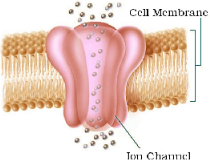
Asymptotic Gradient Flow Structures in Interacting Particle Systems

Helene Ranetbauer

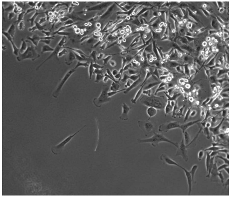
joint work with Maria Bruna, Martin Burger, Helene Ranetbauer and Marie-Therese Wolfram

AANMPDE
August 07, 2018

Interacting Particle Systems



(a) ion channels



(b) chemotaxis

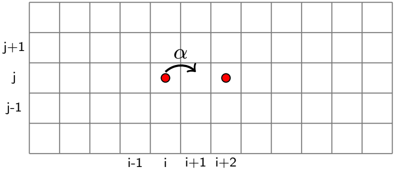
(c) fish school

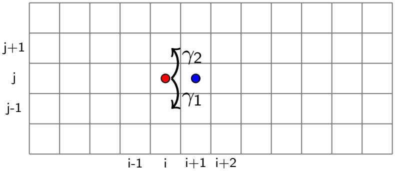
(d) pedestrian dynamics

- microscopic vs. macroscopic models

Microscopic Models

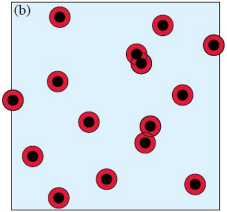
- Lattice Based Models
  - example for two groups of particles (red and blue) going in opposite direction





Microscopic Models

- Off-Lattice Based Models



  - Newton's laws of motion
  - Langevin/Brownian dynamics
  - optimal control approaches

Macroscopic Models

Macroscopic models are often based on mass and/or momentum principles or derived from a microscopic model by taking an appropriate limit.

$\Rightarrow$ Nonlinear PDE models with a 'full', perturbed or asymptotic gradient flow structure, i.e.

$$\partial_t \rho = \nabla \cdot \left(m(\rho)\, \nabla \frac{\partial E}{\partial \rho} \right).$$

$\rho = \rho(x,t)$ ... particle density depending on space and time
$m(\rho)$ ... mobility matrix
$E(\rho)$ ... entropy functional

Macroscopic Models

Macroscopic models are often based on mass and/or momentum principles or derived from a microscopic model by taking an appropriate limit.

$\Rightarrow$ Nonlinear PDE models with a 'full', perturbed or asymptotic gradient flow structure, i.e.

$$\partial_t \rho = \nabla \cdot \left(m(\rho) \, \nabla \frac{\partial E}{\partial \rho} \right) + f(\rho).$$

$\rho = \rho(x,t)$ ... particle density depending on space and time
$m(\rho)$ ... mobility matrix
$E(\rho)$ ... entropy functional
$f(\rho)$ ... perturbation term

Macroscopic Models

Macroscopic models are often based on mass and/or momentum principles or derived from a microscopic model by taking an appropriate limit.

$\Rightarrow$ Nonlinear PDE models with a 'full', perturbed or asymptotic gradient flow structure, i.e.

$$\partial_t \rho = \nabla \cdot \left(m(\rho)\, \nabla \frac{\partial E}{\partial \rho} \right) + f(\rho; \varepsilon).$$

$\rho = \rho(x, t)$ ... particle density depending on space and time
$m(\rho)$ ... mobility matrix
$E(\rho)$ ... entropy functional
$f(\rho; \varepsilon)$ ... perturbation term of order $\mathcal{O}(\varepsilon)$ with $0 < \varepsilon \ll 1$

Microscopic Particle Model

We consider a system of two types of particles r, b in dimension $d = 2, 3$ with different diameter $\varepsilon_r, \varepsilon_b$. Each particle evolves according to the overdamped Langevin stochastic differential equation

$$
\begin{aligned}
d\mathbf{X}_i(t) &= \sqrt{2D_r}\, d\mathbf{W}_i(t) - \nabla V_r(\mathbf{X}_i)\, dt \qquad 1 \leq i \leq N_r, \\
d\mathbf{X}_i(t) &= \sqrt{2D_b}\, d\mathbf{W}_i(t) - \nabla V_b(\mathbf{X}_i)\, dt \qquad N_r + 1 \leq i \leq N.
\end{aligned}
$$

