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From microscopic to macroscopic descriptions of complex systems

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Abstract

Complex systems that can be described at the macroscopic level in terms of bilinear ODEs or bilinear reaction–diffusion equations are considered. The corresponding microscopic description at the level of stochastically interacting entities is defined. The mathematical relationships between these two descriptions are formulated. The solutions of bilinear macroscopic equations are approximated by stochastic (linear) semigroups and the order of approximation is given. ***To cite this article: M. Lachowicz, C. R. Mecanique 331 (2003).***

Résumé

De la description microscopique à la description macroscopique des systèmes complexes. Nous considérons ici des systèmes complexes descrits au niveau macroscopique par des EDOs bilinéaires ou par des équations de réaction–diffusion bilinéaires. La description microscopique correspondante est définie. Les relations mathématiques entre les deux descriptions sont formulées. Les solutions des équations macroscopiques bilinéaires sont approximées par des semigroupes stochastiques (linéaires) et l'ordre d'approximation est donné. ***Pour citer cet article : M. Lachowicz, C. R. Mecanique 331 (2003).***

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Mots-clés : Millieux continus ; Systèmes complexes ; EDO ; Équations de réaction-diffusion ; Semigroupes stochastiques

1. Macroscopic description

In the present paper complex systems that at the macroscopic level admit description by either a system of bilinear ODEs or a system of bilinear reaction–diffusion equations are considered. The present approach however is more general, in fact one may consider at the macroscopic level more complicated systems than bilinear by using small perturbation methods (cf. [1]).

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In the present paper we state the link between two possible descriptions: at microscopic level of stochastically interacting entities (particles, cells, individuals, ...) in terms of continuous linear semigroups of Markov operators (continuous stochastic semigroups); at macroscopic level of densities of interacting entities (in terms of dynamical systems related to bilinear equations either spatially homogeneous or inhomogeneous with weak diffusion).

We consider the following system of equations

$$\dot{\rho}_j = \sum_{k=1}^{r} \alpha_{j,k}\rho_k + \rho_j \sum_{k=1}^{r} \beta_{j,k}\rho_k, \quad j = 1, 2, \ldots, r \tag{1}$$

where $\alpha_{j,k}$, $\beta_{j,k}$ are real constants (they can be positive, negative or zero), $\alpha_{j,k}$ ($j \neq k$) are non-negative constants; $\rho_j = \rho_j(t)$; $t \geqslant 0$ is the time variable, $\dot{\rho}_j = \frac{\mathrm{d}}{\mathrm{d}t}\rho_j$.

Eq. (1) such that $\alpha_{j,k} = 0$, $\beta_{j,k}\beta_{k,j} < 0$ (for all $j \neq k$) and $\beta_{j,j} = 0$ ($\forall j = 1, \ldots, r$) is called the Lotka–Volterra system whereas such that $\alpha_{j,k} = 0$, $\beta_{j,k}\beta_{k,j} < 0$ (for all $j \neq k$) and $\beta_{j,j} < 0$ ($\forall j = 1, \ldots, r$) is called the Verhulst–Volterra system. Eq. (1) such that $\alpha_{j,k} = 0$ (for all $j \neq k$), $\beta_{j,k} \leqslant 0$ ($\forall j, k = 1, \ldots, r$) and for any $j = 1, \ldots, r$ there is $k = 1, \ldots, r$ such that $\beta_{j,k} < 0$ is called the competitive system. The parameters $\alpha_{j,j}$ are intrinsic growth or decay rates of the j-subpopulation, and $\beta_{j,k}$ are the interaction rates (positive, negative or zero) between the j-th and k-th subpopulations.

Next we consider the following (spatially inhomogeneous) system with diffusion

$$\partial_t \varrho_j - \sigma_j \Delta \varrho_j = \sum_{k=1}^{r} \alpha_{j,k}\varrho_k + \varrho_j \sum_{k=1}^{r} \beta_{j,k}\varrho_k, \quad j = 1, 2, \ldots, r \tag{2}$$

where $\alpha_{j,j}$, $\beta_{j,k}$ are real constants; $\alpha_{j,k}$ ($j \neq k$), σ_j ($j \in \{1, 2, \ldots, r\}$) are non-negative constants; $\varrho_j = \varrho_j(t, x)$; $t \geqslant 0$ is the time variable and $x \in \mathbb{T}^d$ is the space variable, $\mathbb{T}^d$ is the d-dimensional torus, $d \geqslant 1$; $\Delta = \sum_{i=1}^{d} \partial_{x_i}^2$.

