Phase Separation in Nonlocal Multispecies Models
Martin Burger, FAU Erlangen-Nürnberg
Many social and biological phenomena can be described by microscopic models for individual agents, using similar paradigms as statistical physics, e.g.

- Crowding effects in molecular biology (ions, cells)
- Swarming / Herding / Flocking (birds, fish, insects)
- Traffic flow / Pedestrian motion
- Opinion formation / Development of social norms
- Price formation, herding in financial markets

Most of them typically involve local repulsion, nonlocal attractions
Macroscopic PDE Models

Single species case

$$\partial_t \rho = \nabla \cdot (m(\rho) \nabla (e'(\rho) - G \ast \rho))$$

Examples of mobility / entropy pairs:

$$m(\rho) = \rho, \quad e(\rho) = \varepsilon \frac{m-1}{m} \rho^m$$

$$m(\rho) = \rho(1 - \rho), \quad e(\rho) = \varepsilon (\rho \log \rho + (1 - \rho) \log(1 - \rho))$$

Gradient flow for energy functional

$$E[\rho] = \int e(\rho) - \frac{1}{2} \rho G \ast \rho \, dx$$
Gradient Flow

Simple example: Wasserstein gradient flow with quadratic entropy

\[ \partial_t \rho = \text{div} \left( \rho \nabla \left( \varepsilon \rho - G * \rho \right) \right) \]

Repulsion strength as scaling parameter (relative to attraction strength encoded in \( G \)).

Mean-field limit of particle system with localized repulsive force

Long time asymptotics: convergence to equilibrium, stationary points of energy functional (mb-DiFrancesco 2008)
Stationary solutions

G regular (no finite-time blow up). Geodesic $\lambda$-convex energy, negative $\lambda$

Note: stationary solutions are regular on their support

On each connected component of support stationary solutions satisfy

$$\varepsilon \rho_\infty = G * \rho_\infty + C[\rho_\infty]$$

Naturally satisfied with single constant by energy minimizers

$$E[\rho] := \frac{\varepsilon}{2} \int_{\mathbb{R}^d} \rho^2(x) \, dx - \frac{1}{2} \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} G(x - y) \rho(y) \rho(x) \, dy \, dx$$
Threshold Phenomenon

Comparison of repulsion and aggregation strength

- Let $\varepsilon < \|G\|_{L^1}$. Then, there exists at least one non trivial $L^1$ steady state, which is also a minimizer for the energy $E[\rho]$.
- Let $\varepsilon \geq \|G\|_{L^1}$. Then, there exist no steady states except $\rho \equiv 0$.

Proof by variational arguments

$E$ is convex in the second case, infimum at zero, no minimizer

Diffusive rescaling to Barenblatt solution in case of nonexistence

Different behaviour on bounded domains, always $L^2$ steady states and energy minimizers
Properties of steady states

Rearrangement: radially symmetric, decreasing energy minimizers

Existence of simply connected steady states with compact support based on integral equation on support

\[ \varepsilon \rho = G \ast \rho + 2E[\rho] \]

Idea: interpretation as eigenvalue equation for fixed support radius. Existence by Krein-Rutman theorem!

Self-organized Cell Sorting

Consider simplest model:

- Two species, same size, different maturation
- Local repulsion, same for all
- Nonlocal aggregation (e.g. chemotaxis), with different strength

Non-intuitive segregation, all cells try to aggregate

Gradient flow for entropy consisting of pressure and aggregation terms

\[ \mathcal{E}[\rho_1, \rho_2] = \int f(\rho_1, \rho_2)dx - \frac{1}{2} \int \rho_1 S_1 * \rho_1 dx - \frac{1}{2} \int \rho_2 S_2 * \rho_2 dx - \int \rho_1 K * \rho_2 dx \]
Self-organized Cell Sorting

Gradient flow

$$\partial_t \rho_1 = \text{div} \left[ \rho_1 \nabla (f_{\rho_1}(\rho_1, \rho_2) - S_1 \ast \rho_1 - K \ast \rho_2) \right]$$

$$\partial_t \rho_2 = \text{div} \left[ \rho_2 \nabla (f_{\rho_2}(\rho_1, \rho_2) - S_2 \ast \rho_2 - K \ast \rho_1) \right]$$

Due to equal size of cells, pressure depends on total density, e.g.