- Particles interact via hard core collisions $\Rightarrow$ they cannot get closer as the sum of their radii, i.e. $\|\mathbf{X}_i - \mathbf{X}_j\| \geq (\varepsilon_i + \varepsilon_j)/2$

Macroscopic Model

- Continuum-level model derived by M. Bruna and J. Chapman using methods of matched asymptotics.

$$\partial_t r = D_r \nabla \cdot \left\{ (1+\varepsilon_r^d \alpha r)\nabla r + \nabla V_r r + \varepsilon_{br}^d \left[\beta_r r \nabla b - \gamma_r b \nabla r + \nabla(\gamma_b V_b - \gamma_r V_r) rb \right] \right\},$$
$$\partial_t b = D_b \nabla \cdot \left\{ (1+\varepsilon_b^d \alpha b)\nabla b + \nabla V_b b + \varepsilon_{br}^d \left[\beta_b b \nabla r - \gamma_b r \nabla b + \nabla(\gamma_r V_r - \gamma_b V_b) rb \right] \right\},$$

where α, β_i and γ_i depend on the dimension and diffusion coefficients and $\varepsilon_{br} = (\varepsilon_b + \varepsilon_r)/2$.

- Only valid if $\varepsilon^d \ll 1$ and in the case of low volume fraction, i.e.

$$\Phi = N_r v_d(\varepsilon_r) + N_b v_d(\varepsilon_b) \ll 1,$$
$$\phi = v_d(\varepsilon_r) r + v_d(\varepsilon_b) b \ll 1.$$

Question

Does the system have a gradient flow structure?

Gradient Flow Structure

$$\begin{aligned}\partial_t r &= D_r \nabla\cdot\left\{(1+\varepsilon_r^d \alpha r)\nabla r + \nabla V_r r + \varepsilon_{br}^d\left[\beta_r\, r\nabla b - \gamma_r b\nabla r + \nabla(\gamma_b V_b - \gamma_r V_r) rb\right]\right\}\\ \partial_t b &= D_b \nabla\cdot\left\{(1+\varepsilon_b^d \alpha b)\nabla b + \nabla V_b b + \varepsilon_{br}^d\left[\beta_b\, b\nabla r - \gamma_b r\nabla b + \nabla\left(\gamma_r V_r - \gamma_b V_b\right) rb\right]\right\}\end{aligned} \qquad (1)$$

The entropy functional

$$E(r,b;\varepsilon) = \int_\Omega r\log r + b\log b + rV_r + bV_b + \frac{\alpha}{2}\left(\varepsilon_r^d\, r^2 + 2\varepsilon_{br}^d\, rb + \varepsilon_b^d\, b^2\right) d\mathbf{x},$$

and the mobility matrix

$$m(r,b;\varepsilon) = \begin{pmatrix} D_r r & 0 \\ 0 & D_b b\end{pmatrix} + \varepsilon_{br}^d rb\begin{pmatrix} -D_r\gamma_r & D_r\gamma_b \\ D_b\gamma_r & -D_b\gamma_b\end{pmatrix}.$$

gives

$$\begin{pmatrix}\partial_t r\\ \partial_t b\end{pmatrix} = \nabla\cdot\left[m\nabla\begin{pmatrix}\frac{\partial E}{\partial r}\\ \frac{\partial E}{\partial b}\end{pmatrix} + f\right] = \nabla\cdot\left[m\nabla\begin{pmatrix}u\\ v\end{pmatrix} + f\right],$$

where $f := f(r,b;\varepsilon) = \mathcal{O}(\varepsilon^2)$.