2. Microscopic description

Following [2] a (large) number N of entities of several $r + 2$ populations is considered. Every entity n ($n \in \{1, \ldots, N\}$) is characterized by $\mathbf{u}_n = (j_n, u_n, x_n) \in \Omega$, where $j_n \in \mathcal{J} = \{0, 1, \ldots, r + 1\}$ is its population, $u_n \in [0, R]$ – its (inner) state (its "*activity*"), $R > 0$, and $x_n \in \mathbb{T}^d$ – its position (center of mass), $\Omega = \mathcal{J} \times [0, R] \times \mathbb{T}^d$. The populations labeled by 0 and $r + 1$ play an auxiliary rôle. The n-entity interacts with the m-entity and the interaction take 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 at point x and the entity of the k-th population with state v at point y is given by the (measurable) function $a = a((j, u, x), (k, v, y))$; $a : \Omega^2 \to \mathbb{R}_+$.

The transition into the j-th population with state u at point x due to the interaction of entities of the k-th population with state v at point y with entities of the l-th population with state w at point z is described by the (measurable) function $A = A((j, u, x); (k, v, y), (l, w, z))$; $A : \Omega^3 \to \mathbb{R}_+$.

The following particular (*conservative*) case is assumed

$$\int_{\Omega} A(\mathbf{u}; \mathbf{v}, \mathbf{w})\, \mathrm{d}\mu(\mathbf{u}) = 1, \quad \text{for } \mu\text{-a.a. } \mathbf{v},\ \mathbf{w} \text{ in } \Omega \text{ such that } a(\mathbf{v}, \mathbf{w}) > 0 \tag{3}$$

where μ is a measure on Ω. We adhere to the obvious convention that the sum on the set $\mathcal{J}$ is expressed by the integral with respect to the counting measure.

In the case of systems related to Eq. (1) we use a simpler space homogeneous model – independent of the space variables x, y, z as well as $\mathcal{J} = \{0, 1, \ldots, r\}$.

In the space homogeneous case let $\mathcal{J} = \{0, 1, \ldots, r\}$; $\Omega = \mathcal{J} \times \mathbb{R}_+$;

$$a_R(j,u,k,v) = a^*(j,u,k,v)\chi(u \leqslant R)\chi(v \leqslant R) \tag{4}$$

$$a^*(j,u,k,v) = \begin{cases} b_{j,k}v & \text{for } j,k = 1,\dots,r \\ b_{j,0} & \text{for } j = 1,\dots,r,\ k = 0 \\ 0 & \text{for } j = 0,\ k = 0,\dots,r \end{cases}$$

$b_{j,k} \geqslant 0$ $(j,k = 0,\dots,r)$, where $R \geqslant R_0 > 0$, $\chi(\text{true}) = 1$, $\chi(\text{false}) = 0$;

$$A_R(j,u;k,v,l,w) = \mathcal{A}^{(R)}_{j,k,l}(u,v)\chi(u \leqslant R)\chi(v \leqslant R)\chi(w \leqslant R) \tag{5}$$

for $j,k,l = 0,\dots,r$,

$$\mathcal{A}^{(R)}_{j,k,l}(u,v) = \frac{\mathcal{A}_{j,k,l}(u,v)}{\sum_{j'=1}^{r}\int_0^R \mathcal{A}_{j',k,l}(u',v)\,\mathrm{d}u'}$$

and $\mathcal{A}_{j,k,l} \geqslant 0$ satisfies

$$\sum_{j'=1}^{r}\int_0^{R_0} \mathcal{A}_{j',k,l}(u,v)\,\mathrm{d}u \geqslant c_1 > 0, \qquad \sum_{j'=1}^{r}\int_0^{\infty} \mathcal{A}_{j',k,l}(u,v)\,\mathrm{d}u = 1, \qquad \int_0^{\infty} u\mathcal{A}_{j,k,l}(u,v)\,\mathrm{d}u = B_{j,k,l}v$$

for all $v > 0$, $j,k,l = 0,\dots,r$, where c_1 is a constant; $R_0 > 0$ is fixed and $R > R_0$; Moreover, $\mathcal{A}_{0,k,l} \equiv 0$ ($\forall k$, $l = 0,\dots,r$), $\mathcal{A}_{j,k,l} \equiv 0$ (if $j \neq k$, $j,k,l = 1,\dots,r$).

