(m+1)\, n_i}\right),\end{aligned} \tag{10}$$

where $f_{ij} = f_{ij}(t)$, $n_i = n_i(f)(t)$, and $J_{ij} = J_{ij}(f)(t)$.

These calculations can be specialized to specific structures, as we shall see in the next section focusing on a number of different applications corresponding to different physical features.

4. Research Perspectives

This section presents some reasonings on the application of the tools developed in Section 3 to different classes of systems in the field of soft sciences. In more detail, we consider applications to social systems, models of multicellular systems, and self-propelled particles. For the first two, we show how Equations (7) and (10) can be adapted to the specific system under consideration and the information that the analysis can provide, while the third class of problems requires additional work to be viewed as a possible research perspective. Some hints to tackle these perspective problems are brought to the attention of the reader.

Social systems: The dynamics of social systems constituted by many interacting entities can be modeled by the kinetic theory methods as shown in [28,34]. Mathematical models have been derived by assuming that the overall system is partitioned into groups of interest characterized by the economical or social strategy they share. The number of entities (active particles) within each group of interest (functional subsystem) can be supposed to be constant when the said entities do not move across functional subsystems, while when this dynamics occurs the assumption simply refers to the total number of active particles. Applications are reviewed in [28], focusing on mathematical topics, and [35] with greater emphasis on economy and social sciences (see also [36]). Here, the functions f are probability distribution functions over discrete variables u.

The reasonings presented in Section 2—which focus on soft variables—suggest modeling approaches by discrete variables. Therefore, when active particles do not move across functional subsystems, the mathematical structure underlying the derivation of specific models is as follows:

$$\begin{cases} \partial_t f_{ij} = \sum_{k=1}^{n} \sum_{p,q=1}^{m} \eta_{ik}^{pq} C_{ik}^{pq}(ip \to ij) f_{ip} f_{kq} - f_{ij} \sum_{k=1}^{n} \sum_{q=1}^{m} \eta_{ik}^{jq} f_{kq}, \\ \partial_t H_i = -\frac{\eta_0}{(m+1)n_i} \sum_{j=1}^{m} J_{ij} \left(1 + \log \frac{f_{ij}}{(m+1)\, n_i}\right), \end{cases} \tag{11}$$

while this structure (11) can be technically modified to account for a dynamics which describes crossing functional subsystems.

The literature on social systems often looks for possible equilibria. The mathematical theory of active particles leads to possible equilibrium configurations defined by the shape of the probability distribution f_{ij} over the activity variable. The dynamics of the entropy follows that of the distributions f_{ij} and describes the specific features of the trend to equilibrium when it exists. Particularly important is analysis of *segregation phenomena* which might be described by Entropy functions [37]. The study of segregation phenomena is also very important in the study of collective learning dynamics [4,38], as it can denote the onset of clusters of extreme levels of education, namely very high and very low levels.

In addition, economical systems might be characterized by turbulence whenever, for instance, political conflicts have an influence on economy markets [39,40]. Therefore, fluctuations and oscillating behaviors of the entropy functions can provide an important measure of the economy of nations.

Multicellular systems: The modeling of multicellular systems requires substantial developments with respect to the mathematical structure used for social systems (Equation 11). According to [26], the competition between immune and tumor cells should include proliferative and destructive events which are typical of the competition. Proliferation might even generate Darwinist-type mutations and subsequently selection. The dynamics includes both an initial transient behavior, where the dynamics include variations of the activity variable of the interacting functional subsystems—namely the progression of cells which are carriers of a pathogen and the immune system which has the ability to deplete these cells.

Subsequently, proliferative/destructive events can become dominant. Focusing on this specific dynamics, the mathematical structure is as follows:

$$\begin{cases} \partial_t f_{ij} = \displaystyle\sum_{h,k=1}^{n} \sum_{p,q=1}^{m} \eta_{hk}^{pq} P_{hk}^{pq}(hk \to ij) f_{hp} f_{kq} \\ \qquad\qquad - \displaystyle\sum_{k=1}^{n} \sum_{q=1}^{m} \mu_{hk}^{pq} D_{ik}^{jq}(ij) f_{ij} f_{kq}, \\ \partial_t H_i = -\dfrac{\eta_0}{(m+1)n_i^2} \displaystyle\sum_{j=1}^{m} \left(J_{ij} \sum_{k=1}^{m} f_{ik} - f_{ij} \sum_{k=1}^{m} J_{ik} \right) \\ \qquad\qquad \times \left(1 + \log \dfrac{f_{ij}}{(m+1)\, n_i} \right), \end{cases} \tag{12}$$