$$f(\rho_1, \rho_2) = \epsilon (\rho_1 + \rho_2)^2 / 2$$

Degenerate Cross-Diffusion system

$$\partial_t \rho_1 = \text{div} \left[ \epsilon \rho_1 \nabla (\rho_1 + \rho_2) - \rho_1 \nabla S_1 \ast \rho_1 - \rho_1 \nabla K \ast \rho_2 \right]$$

$$\partial_t \rho_2 = \text{div} \left[ \epsilon \rho_2 \nabla (\rho_1 + \rho_2) - \rho_2 \nabla S_2 \ast \rho_2 - \rho_2 \nabla K \ast \rho_1 \right]$$
Canonical Model

What is the basis of segregation? Degeneracy of diffusion and difference of other forces

\[ \partial_t \rho_1 = \text{div} (\epsilon \rho_1 \nabla (\rho_1 + \rho_2) - \rho_1 \nabla V_1) \]
\[ \partial_t \rho_2 = \text{div} (\epsilon \rho_2 \nabla (\rho_1 + \rho_2) - \rho_2 \nabla V_2) \]

No external potentials, 1D: segregated initial values remain segregated, Bertsch et al 1995 (multi-D: Schmidtchen et al 2019)

Segregation with additional reaction terms promoting repulsion of the species, Bertsch et al 2012
Interaction Model

Equal size (repulsion force) but different potential forces leads to segregation

**Proposition** Let $V_i \in L^1_{loc}(\mathbb{R}^d) \cap W^{1,\infty}(\mathbb{R}^d)$ be given external potentials. If $(\rho_1^\infty, \rho_2^\infty)$ is a $C^1$ (weak) stationary solution of (*) then we have

$$\text{supp}(\rho_1^\infty) \cap \text{supp}(\rho_2^\infty) \subseteq \{\nabla V_1 = \nabla V_2\}.$$  \hspace{1cm} (10)

**Proof.** Let $x \in \text{supp}(\rho_1^\infty) \cap \text{supp}(\rho_2^\infty)$. Then the weak formulation of (*) implies

$$\epsilon \nabla (\rho_1^\infty + \rho_2^\infty)(x) = \nabla V_1(x) = \nabla V_2(x),$$

from which the assertion follows.

(mb-DiFrancesco-Fagioli-Stevens 2018)
Interaction Model

Direct consequence: segregation for the interaction model with Newtonian potential

**Proposition** Let $K$ be the fundamental solution of the Laplace equation in $\mathbb{R}^d$, and $S_1 = \sigma_1 K$, $S_2 = \sigma_2 K$ with $\sigma_1 \leq 1 \leq \sigma_2$ and $\sigma_1 \neq \sigma_2$. Then, every $C^1$ stationary solution $(\rho_1, \rho_2)$ of (*) is fully segregated, i.e. $\text{supp}(\rho_1) \cap \text{supp}(\rho_2)$ has empty interior.

(mb-DiFrancesco-Fagioli-Stevens 2018)
Interaction Model

General Kernels, entropy minimizers:

\[ \mathcal{F}[\rho_1, \rho_2] = \frac{\epsilon}{2} \int_{\mathbb{R}} (\rho_1 + \rho_2)^2 dx - \frac{1}{2} \int_{\mathbb{R}} \rho_1 S_1 \ast \rho_2 dx - \frac{1}{2} \int_{\mathbb{R}} \rho_2 S_2 \ast \rho_2 dx - \int_{\mathbb{R}} \rho_1 K \ast \rho_2 dx, \]

**Theorem**  Assume that \( K \in C(\mathbb{R}) \) with a unique maximum at zero and being strictly radially decreasing in a neighbourhood. Let \( S_i = \sigma_i K \) for some \( \sigma_1, \sigma_2 > 0 \) with \( \sigma_1 + \sigma_2 > 2 \). Let \((\rho_1^\infty, \rho_2^\infty)\) be a local minimizer of \( \mathcal{F} \) on \( \mathcal{M} \), and

\[ S := \text{supp}(\rho_1^\infty) \cap \text{supp}(\rho_2^\infty). \]

Then \( S \) has zero Lebesgue measure.