In the space inhomogeneous case let $\mathcal{J} = \{0,1,\dots,r+1\}$; $\Omega = \mathcal{J} \times \mathbb{R}_+ \times \mathbb{T}^d$; $\varepsilon > 0$; $\kappa_\varepsilon^d = \frac{\varepsilon^d}{d}|\mathbb{S}^{d-1}|$; $\mathbb{S}^{d-1} = \{\eta \in \mathbb{R}^d\colon |\eta| = 1\}$; $|\mathbb{S}^{d-1}| = \int_{\mathbb{S}^{d-1}} \mathrm{d}\eta$;

$$a_{R,\varepsilon}(j,u,x,k,v,y) = a^*(j,u,x,k,v,y)\chi(u \leqslant R)\chi(v \leqslant R) \tag{6}$$

$$a^*(j,u,x,k,v,y) = \begin{cases} \frac{1}{\kappa^d_{\varepsilon^3}}\chi\big(|y-x| < \varepsilon^3\big)b_{j,k}v & \text{for } j,k = 1,\dots,r \\ b_{j,k} & \text{for } j = 1,\dots,r,\ k = 0, r+1 \\ 0 & \text{for } j = 0, r+1,\ k = 0,\dots,r+1 \end{cases}$$

$$A_{R,\varepsilon}(j,u,x;k,v,y,l,w,z) = \frac{1}{\kappa^d_{\varepsilon^3}}\chi\big(|y-x| < \varepsilon^3\big)\mathcal{A}^{(R)}_{j,k,l}(u,v)\chi(u \leqslant R)\chi(v \leqslant R)\chi(w \leqslant R) \tag{7}$$

$j,k = 0,\dots,r+1$, $l = 0,\dots,r$, where $\mathcal{A}^{(R)}_{j,k,l}(u,v)$ is given by (3) for $j,k,l = 0,\dots,r$,

$$\mathcal{A}^{(R)}_{r+1,k,l} \equiv 0, \quad \forall k,l = 0,\dots,r+1$$

$$A_{R,\varepsilon}(j,u,x;k,v,y,r+1,w,z) = \frac{\delta_{j,k}}{\kappa^d_\varepsilon}\chi\big(|y-x| < \varepsilon\big)\mathcal{A}^{(R)}_j(u,v)\chi(u \leqslant R)\chi(v \leqslant R)\chi(w \leqslant R)$$

for $j,k = 1,\dots,r$, $\delta_{j,j} = 1$, $\delta_{j,k} = 0$ $(j \neq k)$,

$$\mathcal{A}^{(R)}_j(u,v) = \frac{\mathcal{A}_j(u,v)}{\sum_{j'=1}^{r}\int_0^R \mathcal{A}_{j'}(u',v)\,\mathrm{d}u'}$$

and $\mathcal{A}_j \geqslant 0$ satisfies

$$\sum_{j'=1}^{r}\int_0^{R_0} \mathcal{A}_{j'}(u,v)\,\mathrm{d}u \geqslant c_2 > 0, \qquad \sum_{j'=1}^{r}\int_0^{\infty} \mathcal{A}_{j'}(u,v)\,\mathrm{d}u = 1, \qquad \int_0^{\infty} u\,\mathcal{A}_j(u,v)\,\mathrm{d}u = v, \quad \forall v > 0$$

for all $j = 1,\dots,r$, where c_2 is a constant.

Let the system be initially distributed according to the probability density $F_N \in L_{1,N}$, where $L_{1,N}$ is the space equipped with the norm $\|f\|_{L_{1,N}} = \int_{\Omega^N} |f(\mathbf{u}_1,\ldots,\mathbf{u}_N)|\,\mathrm{d}\mu(\mathbf{u}_1)\cdots\mu(\mathbf{u}_N)$. The time evolution is described by

$$\partial_t f_N = \Lambda_N^* f_N; \quad f_N|_{t=0} = F_N \tag{8}$$

where

$$\Lambda_N^* f(\mathbf{u}_1,\mathbf{u}_2,\ldots,\mathbf{u}_N) = \frac{1}{N}\sum_{\substack{1\leqslant n,m\leqslant N\\ n\neq m}}\biggl(\int_\Omega A(\mathbf{u}_n;\mathbf{v},\mathbf{u}_m)a(\mathbf{v},\mathbf{u}_m)f(\mathbf{u}_1,\ldots,\mathbf{u}_{n-1},\mathbf{v},\mathbf{u}_{n+1},\ldots,\mathbf{u}_N)\,\mathrm{d}\mu(\mathbf{v}) \\ - a(\mathbf{u}_n,\mathbf{u}_m)f(\mathbf{u}_1,\ldots,\mathbf{u}_N)\biggr)$$