- $f = 0 \iff D_r = D_b$ and $\varepsilon_r = \varepsilon_b$

Asymptotic gradient flow structure

Let $\varepsilon > 0$ be a small parameter. Consider a gradient flow structure of the form

$$\partial_t \rho = \nabla \cdot (m(\rho, \varepsilon) \nabla E'(\rho, \varepsilon)),$$

where

$$m(\rho, \varepsilon) = \sum_{j=0}^{\infty} \varepsilon^j m_j(\rho), \qquad E'(\rho, \varepsilon) = \sum_{j=0}^{\infty} \varepsilon^j E_j'(\rho),$$

we find

$$\partial_t \rho = \sum_{k=0}^{\infty} \varepsilon^k \nabla \cdot \left(\sum_{j=0}^{k} m_j(\rho) \nabla E_{k-j}'(\rho) \right).$$

Truncating the expansion at a finite k does not yield a gradient flow structure in general, but up to terms of order ε^k it coincides with the gradient flow structure with mobility $\sum_{j=0}^{k} \varepsilon^j m_k(\rho)$ and entropy $\sum_{j=0}^{k} \varepsilon^j E_k(\rho)$.

How can we use it?

Asymptotic gradient flow structure of first order:

$$\begin{pmatrix} \partial_t r \\ \partial_t b \end{pmatrix} = \nabla \cdot \left[m(r,b) \nabla \begin{pmatrix} u \\ v \end{pmatrix} + \varepsilon^{2d} f(r,b) \right].$$

- existence of stationary solutions (u_*, v_*): compute equilibrium solution (u_∞, v_∞) of full gradient flow system (energy minimization) and use a perturbation argument.

$$-\nabla \cdot \left(m(r_\infty, b_\infty) \begin{pmatrix} \nabla u \\ \nabla v \end{pmatrix} \right) = \nabla \cdot \left(\varepsilon^{2d} f(r,b) + (m(r,b) - m(r_\infty, b_\infty)) \begin{pmatrix} \nabla(u - u_\infty) \\ \nabla(v - v_\infty) \end{pmatrix} \right)$$
$$=: G(u,v)$$

We have as a consequence that

$$\|u_* - u_\infty\|_X + \|v_* - v_\infty\|_X \leq C\varepsilon^{2d}.$$

How can we use it?

- behavior of transient solutions locally around stationary solutions

$$\partial_t(r,b) - \nabla\cdot\left(m(r_\infty,b_\infty)\begin{pmatrix}\nabla u\\ \nabla v\end{pmatrix}\right) = \nabla\cdot\Bigg(\varepsilon^{2d} f(r,b) + (m(r,b)-m(r_\infty,b_\infty))\begin{pmatrix}\nabla(u-u_\infty)\\ \nabla(v-v_\infty)\end{pmatrix}\Bigg)$$

We were able to show linear stability close to stationary solution (u_*, v_*) and $\varepsilon > 0$ sufficiently small.

- How to use asymptotic gradient flow structure for proving global existence?

Numerics

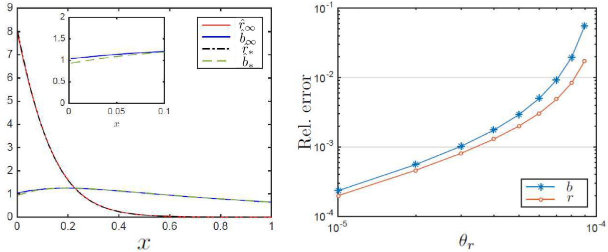


Figure: $(\hat{r}_*, \hat{b}_*) = (r_*/N_r, b_*/N_b)$ denote the stationary solutions from solving the long-time limit of the asymptotic gradient flow structure and $(\hat{r}_\infty = r_\infty/N_r, \hat{b}_\infty = b_\infty/N_b)$ denote the equilibrium solutions obtained from minimizing the entropy. The right Figure illustrates the error between the stationary solution $(\hat{r}_*, \hat{b}_*)$ and the equilibrium solution $(\hat{r}_\infty, \hat{b}_\infty)$ as a function of θ_r. The parameters are $d = 2$, $D_b = 1$, $\varepsilon_r = \varepsilon_b = 0.01$, $N_b = N_r = 200$, $V_r = 2x$, $V_b = x$ and $\theta_r = 8 \cdot 10^{-5}$ and $D_r = 0.2$ (in the left Figure).