Similarly to the case of social systems, the dynamics of entropy can provide important information on the biological properties of the systems under consideration [41]. In addition, it can contribute to the assessment of chaotic behaviors which may be related to the onset of pathological states [5]. In some cases, these are enhanced by segregation phenomena already mentioned in the preceding paragraph.

Self-propelled particles: The dynamics of self-propelled particles can be referred to a vast body of literature generated by the celebrated book by Prigogine and Hermann [42] on vehicular traffic, by the Cucker and Smale paper [43] on swarm dynamics, up to recent developments [44], by the kinetic theory approach to crowd dynamics [10], and the dynamics of multicellular systems [27,45]. Without citing a huge amount of literature, we limit our bibliographic indications simply by stressing the interest on this topic witnessed in a recent special issue [46] and in the edited book [1].

The study of the entropy dynamics for the aforementioned classes of equations cannot be treated as a straightforward generalization of the mathematical tools proposed in Section 3. In fact, the presence of a space variable requires that the space inhomogeneity be accounted for so that both dependent variables of the dynamical system and Entropy function depend on space as well. Two possible approaches have been developed. The first one starts with a detailed modeling of the interactions involving not only social-biological states at the microscopic scale, but also localization of the interacting active particles; applications refer to crowd dynamics [9], vehicular traffic [5,6], and multicellular systems [27]. The second approach is based on the conjecture that space dynamics is induced by a velocity jump perturbation of the spatially homogeneous activity dynamics; see for example [25,30]. The latter has been introduced by the pioneer paper [47], where the aforementioned perturbation of the transport equation is used to derive diffusion models (parabolic) and models with finite speed of propagation (hyperbolic) [48]. The use of entropy estimate is important not only toward an assessment of the physical properties of the solution, but also toward the interpretation of empirical data [49] for systems, where the available data are often not complete [50].

It is worth mentioning that the aforementioned micro-macro derivation generates challenging analytic problems related to the qualitative analysis of the solutions to mathematical problems at different scales—say at the level of kinetic equations [51] or at that of tissues [52]. Hence, one also has to look for a multiscale validity of the entropy function by looking at it as a tool that can contribute to the qualitative analysis of mathematical problems [53]. Segregation phenomena in swarms and crowds means subdivision into different groups sharing a certain behavior (e.g., multilane fingering in crowd dynamics as studied in [11]). It can be a local phenomenon, and hence it might require the definition of a local Entropy function.

As mentioned, investigations on the dynamics of Entropy functions have not been exhaustively treated for the class of dynamical systems with space structure, while various motivations—including those proposed in this paragraph—suggest that this challenging topic be tackled. A possible further development suggested by one of the referees which definitely deserves attention would consist of comparing the expression of the entropy function proposed in our paper with various ones known in the literature—as an example, the celebrated Shannon entropy. A similar idea is also proposed in the open source paper by the Abel prize laureate Michail Gromov [54]. He refers, with examples, the choice of the entropy to the mathematical structure. Here, the first step is the derivation of a mathematical structure consistent with the complexity features of living systems. A recently published book has been devoted to this topic [3], while a specific structure has been presented in our paper. Actually, we do believe that a further step would be particularizing the selection of the entropy to each specific structure corresponding to different classes of systems. Indeed, living systems show common features, but need to be particularized by specific differences. Hence, the most appropriate expression should be referred to each class of systems. Indeed, this challenging perspective is in a research program we feel engaged to.

A general research topic which definitely worth investigation consists of the study of systems where nonlinear interactions occur—namely, the output of interaction depends not only on the microscopic state of the interacting entities, but also on the probability distribution function of the active particles involved in the game. This additional nonlinearity appears in various models, including the literature presented in our paper. This additional nonlinearity modifies the dynamics and hence also the behavior of the entropy. A detailed analysis of this matter should be specialized for each model, and it is definitely worth further research activity already scheduled in our research plan.

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