Probabilistic Engineering Mechanics 26 (2011) 54–60

Contents lists available at ScienceDirect

Probabilistic Engineering Mechanics

journal homepage: www.elsevier.com/locate/probengmech

Microscopic, mesoscopic and macroscopic descriptions of complex systems

Mirosław Lachowicz *

Institute of Applied Mathematics and Mechanics, Faculty of Mathematics, Informatics and Mechanics, University of Warsaw, ul. Banacha, 2, 02097 Warsaw, Poland

ARTICLE INFO

Article history:
Received 12 December 2009
Received in revised form
13 April 2010
Accepted 21 June 2010
Available online 30 June 2010

Dedicated to Professor Kazimierz Sobczyk on his 70th birthday

Keywords:
Markov jump processes
Microscopic models
Integro-differential equations
Verhulst equation
DNA denaturation
Lotka–Volterra equation

ABSTRACT

In the present paper the general approach that relates microscopic models with those at the mesoscopic scale and then the macroscopic scale is reviewed. The models at the micro-scale level are defined by a large number of interacting entities (particles, agents, cells, individuals, etc), and is in terms of a Markov jump process and related linear evolution equations. The intermediate models refer to the meso-scale level of description of test entities and are given in terms of bilinear Boltzmann-type equations. Mathematical relationships between these three possible descriptions are presented and explicit error estimates are given. The general framework is applied to propose the microscopic and mesoscopic models that correspond to very well known models in biomathematics: the Verhulst logistic equation and the Lotka–Volterra system of equations. The asymptotic time behaviour for the mesoscopic model corresponding to the Verhulst logistic equation is defined. The mesoscopic model corresponding to the Verhulst equation is modified to a new mesoscopic model of DNA denaturation.

1. Introduction

There are various examples of methods of mechanics, including statistical mechanics, that are successfully applied to complex systems in biological and medical sciences—see e.g. Refs. [1–11] and references therein.

The description of biological populations is usually carried out on the macroscopic level of interacting subpopulations within the system. Such an approach is usually related to deterministic systems of ordinary differential equations or systems of reaction–diffusion equations. They describe the (deterministic) evolution of densities of subpopulations of the system rather than the individual entities. However, in many cases the description on a micro-scale (or meso-scale) of interacting entities (e.g. particles, cells, individuals, agents, factors, persons, etc) seems to be more appropriate, see [3,4,6,7] and references therein.

It is very well known that such a process as evaporation cannot be successfully described by using only macroscopic equations: the Navier–Stokes system (for water) – cf. [12] – and the Euler system (for vapor) with the proper matching. There is a thin layer, known as the Knudsen layer, between liquid and vapour, and the description should have a multi-scale character taking into consideration the microscopic phenomena in the framework of kinetic theory.

The situation is even more evident for biological phenomena. For example, in the case of tumour cells in competition with the immune system, the following steps of the evolution:

- Loss of differentiation and replication; Reproducing of the cells; Interaction (activation or inhibition) and competition at the cellular level with immune and environmental cells e.g. through the emission of cytokine signals;

are related to cellular and subcellular interactions between tumour cells, and agents of the immune system. The subcellular scale refers to processes that take place within the cells or at the cell membrane, e.g. synthesis of DNA and the activities of chemical signals between cells. The cellular scale refers to various types of interaction between cells, e.g. interactions between tumour cells and immune system cells. Therefore, those scales may be connected with a microscopic level of description, i.e. the level of interacting individual entities of the system or, with some suitable reduction of the description, to the mesocopic scale of test entities.

As a prototype of the mathematical setting and relationships between three possible scales of description – micro, meso and macro – can be the kinetic theory of rarefied gases, see e.g. [13,2] and references therein. There is however an important difference: in the case of biological systems a basic microscopic theory, like Newton's laws in the kinetic theory case, is not available. Therefore it is reasonable to apply the following strategy. One may start with

* Fax: +48 022 55444300.
E-mail address: lachowic@mimuw.edu.pl.