Example: Scalar diffusion equation

$$\partial_t r = \nabla \cdot \left[(1 + \varepsilon_1 r - \varepsilon_2 b) \nabla r + \varepsilon_3 r \nabla b \right], \qquad t > 0, \mathbf{x} \in \Omega,$$

where $\mathbf{x} \in \Omega \subset \mathbb{R}^d$, $d = 2, 3$.

- describes the density of interacting particles diffusing through a porous medium represented by a fixed porosity density $b(x)$
- diffusing (Brownian) red and immobile (obstacle) blue particles using the asymptotic method in the limit of low volume fraction
- nonlinear Fokker-Planck equation lacking a full GF structure
- use AGF to understand properties of its solutions such as existence, uniqueness, or long-time behavior

Asymptotic gradient flow structures

$$\partial_t r = \nabla \cdot [(1 + \varepsilon_1 r - \varepsilon_2 b)\nabla r + \varepsilon_3 r \nabla b]$$

$$\partial_t r = \nabla \cdot \left[m(r,\varepsilon) \nabla \frac{\delta E}{\delta r}(r,\varepsilon) + f(r,\varepsilon) \right], \qquad f = \mathcal{O}(\varepsilon^2).$$

(1)
- $E_1(r) = \int_\Omega \left[r(\log r - 1) + \frac{1}{2}\varepsilon_1 r^2 + \varepsilon_3 rb \right] \mathrm{d}\mathbf{x}$
- $m_1(r) = r(1 - \varepsilon_2 b)$
- $f_1(r) = rb(\varepsilon_1\varepsilon_2 \nabla r + \varepsilon_2\varepsilon_3 \nabla b)$

(2)
- $E_2(r) = \int_\Omega r \left[\log\left(\frac{r}{1 - \varepsilon_1 r - \varepsilon_3 b} \right) - 1 \right] \mathrm{d}\mathbf{x}$
- $m_2(r) = r(1 - \varepsilon_1 r - \varepsilon_2 b)$
- $f_2(r) = -\varepsilon_1 r^2 (\varepsilon_1 \nabla r + \varepsilon_3 \nabla b) + (\varepsilon_2 - \varepsilon_3) rb \,(2\varepsilon_1 \nabla r + \varepsilon_3 \nabla b) + O(\varepsilon^3)$

(3)
- $E_3(r) = \int_\Omega r \left[\log\left(\frac{r}{1 - \alpha\varepsilon_1 r - \varepsilon_3 b} \right) - 1 \right] \mathrm{d}\mathbf{x}$
- $m_3(r) = r(1 - \beta\varepsilon_1 r - \varepsilon_2 b)$

Properties

Definition

Two AGF structures defined by a entropy-mobility pair (E_i, m_i) and entropy variables $u_i = \delta E_i / \delta r$ are equal up to order ε^k, if

(i) the asymptotic expansions $m_i \nabla u_i$ are equal up to order ε^k.

(ii) the asymptotic expansions of their corresponding stationary solutions, found setting $u_i = \chi_i$ constant, are equal up to order ε^k.

- $(E_1(r), m_1(r))$, $(E_2(r), m_2(r))$ and $(E_3(r), m_3(r))$ are equivalent up to order ε.
- Questions: Which entropy-mobility pair should you choose? What is the 'right' one?

