On a nonlocal model of biological aggregation

Aspects of Optimal Transport in Geometry and Calculus of Variations

Dejan Slepčev

IPAM

Biological Aggregation



- Large scale collective behavior
- No leader
- Group size $\gg$ interaction length scale
- Sharp boundaries, approximately constant density

Models

- Lagrangian
- Eulerian

Recent references

- Parrish and Keshet (1999) *Science*
- Mogilner, Keshet, Bent, and Spiros (2003) *Math. Bio.*
- Okubo and Levin (Editors) (2001) *Springer*
- Burger, Capasso, and Morale (2007) *Nonlin. Anal. Real. World. Appl.*
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Continuum model

- mechanisms
  - attraction at a distance
  - local dispersal
- ρ density

Individual's velocity

$$V = V_a + V_r$$

$$V_a = \nabla(K * \rho) \qquad V_r = -\rho\nabla\rho$$

K "sensing kernel", $K \geq 0$, smooth, $\int K = 1$, $K(x) = K(|x|)$

Equation

$$\rho_t = -\nabla(\rho\nabla(K * \rho - \rho^2))$$

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$$\rho_t = -\nabla(\rho\nabla(K * \rho - \rho^2))$$

The problem

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\begin{aligned}
\rho_t - \nabla \cdot \Big(\rho \nabla \big(\frac{3}{4}\rho^2 - K * \rho\big)\Big) &= 0 && \text{on } \Omega \times (0,T) =: \Omega_T \\
\nabla\Big(\frac{3}{4}\rho^2 - K * \rho\Big) \cdot \nu &= 0 && \text{on } \partial\Omega \times (0,\infty) \\
\rho(\,\cdot\,,0) &= \rho_0 && \text{in } \Omega
\end{aligned}
$$

Theorem (existence and uniqueness)

Assume that Ω is convex. Let $\rho_0 \in L^\infty(\Omega)$, and $\rho_0 \geq 0$. There exists a unique weak solution $\rho \in L^\infty(\Omega_T)$ with $\rho^3 \in L^2(0,T,H^1(\Omega))$, $\rho_t \in L^2(0,T,H^{-1}(\Omega))$, and $\rho \in C(0,T,L^p(\Omega))$ for all $p \in [1,\infty)$.

- Related results by Burger, Capasso, and Morale and Burger and Di Francesco

Weak Solutions

The problem

$$\rho_t - \nabla \cdot \Big(\rho\nabla\big(\frac{3}{4}\rho^2 - K * \rho\big)\Big) = 0 \qquad \text{on } \Omega \times (0,T) =: \Omega_T$$

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Properties of Solutions

- The solutions are nonnegative
- Mass (i.e. L^1 norm) is preserved
- *formally:* Center of mass is preserved if $\Omega = \mathbb{R}^n$
- Energy is dissipated

Energy

$$E = \int \frac{1}{4}\rho^3 - \frac{1}{2}\rho K * \rho dx$$

Gradient flow structure

Equation

$$\rho_t = \nabla \cdot (\rho \nabla (\frac{3}{4}\rho^2 - K * \rho))$$

The equation is a gradient flow of the energy in Wasserstein metric.

Metric (inner product)

Let u_1, u_2 be tangent vectors at ρ, that is zero-mean functions

$$\langle u_1, u_2 \rangle_\rho = \int \rho \nabla p_1 \cdot \nabla p_2$$

where $\quad -\nabla \cdot (\rho \nabla p_i) = u_i \quad$ for $i = 1, 2$.

Gradient flow

$$\langle \rho_t, u \rangle_\rho = -\frac{\delta E}{\delta \rho}[u]$$

for all tangent vectors u.

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Modified energy

Energy

$$E(\rho) = \frac{1}{4}\iint K(x-y)(\rho(x)-\rho(y))^2 dxdy + \frac{1}{4}\int \rho(1-\rho)^2 dx$$

Local energy

$$E_{loc}(\rho) = \frac{1}{2}\int |\nabla\rho|^2 + \int \rho(1-\rho)^2 dx$$

- De Masi, Gobron, Pressuti (1995) *K radial, W regular*
- Bates, Fife, Ren, and Wang (1997) *W regular*
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- Fife (1997) *W of obstacle type*

Properties

- Speed is zero
- Profile is monotone
- Supported on half-plane

Traveling waves

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Gamma convergence

Let $K_\varepsilon(x) := \frac{1}{\varepsilon^n} K(\frac{x}{\varepsilon})$. Rescale space $x_{new} = \varepsilon\, x$.

Rescaled energy

$$E_\varepsilon(\rho) := \frac{1}{4\varepsilon} \iint K_\varepsilon(x-y)(\rho(x)-\rho(y))^2 dxdy + \frac{1}{\varepsilon} \int W(\rho)dx$$

Sharp interface functional

For $\chi \in BV(\Omega, \{0,1\})$

$$E_{sh}(u) := \int |\nabla \chi|$$

Gamma Convergence (Alberti and Bellettini)

$$E_\varepsilon \xrightarrow{\Gamma} E_{sh} \quad \text{as } \varepsilon \to 0$$

Minimizers of E_ε converge towards minimizers of E_{sh}.