The operator Λ_N^* for $A = A_R$, $a = a_R$ or $A = A_{R,\varepsilon}$, $a = a_{R,\varepsilon}$ is a bounded linear operator in the space $L_{1,N}$. Therefore the Cauchy problem (8) has the unique solution $f_N(t) \in L_{1,N}$ for all $t \geqslant 0$. Moreover, by standard argument, we see that the solution is non-negative and the $L_{1,N}$-norm is conserved

$$\bigl\|f_N(t)\bigr\|_{L_{1,N}} = \|F_N\|_{L_{1,N}} = 1, \quad \text{for } t > 0 \tag{9}$$

Thus $\exp(t\Lambda_N^*)$ defines a continuous linear semigroup of Markov operators (continuous stochastic semigroups) – cf. [3].

The s-individual marginal density ($1 \leqslant s < N$) is defined by

$$f_{N,s}(\mathbf{u}_1,\ldots,\mathbf{u}_s) = \int_{\Omega^{N-s}} f_N(\mathbf{u}_1,\ldots,\mathbf{u}_N)\,\mathrm{d}\mu(\mathbf{u}_{s+1})\cdots\mathrm{d}\mu(\mathbf{u}_N) \tag{10}$$

and $f_{N,N} = f_N$. We assume that the process starts with chaotic (i.e., factorized) probability density and we consider initial data

$$F_{N,s} = (F)^{s\otimes} = \underbrace{F\otimes\ldots\otimes F}_{s\times}, \quad s = 1,\ldots,N \tag{11}$$

i.e., s-fold outer product of a probability density F defined on Ω.

In the limit $N \to \infty$ the linear equation (8) results [2] in a bilinear system of Boltzmann-like integro-differential equations in the form proposed in [4].

Various Boltzmann-like equations in the context of biological systems were considered by various authors (see, e.g., [4–9] and references therein). In the literature the Boltzmann-like equations are referred to as GKM – Generalized Kinetic (Boltzmann) Models (cf. [6]). They can be related to mesoscopic description.

The relationships between the GKM and some hydrodynamic systems were discussed in [9].

3. Links

We may state the asymptotic result in the space homogeneous case (all functions are assumed to be independent of the position variables).

Theorem 3.1. *Given parameters* $\alpha_{j,k}$, $\beta_{j,k}$ $(j,k \in \{1,2,\ldots,r\})$ *and* $(\rho_1^{(0)},\ldots,\rho_r^{(0)}) \in \mathbb{R}_+^r$. *Then there exist* a_R, A_R *satisfying* (4), (5) *with* $R > R_0$; $t_1 > 0$; F *being a probability density on* $\mathcal{J}\times\mathbb{R}_+$ *such that* $(\overline{F}(1),\ldots,\overline{F}(r)) = (\rho_1^{(0)},\ldots,\rho_r^{(0)}) \in \mathbb{R}_+^r$; *the unique non-negative solution* $(\rho_1,\ldots,\rho_r)$ *of Eq.* (1) *corresponding to the initial datum* $(\rho_1^{(0)},\ldots,\rho_r^{(0)})$; *such that for sufficiently large* N *and* R

$$\sup_{t\in[0,t_1]}\sum_{j=1}^r\bigl|\bar{f}_{N,1}(t,j) - \rho_j(t)\bigr| \leqslant \frac{c_1}{N^{\eta_1}} + \frac{c_2}{R} \tag{12}$$

where the non-negative function $f_N \in L_{1,N}$ *is the unique solution of Eq.* (8) *with* $a = a_R$, $A = A_R$ *and corresponding to the initial datum* $F^{N\otimes}$; η_1, c_1 *are positive constants that depend on* R; c_2 *is a constant*; *and* $\bar{f} = \int_0^R u f(u)\,\mathrm{d}u$.