(mb-DiFrancesco-Fagioli-Stevens 2018)
Interaction Model

More structure for entropy minimizers in 1D (or radial symmetry):

$$\mathcal{F}[\rho_1, \rho_2] = \frac{\epsilon}{2} \int (\rho_1 + \rho_2)^2 dx - \frac{1}{2} \int \rho_1 S_1 \ast \rho_2 dx - \frac{1}{2} \int \rho_2 S_2 \ast \rho_2 dx - \int \rho_1 K \ast \rho_2 dx,$$

**Proposition** Let $\sigma_1, \sigma_2 > 0$, $K$ be strictly decreasing with respect to the radial variable and $(\rho_1^{\infty}, \rho_2^{\infty}) \in \mathcal{M}$ be a minimizer of $\mathcal{F}$. Then $\text{supp}(\rho_1^{\infty} + \rho_2^{\infty})$ is a connected interval.

**Theorem** Assume that $K \in C(\mathbb{R})$ is strictly radially decreasing. Let $\sigma_1, \sigma_2 > 0$ with $\sigma_1 + \sigma_2 > 2$ and $\sigma_2 < 1$. Let $(\rho_1^{\infty}, \rho_2^{\infty})$ be a global minimiser with compact support of $\mathcal{F}$ on $\mathcal{M}$ with $m_1 = m_2$. Then $\rho_1^{\infty} + \rho_2^{\infty}$ is radially symmetric around its center of mass $X_0$ and there exist $b > a > 0$ such that

$$\text{supp}(\rho_1^{\infty}) = [X_0 - a, X_0 + a], \quad \text{supp}(\rho_2^{\infty}) = [X_0 - b, X_0 - a] \cup [X_0 + a, X_0 + b].$$

(mb-DiFrancesco-Fagioli-Stevens 2018)
Regularity Issues

Issues in the analysis of the gradient flow reflected in the analysis of stationary solutions vs. energy minimizers

Weak solution concept for stationary solutions

\[ \rho_1 + \rho_2 \in \text{Lip}(\mathbb{R}), \quad \text{and} \]

\[ 0 = \int \rho_1 \left( \epsilon (\rho_1 + \rho_2)_x - S'_1 * \rho_1 - K' * \rho_2 \right) U_x \, dx \]

\[ 0 = \int \rho_2 \left( \epsilon (\rho_1 + \rho_2)_x - S'_2 * \rho_2 - K' * \rho_1 \right) V_x \, dx \]

Easy result: energy minimizer with Lipschitz regularity of total density is stationary solution (variation along transport with U and V) (mb-DiFrancesco-Fagioli-Stevens 2018)
Regularity Issues

Proof of Lipschitz regularity in the segregated case

**Theorem.** Assume $K \in C^1(\mathbb{R})$ to be strictly radially decreasing. Let $\sigma_1, \sigma_2 > 0$ and let $(\rho_1^\infty, \rho_2^\infty)$ be a global minimiser with compact support of $\mathcal{F}$ on $\mathcal{M}$. Moreover, assume that for some $M > 1$ there exist $a_1 < a_2 < \ldots < a_M$ such that $\text{supp}(\rho_1^\infty + \rho_2^\infty)$ equals $\bigcup_{i=1}^{M-1} [a_i, a_{i+1}]$ and for each $i = 1, \ldots, M - 1$ we have

$$\rho_k^\infty > 0, \rho_\ell^\infty = 0 \text{ on } (a_i, a_{i+1}),$$

with $\{k, \ell\} = \{1, 2\}$. Then $\rho_1^\infty + \rho_2^\infty$ is Lipschitz-continuous.

Difficulty in the proof: glueing together different parts. Can be shown by constructing appropriate energy perturbations

(mb-DiFrancesco-Fagioli-Stevens 2018)
Consider two-species model with one parameter

\[
\frac{\partial}{\partial t} \rho = \frac{\partial}{\partial x} \left( \rho \frac{\partial}{\partial x} \left( \frac{\delta \mathcal{F}}{\delta \rho} \right) \right) = \frac{\partial}{\partial x} \left( \rho \frac{\partial}{\partial x} \left( (1 + \delta) \rho + \eta \right) \right)
\]

\[
\frac{\partial}{\partial t} \eta = \frac{\partial}{\partial x} \left( \eta \frac{\partial}{\partial x} \left( \frac{\delta \mathcal{F}}{\delta \eta} \right) \right) = \frac{\partial}{\partial x} \left( \rho \frac{\partial}{\partial x} \left( \rho + (1 + \delta) \eta \right) \right)
\]

\[
\mathcal{F}_L(\rho, \eta) = \frac{1 + \delta}{2} \int_{\Omega} (\rho + \eta)^2 dx - \delta \int_{\Omega} \rho \eta dx \quad \delta \in (-1, \infty)
\]

\[
\mathcal{F}_{NL}(\rho, \eta) = \frac{1 + \delta}{2} \int_{\Omega} (\rho + \eta)^2 dx - \delta \int_{\Omega} \rho (K * \eta) dx
\]
Three regimes for energy minimizers (mb-Carillo-Pietschmann-Schmidtchen 2019)