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Sharp interface evolution

	Local	Nonlocal	Sharp
Energy	E_{loc}	E	E_{sh}
L^2	Allen–Cahn	nonlocal Allen–Cahn	$v=$mean curvature
H^{-1}	Cahn–Hilliard	nonlocal Cahn–Hilliard	Mullins–Sekerka
Wass.	thin-film eq.	bio. aggregation	Hele–Shaw

Hele–Shaw problem

$$\begin{aligned} \Delta p &= 0 && \text{in } O_t \\ p &= \kappa && \text{on } \partial O_t \\ v &= \nabla p \cdot \nu && \text{normal velocity of } \partial O_t \end{aligned}$$

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Remarks

- Using matched asymptotic expansion as in Rubinstein, Sternberg, and Keller, Pego, and Giacomin and Lebowitz one can demonstrate that Hele-Shaw problem is the sharp interface limit of the bio-aggregation equation.

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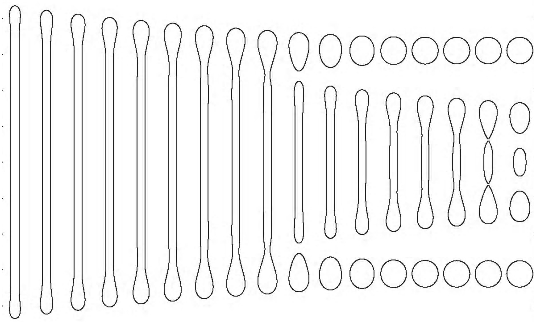
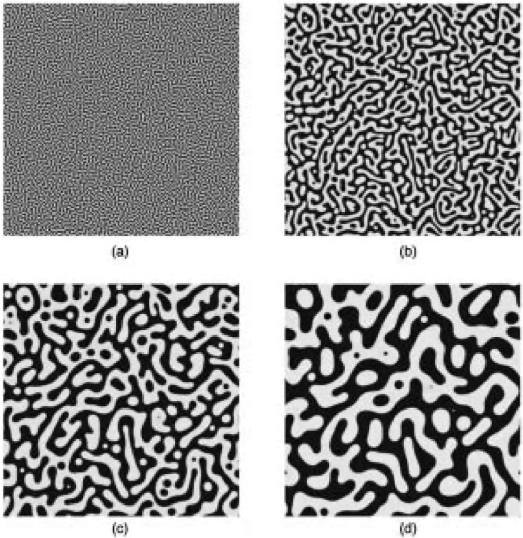


Hele–Shaw dynamics computed by Glasner (2002)

Coarsening behavior in interfacial systems



Coarsening in Cahn-Hilliard equation, computed by Zhu, Chen, Shen, and Tikare (1999)

Interfacial evolutions

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Kohn-Otto Framework

- $\overline{E} = E/|\Omega|$ — energy density
- L — an order parameter

Interpolation inequality

If $\overline{E}$ small

$$\overline{E}\,L^{\alpha} \geq C > 0$$

Dissipation relation

For example

$$(\dot{L})^2 \leq C(-\dot{\overline{E}})$$

Upper bound on coarsening rate

For T large and $\sigma \in (1, 1 + \frac{2}{\alpha})$

$$\frac{1}{T}\int_0^T \overline{E}(t)^{\sigma}\,dt > C\frac{1}{T}\int_0^T \left(t^{-\frac{\alpha}{\alpha+2}}\right)^{\sigma}\,dt$$

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Coarsening rate: related results

- Kohn and Otto *Upper bounds of coarsening rates* in Cahn–Hiliard equations 2002.
- Kohn and Yan, *Epitaxial growth*
- Kohn and Yan, *Multicomponent phase separation*
- Conti, Niethammer, and Otto *Mullins–Sekerka*
- Dai and Pego *Mean-field models of phase transitions*
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Dissipation Inequality

We choose L to be the (appropriately averaged) Wasserstein distance to $\overline{\rho}$, the average of ρ:

$$L = \frac{1}{|\Omega|^{1/2}} d_W(\rho, \overline{\rho})$$

Dissipation relation follows from gradient-flow structure:

$$\begin{aligned}
\left(\frac{dL}{dt}\right)^2 &= \frac{1}{|\Omega|}\left(\frac{d}{dt} d_W(\rho, \overline{\rho})\right)^2 \\
&\leq \frac{1}{|\Omega|}\langle \rho_t, \rho_t \rangle_\rho \\
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Interpolation Inequality

$$E = \int W(\rho)dx + \iint (\rho(x) - \rho(y))^2 K(x-y)dxdy.$$

Need to show

$$\overline{E}\, L \gtrsim 1 \quad \text{if } \overline{E} \ll 1$$

- Consider the case $\overline{\rho} = \frac{1}{2}$.
- We can assume $K = \frac{1}{\omega_n}\chi_{B(0,1)}$.
- When $\overline{E} \ll 1$ then ρ is interfacial (close to either 0 or 1 on most of Ω)
- Let $K_r(x) := \frac{1}{r^n}K(\frac{x}{r})$.
- To show $L \gtrsim l$ it suffices to show $\rho * K_l$ is interfacial
- It suffices to show that $\int |\rho - \rho * K_l|$ is small (say $< 1/64$)