0266-8920/$ – see front matter © 2010 Elsevier Ltd. All rights reserved.
doi:10.1016/j.probengmech.2010.06.007

the deterministic macroscopic model for which the identification of parameters by an experiment is easier. Then one provides the theoretical framework for modelling at the microscopic scale in such a way that the corresponding models at the macro- and micro-scales are asymptotically equivalent, i.e. the solutions are close each to other in a properly chosen norm. Then, if the parameters of the microscopic model are suitably chosen, one may hope that it covers not only macroscopic behaviour of the system in question, but also some of its microscopic features. The microscopic model by its nature can be richer and can describe a larger variety of phenomena.

The present paper reviews a general framework for the program [14,15,6] of finding possible transitions between the different levels of description i.e.

(Mi) —at the level of interacting entities ("*micro-scale*"), in mathematical terms of jump Markov processes, that lead to continuous (linear) stochastic semigroups;
(Me) —at the level of the statistical description of a test entity ("*meso-scale*"), in terms of continuous nonlinear semigroups related to the solutions of bilinear Boltzmann-type;
(Ma) —at the level of densities of subpopulations ("*macro-scale*"), in terms of dynamical systems related to bilinear systems of ODEs or reaction–diffusion(–chemotaxis) equations

and we discusses some important examples.

Refs. [14,15,6] provide such a conceptual framework for various situations of biological interest. In particular, Ref. [14] deals with the mathematical theory for a large class of ODEs of Lotka–Volterra-type and reaction–diffusion systems (with small diffusion). Ref. [15] shows that the theory can be generalized to take into account reaction–diffusion–chemotaxis systems (i.e. reaction–diffusion equations with a chemotaxis-type term) in the context of tumour invasion. These methods may lead to new and more accurate modelling of complex processes.

There is a huge literature related to the rigorous derivation of macroscopic equations from microscopic models. The interested reader is referred e.g. to Refs. [16,6,17,9,18] and references therein.

The plan of the paper is as follows. Section 2 reviews the general framework leading to the description on the microscopic level. The Markov jump processes of N interacting entities and the corresponding linear evolution equations for densities are defined. Section 3 deals with the mesoscopic model obtained "in the limit $N \to \infty$". In Section 4 we consider a simple but illuminating example of the Verhulst logistic equation at the macroscopic level and the corresponding microscopic and mesoscopic equations. The asymptotic time behaviour of the solution to the mesoscopic model is proved. In Section 5 a new preliminary mesoscopic model of DNA denaturation is proposed. The model is based on the mesoscopic model in Section 4. In Section 6 the microscopic and mesoscopic models related to the classical Lotka–Volterra system of equations are defined. The paper concludes in Section 7 with concluding remarks.

2. Microscopic model: the general framework

In this section we present the general framework [14,15,6] that allows us to construct the microscopic model that corresponds to the large class of macroscopic models. The microscopic model is constructed in terms of a Markov jump process. We introduce the linear generator that completely describes the evolution of the density probability at the microscopic scale that may approximate the solution of the corresponding macroscopic model.

In what follows, a (large) number N of entities of various subpopulations is considered. Every entity n ($n \in \{1, \ldots, N\}$) is characterized by

$$\mathbf{u}_n = (j_n, u_n) \in \mathbf{U} = \mathcal{J} \times \mathcal{U} \tag{1}$$

where $j_n \in \mathcal{J} \subset \{1, 2, 3, \ldots\}$ is its subpopulation, $u_n \in \mathcal{U}$—its (inner, microscopic) state (its *activity*, *energy*, *dominance*, *fitness*, *position*, *velocity*, etc).

The n-entity interacts with the m-entity, and the interaction takes place at random times. After the interaction both entities may change their populations and/or their states.

The rate of interaction between the entity of the j-th population with state u and the entity of the k-th population with state v is given by the measurable function $a = a(\mathbf{u}, \mathbf{v})$ such that

$$0 \le a(\mathbf{u}, \mathbf{v}) \le a_+ < \infty, \quad \forall \mathbf{u}, \mathbf{v} \in \mathbf{U}, \tag{2}$$

where a_+ is a constant and "$\forall$" is understood "*for all*" with respect to discrete variables and "*for almost all*" with respect to continuous variables.