Comparison of Entropy-Mobility Pair (1) and (2)

- $E_1(r) = \int_\Omega \left[r(\log r - 1) + \frac{1}{2}\varepsilon_1 r^2 + \varepsilon_3 rb\right] \mathrm{d}\mathbf{x}$ and $m_1(r) = r(1 - \varepsilon_2 b)$
  - global existence of the corresponding AGF *with* modification of the flux term
  - exponential convergence to equilibrium
- $E_2(r) = \int_\Omega r \left[\log\left(\frac{r}{1-\varepsilon_1 r - \varepsilon_3 b}\right) - 1\right] \mathrm{d}\mathbf{x}$ and $m_2(r) = r(1 - \varepsilon_1 r - \varepsilon_2 b)$
  - global existence of the corresponding full GF *without* modification of the flux term
  - not clear how to control the higher order terms in order to pass to the AGF model

Global Existence of $\partial_t r = \nabla \cdot [(1+\varepsilon_1 r - \varepsilon_2 b)\nabla r + \varepsilon_3 r \nabla b]$

$$
\begin{aligned}
E_1(r) &= \int_\Omega \left[r(\log r - 1) + \frac{1}{2}\varepsilon_1 r^2 + \varepsilon_3 r b \right] \mathrm{d}\mathbf{x} \\
m_1(r) &= r(1-\varepsilon_2 b)
\end{aligned}
$$

allows to prove global existence of a weak solution r to the equation

$$
\begin{aligned}
\partial_t r &= \nabla \cdot J_r \\
(1-\varepsilon_1 r - \varepsilon_2 b) J_r &= (1-\varepsilon_1 r - \varepsilon_2 b) \left[(1+\varepsilon_1 r - \varepsilon_2 b)\nabla r + \varepsilon_2 r \nabla b) \right],
\end{aligned}
$$

in the sense of

$$
\int_0^T \left[\langle \partial_t r, \Phi \rangle_{H^{-1},H^1} + \int_\Omega J_r \cdot \nabla \Phi \, \mathrm{d}\mathbf{x} \right] \mathrm{d}t = 0,
$$

for all $\Phi \in L^2(0,T,H^1(\Omega))$.

Global Existence of $\partial_t r = \nabla \cdot [(1 + \varepsilon_1 r - \varepsilon_2 b)\nabla r + \varepsilon_3 r \nabla b]$

$$
\begin{aligned}
E_2(r) &= \int_\Omega r \left[\log\left(\frac{r}{1 - \varepsilon_1 r - \varepsilon_3 b} \right) - 1 \right] \mathrm{d}\mathbf{x} \\
m_2(r) &= r(1 - \varepsilon_1 r - \varepsilon_2 b)
\end{aligned}
$$

automatically provides the necessary bounds on r with the help of the boundedness by entropy method and allows to prove global existence of a weak solution r to the equation

$$
\int_0^T \left[\langle \partial_t r, \Phi \rangle_{H^{-1}, H^1} + \int_\Omega \left(m_2(r) \nabla \frac{\partial E_2}{\partial r} \right) \cdot \nabla \Phi \mathrm{d}\mathbf{x} \right] \mathrm{d}t = 0,
$$

for all $\Phi \in L^2(0, T, H^1(\Omega))$.

Conclusion

- definition of the concept of asymptotic gradient flow structures
- full GF: global in time existence, exponential convergence to equilibrium solutions
- AGF: existence and linear stability of stationary solutions, global in time existence with modification of the flux term
- TO DO: prove that time dependent solutions of full GF and AGF are sufficiently close to each other, i.e. of order $\mathcal{O}(\varepsilon^2)$

References

- Bruna, M., Burger, M., Ranetbauer, H., Wolfram, M. T. (2017). Cross-diffusion systems with excluded-volume effects and asymptotic gradient flow structures. Journal of Nonlinear Science, 27(2), 687-719.
- Bruna, M., Burger, M., Ranetbauer, H., Wolfram, M. T. (2018). Asymptotic gradient flow structures of a nonlinear Fokker-Planck equation. Submitted to CMS.
- Bruna, M., Chapman, S. J. (2012). Diffusion of multiple species with excluded-volume effects. The Journal of chemical physics, 137(20), 204116.
- Bruna, M., Chapman, S. J. (2012). Excluded-volume effects in the diffusion of hard spheres. Physical Review E, 85(1), 011103.