Theorem:

$$\delta > 0, \text{ the unique minimisers } \rho = \frac{m_1}{|\Omega|}, \text{ and } \eta = \frac{m_2}{|\Omega|}$$

$$\delta = 0, \text{ infinite family of minimisers}$$

$$\sigma = \rho + \eta = \frac{m_1 + m_2}{|\Omega|} = \text{const.}$$

$$-1 < \delta < 0, \text{ infinite family of minimisers}$$

$$|\text{supp } \rho \cap \text{supp } \eta| = 0.$$
Repulsive Segregation

Transient behaviour for segregated initial data: JKO scheme preserves segregation and converges to a solution of

\[
\frac{\partial \rho}{\partial t} = (1 + \delta) \frac{\partial}{\partial x} \left( \rho \frac{\partial}{\partial x} (\rho + \eta) \right)
\]

\[
\frac{\partial \eta}{\partial t} = (1 + \delta) \frac{\partial}{\partial x} \left( \eta \frac{\partial}{\partial x} (\rho + \eta) \right)
\]

(a) \( \delta = -0.9 \).

(b) \( \delta = 0 \).

(c) \( \delta = 0.9 \).
Gap Formation

Nonlocal system: gap formation can be shown depending also on the range of the kernel.
Nonquadratic pressure

Steady states with simply connected support solve nonlinear fixed point equation

\[ \varepsilon \rho_\infty^{m-1} = G * \rho_\infty + C[\rho_\infty] \]

Phase transition at \( m = 2 \)

For \( m > 2 \) compactly supported unique stationary solutions
For \( m < 2 \) stationary solutions with global support, nonuniqueness, no thresholding phenomenon

(mb-Fetecau-Huang 2014, Delgadino-Yao-Yan 2019)
Size Exclusion Models

Gradient flow

$$\frac{\partial \rho}{\partial t} = \nabla \cdot (\rho (1 - \rho) \nabla (E'[\rho]))$$

for entropy

$$E[\rho] = -\frac{1}{2} \int \rho G * \rho \, dx + \frac{\sigma^2}{2} \int (\rho \log \rho + (1 - \rho) \log(1 - \rho)) \, dx$$

Cluster formation and coarsening in the large time limit

Figure 1: Numerical solution of the parabolic system (1)-(4) with random initial data $g_1 \in [0.1, 0.11]$ and $\varepsilon = 10^{-4}$. 
Multispecies Model

Two-species model

$$\rho = r + b,$$

\[
\partial_t r = \nabla \cdot (\varepsilon (1 - \rho) \nabla r + \varepsilon r \nabla \rho + r (1 - \rho) [\nabla (c_{11} K * r - K * b) + \nabla V]),
\]

\[
\partial_t b = \nabla \cdot (D\varepsilon (1 - \rho) \nabla b + D\varepsilon b \nabla \rho + Db (1 - \rho) [\nabla (c_{22} K * b - K * r) + \nabla V])
\]

Global existence of bounded weak solutions by gradient flow techniques and boundedness by entropy

Convergence (along subsequences) to stationary solutions

Sobolev regularity only for total density

mb-DiFrancesco-Pietschmann-Schlake 2010

Berendsen-mb-Pietschmann 2017
Gradient flow

Formulation with diagonal mobility matrix

\[ \partial_t (r, b) = \nabla \cdot \left( M(r, b) : \nabla E'[r, b] \right) \]

\[ M(r, b) = \begin{pmatrix}
    r(1 - \rho) & 0 \\
    0 & Db(1 - \rho)
\end{pmatrix} \]

Energy functional

\[ E[\rho] = \int \left( \epsilon (\rho \log \rho + (1 - \rho) \log(1 - \rho)) + \frac{c_{11}}{2} rK \ast r + \frac{c_{22}}{2} bK \ast b - rK \ast b \right) dx \]
Two-Species Cahn-Hilliard