The analog of Theorem 3.1 in the space inhomogeneous case with weak diffusion can be written as follows

Theorem 3.2. *Given parameters* $\alpha_{j,k}$, $\beta_{j,k}$, σ_j^* $(j, k \in \{1, 2, \ldots, r\})$ *and* $(\varrho_1^{(0)}, \ldots, \varrho_r^{(0)}) \in C^3(\mathbb{T}^d; \mathbb{R}_+^r)$. *Then there exist*

(i) $a_{R,\varepsilon}$, $A_{R,\varepsilon}$ *satisfying* (6), (7) *with* $R > R_0$ *and* $\varepsilon > 0$;
(ii) $t_2 > 0$;
(iii) F *being a* (*smooth*) *probability density on* Ω, *such that* $(\overline{F}(1,\cdot), \ldots, \overline{F}(r,\cdot)) = (\varrho_1^{(0)}, \ldots, \varrho_r^{(0)})$;
(iv) *the unique classical non-negative solution* $(\varrho_1, \ldots, \varrho_r)$ *of Eq.* (2) *with* $\sigma_j = \varepsilon^2 \sigma_j^*$ *and initial data* $(\varrho_1^{(0)}, \ldots, \varrho_n^{(0)})$;

such that for sufficiently large N, R *and small* $\varepsilon > 0$

$$\sup_{t\in[0,t_2]} \sum_{j=1}^{r} \int_{\mathbb{T}^d} \left| \bar{f}_{N,1}(t, j, x) - \varrho_j(t, x) \right| \mathrm{d}x \leqslant \frac{c_3}{N^{\eta_2}} + \frac{c_4}{R} + c_5 \varepsilon^3 \tag{13}$$

where the non-negative function $f_N \in L_{1,N}$ *is the unique solution of Eq.* (8) *with* $a = a_{R,\varepsilon}$, $A = A_{R,\varepsilon}$ *and corresponding to the initial datum* $F^{N\otimes}$; η_2 *and* c_3 *are positive constants that depend on* R *and* ε; c_4 *is a positive constant that depends on* ε; c_5 *is a constant.*

Theorems 3.1 and 3.2 show that the conservative (i.e., satisfying (3)) linear equation (8) can result (in properly chosen limits) in the nonlinear equations (1) and (2) in the space homogeneous and inhomogeneous cases, respectively, which need not be conservative. The proofs follow two steps: the transition from the microscopic level (Eq. (8)) to the mesoscopic level and then from mesoscopic level to the macroscopic level (Eqs. (1) and (2)). The detailed proofs of the first step will appear in [2] (where the idea of [10] will be used) and of the second step in the forthcoming paper [11]. A simpler case of competitive systems was discussed in [12].

In the general case, Theorems 3.1 and 3.2 have a local in time character, but for a large class of Eqs. (1) and (2) for which the global existence results hold the global (on any compact time interval) result is possible.

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References

[1] R. O'Malley Jr., Singular Perturbation Methods for ODE, Springer, New York, 1991.
[2] M. Lachowicz, On bilinear kinetic equations. Between micro and macro description of biological populations, Banach Center Publ., in press.
[3] A. Lasota, M.C. Mackey, Chaos, Fractals, and Noise, Springer, New York, 1994.

[4] M. Lachowicz, D. Wrzosek, Nonlocal bilinear equations. Equilibrium solutions and diffusive limit, Math. Models Methods Appl. Sci. 11 (2001) 1375–1390.
[5] L. Arlotti, N. Bellomo, Population dynamics with stochastic interaction, Transport Theory Statist. Phys. 24 (1995) 431–443.
[6] L. Arlotti, N. Bellomo, E. De Angelis, Generalized kinetic Boltzmann models: Mathematical structures and applications, Math. Models Methods Appl. Sci. 12 (2002) 571–596.
[7] L. Arlotti, N. Bellomo, M. Lachowicz, Kinetic equations modelling population dynamics, Transport Theory Statist. Phys. 29 (2000) 125–139.
[8] E. Jäger, L. Segel, On the distribution of dominance in a population of interacting anonymous organisms, SIAM J. Appl. Math. 52 (1992) 1442–1468.
[9] M. Lachowicz, From microscopic to macroscopic description for generalized kinetic models, Math. Models Methods Appl. Sci. 12 (2002) 985–1005.
[10] M. Lachowicz, M. Pulvirenti, A stochastic particle system modeling the Euler equation, Arch. Rational Mech. Anal. 109 (1990) 81–93.
[11] M. Lachowicz, General population systems. Macroscopic limit of a class of stochastic semigroups, in press.
[12] M. Lachowicz, Describing competitive systems at the level of interacting individuals, in: Proceedings of the Eight National Conference on Applications of Mathematics in Biology and Medicine, Łajs, 25–28 September, 2002, pp. 95–100.