The transition into the j-th population with state u of an entity of the k-th population with state v, due to the interaction with an entity of the l-th population with state w, is described by the measurable function

$$A = A(\mathbf{u}; \mathbf{v}, \mathbf{w}) \ge 0, \quad \forall \mathbf{u}, \mathbf{v}, \mathbf{w} \in \mathbf{U}, \tag{3}$$

A is the transition probability and therefore

$$\sum_{j \in \mathcal{J}} \int_{\mathcal{U}} A\left((j, u); \mathbf{v}, \mathbf{w}\right)\, \mathrm{d}u = 1, \tag{4}$$

for all $\mathbf{v}, \mathbf{w} \in \mathbf{U}$, such that $a(\mathbf{v}, \mathbf{w}) > 0$.

The stochastic model (at the microscopic level) will be completely determined by the choice of functions a and A. Different choices of a and A give rise to different microscopic models (Markov jump processes)— [14,15,6].

Given N, a and A, we assume that the stochastic system is defined by the Markov jump process of N entities through the following generator Λ_N

$$\begin{aligned}
&\Lambda_N \phi(\mathbf{u}_1, \ldots, \mathbf{u}_N) \\
&\quad = (N-1) a_+ \int_{\mathbf{U}^N} \left(\phi(\mathbf{v}_1, \ldots, \mathbf{v}_N) - \phi(\mathbf{u}_1, \ldots, \mathbf{u}_N)\right) \\
&\qquad \times \nu\left(\mathrm{d}\mathbf{v}_1, \ldots, \mathrm{d}\mathbf{v}_N; \mathbf{u}_1, \ldots, \mathbf{u}_N\right),
\end{aligned} \tag{5}$$

with the transition function ν defined by

$$\begin{aligned}
&\nu\left(\mathrm{d}\mathbf{v}_1, \ldots, \mathrm{d}\mathbf{v}_N; \mathbf{u}_1, \ldots, \mathbf{u}_N\right) \\
&\quad = \left(1 - \sum_{\substack{1 \le n, m \le N \\ n \ne m}} \frac{a(\mathbf{u}_n, \mathbf{u}_m)}{N(N-1)a_+}\right) \delta_{\mathbf{u}_1}(\mathrm{d}\mathbf{v}_1) \cdots \delta_{\mathbf{u}_N}(\mathrm{d}\mathbf{v}_N) \\
&\qquad + \sum_{\substack{1 \le n, m \le N \\ n \ne m}} \frac{a(\mathbf{u}_n, \mathbf{u}_m)}{N(N-1)a_+} A(\mathrm{d}\mathbf{v}_n; \mathbf{u}_n, \mathbf{u}_m) \\
&\qquad \times \delta_{\mathbf{u}_1}(\mathrm{d}\mathbf{v}_1) \cdots \delta_{\mathbf{u}_{n-1}}(\mathrm{d}\mathbf{v}_{n-1}) \delta_{\mathbf{u}_{n+1}}(\mathrm{d}\mathbf{v}_{n+1}) \cdots \delta_{\mathbf{u}_N}(\mathrm{d}\mathbf{v}_N),
\end{aligned} \tag{6}$$

where ϕ is a test function (a real-valued, Borel measurable bounded function). We have adopted the convention that for $\mathbf{u} = (j, u)$, $\mathbf{v} = (k, v)$,

$$\delta_{\mathbf{u}}(\mathrm{d}\mathbf{v}) = \delta_{j,k} \delta_u(\mathrm{d}v), \tag{7}$$

and

$$\int_{\mathbf{G}} A(\mathrm{d}\mathbf{u}; \mathbf{v}, \mathbf{w}) = \sum_{j \in \mathcal{J}_1} \int_{\mathcal{U}_1} A\left((j, u); \mathbf{v}, \mathbf{w}\right)\, \mathrm{d}u, \tag{8}$$

for $\mathbf{G} = \mathcal{J}_1 \times \mathcal{U}_1$, where $\mathcal{J}_1 \subset \mathcal{J}$, and $\mathcal{U}_1$ is a measurable set in $\mathbf{U}$, δ_u is the atom measure concentrated in u and $\delta_{j,k}$ is the Kronecker delta.

Λ_N is the generator for a Markov jump process in $\mathbf{U}^N$ that can be constructed as in Ref. [19], Section 4.2.