Defining a nonlocal Laplacian (similar Slepcev 08)

\[-\Delta_K u = u - \frac{1}{k} K * u.\]

\[k = \int_{\mathbb{R}^N} K(x) \, dx.\]

the system can be written as

\[\partial_t r = \nabla \cdot (kr(1 - \rho) \nabla (c_{11}\Delta_K r - \Delta_K b + \partial_r W(r, b)))\]

\[\partial_t b = \nabla \cdot (Dkb(1 - \rho) \nabla (c_{22}\Delta_K b - \Delta_K r + \partial_b W(r, b))))\]

with multi-well potential

\[W(r, b) = \varepsilon(r \log r + b \log b + (1 - \rho) \log(1 - \rho)) + \frac{c_{11}}{2} r^2 - rb + \frac{c_{22}}{2} b^2 - \frac{c_{11}}{2} r - \frac{c_{22}}{2} b.\]
Two-Species Cahn-Hilliard

Convergence to minimizer of the energy minimizer in the large time limit

Gamma-convergence of energy to binary model in the deep-quench limit

Multispecies (nonlocal) isoperimetric problem

Berendsen-mb-Pietschmann 2017, Berendsen-Pagliari 2018
Energy minimizers

Gamma Limit of energy

\[ E[\rho] = \int \epsilon(\rho \log \rho + (1 - \rho) \log(1 - \rho)) + \frac{c_{11}}{2} rK * r + \frac{c_{22}}{2} bK * b - rK * b \] \, dx

given by

\[ E_0[\rho] = \int \frac{c_{11}}{2} rK * r + \frac{c_{22}}{2} bK * b - rK * b \] \, dx + \chi(r, b)

With characteristic function of admissible set

\[ 0 \leq r, 0 \leq b, r + b \leq 1 \]

Cicalese-DeLuca-Novaga-Ponsiglione 2016, Berendsen-mb-Pietschmann 2017
Radially decreasing K

<table>
<thead>
<tr>
<th>general $K$</th>
<th>$-1 &lt; c_{22} \leq 0$</th>
<th>$c_{22} = -1$</th>
<th>$c_{22} &lt; -1$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$-1 &lt; c_{11} \leq 0$</td>
<td><img src="image1" alt="Diagram" /></td>
<td><img src="image2" alt="Diagram" /></td>
<td><img src="image3" alt="Diagram" /></td>
</tr>
<tr>
<td>if $(c_{11} + 1)m_1 = (c_{22} + 1)m_2$ and $K$ positive definite</td>
<td></td>
<td>if $c_{11} + c_{22} \leq -2$</td>
<td></td>
</tr>
<tr>
<td>$c_{11} = -1$</td>
<td><img src="image4" alt="Diagram" /></td>
<td><img src="image5" alt="Diagram" /></td>
<td><img src="image6" alt="Diagram" /></td>
</tr>
<tr>
<td>$c_{11} &lt; -1$</td>
<td><img src="image7" alt="Diagram" /></td>
<td><img src="image8" alt="Diagram" /></td>
<td><img src="image9" alt="Diagram" /></td>
</tr>
<tr>
<td>if $c_{11} + c_{22} \leq -2$</td>
<td></td>
<td>if $N = 1$</td>
<td></td>
</tr>
</tbody>
</table>

Cicalese-DeLuca-Novaga-Ponsiglione 2016
Radially decreasing $K$

<table>
<thead>
<tr>
<th>$K$ Coulomb</th>
<th>$-1 &lt; c_{22} \leq 0$</th>
<th>$c_{22} = -1$</th>
<th>$c_{22} &lt; -1$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$-1 &lt; c_{11} \leq 0$</td>
<td><img src="image1" alt="Image" /></td>
<td><img src="image2" alt="Image" /></td>
<td><img src="image3" alt="Image" /></td>
</tr>
<tr>
<td>$c_{11} = -1$</td>
<td><img src="image4" alt="Image" /></td>
<td><img src="image5" alt="Image" /></td>
<td><img src="image6" alt="Image" /></td>
</tr>
<tr>
<td>$c_{11} &lt; -1$</td>
<td><img src="image7" alt="Image" /></td>
<td><img src="image8" alt="Image" /></td>
<td><img src="image9" alt="Image" /></td>
</tr>
</tbody>
</table>

*Cicalese-DeLuca-Novaga-Ponsiglione 2016*
Strong self-attraction

\[ c_{11} + c_{22} < -2 \]

Intersection of support has zero Lebesgue measure

*Berendsen-mb-Pietschmann 2017*

Conjecture: union of support is a ball, each support simply connected

How are local interfaces determined?
Future: Social Network Interaction

Particles interact on a network with edges / weights changing in time

Phase separation will mean connected subclusters (echo chambers)
Macroscopic description?