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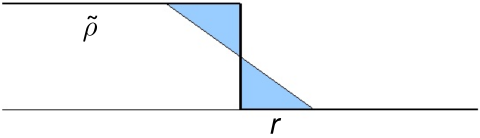
Interpolation Inequality (cont.)

Recall $K_r(x) := \frac{1}{r^n} K(\frac{x}{r})$. Let $\tilde{\rho} = \chi_{\{\rho > 7/8\}}$.

Good measure of the perimeter

$$\phi(r) := \frac{1}{|\Omega|} \int |\tilde{\rho} - K_r * \tilde{\rho}|$$



Energy bounds the perimeter

$$\phi(1) \lesssim \overline{E}$$

$$\int |\tilde{\rho} - K * \tilde{\rho}| \lesssim \int W(\rho) + \iint (\rho(x) - \rho(y))^2 K(x-y) dx dy$$

Subadditivity

We have

$$\phi(1) = \frac{1}{|\Omega|} \int |\tilde{\rho} - K * \tilde{\rho}| \lesssim \overline{E}$$

We want

$$\phi(l) = \frac{1}{|\Omega|} \int |\tilde{\rho} - K_l * \tilde{\rho}| \leq \frac{1}{64} \tag{2}$$

Subadditivity

ϕ is subadditive: $\phi(r_1 + r_2) \leq \phi(r_1) + \phi(r_2)$

and therefore $\phi(l) \lesssim l\phi(1)$

Thus (2) holds for $l \sim 1/\overline{E}$. So $L \gtrsim l \gtrsim 1/\overline{E}$.

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$$\phi(1) = \frac{1}{|\Omega|}\int |\tilde{\rho} - K * \tilde{\rho}| \lesssim \overline{E}$$

We want

$$\phi(l) = \frac{1}{|\Omega|}\int |\tilde{\rho} - K_l * \tilde{\rho}| \leq \frac{1}{64} \tag{2}$$

Subadditivity

ϕ is subadditive: $\phi(r_1 + r_2) \leq \phi(r_1) + \phi(r_2)$

and therefore $\phi(l) \lesssim l\phi(1)$

Thus (2) holds for $l \sim 1/\overline{E}$. So $L \gtrsim l \gtrsim 1/\overline{E}$.

Nonlocal Cahn–Hiliard equation

Equation:

$$\rho_t = \nabla \cdot (\mu(\rho)\nabla(\rho - K * \rho + W'(\rho))) = \nabla \cdot (\mu(\rho)\nabla(\frac{\delta E}{\delta \rho}))$$

with $\mu > 0$.

Metric (inner product)

Let u_1, u_2 be tangent vectors at ρ, that is zero-mean functions

$$\langle u_1, u_2 \rangle_\rho = \int \mu(\rho)\nabla p_1 \cdot \nabla p_2$$

$$\text{where} \qquad -\nabla \cdot (\mu(\rho)\,\nabla p_i) = u_i \qquad \text{for } i = 1, 2.$$

Gradient flow

$$\langle \rho_t, u \rangle_\rho = -\frac{\delta E}{\delta \rho}[u]$$

for all tangent vectors u.

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Gradient flow

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for all tangent vectors u.

Length L

Admissible paths between ρ_0 and ρ_1:

$$\mathcal{A}(\rho_0,\rho_1) := \Big\{(\rho, J) \ : \rho : [0,1] \to L^1(\Omega), J \in L^1(\Omega \times [0,1], \mathbb{R}^N)$$
$$\rho_t + \nabla \cdot J = 0 \quad \text{on } \Omega \times [0,1] \text{ weakly,}$$
$$\rho \in C^{weak}([0,1], L^1(\Omega))$$
$$\int_0^1 \int_\Omega \frac{1}{\mu(\rho(x,t))} |J(x,t)|^2 dxdt < \infty\Big\}.$$

Distance

$$d^2(\rho_0,\rho_1) := \inf_{(u,J)\in\mathcal{A}} \int_0^1 \int_\Omega \frac{1}{\mu(\rho(x,t))} |J(x,t)|^2 dxdt.$$

Length L

$$L(t) := d(\rho(t), \overline{\rho}) \qquad \overline{L}(t) := \frac{1}{\sqrt{|\Omega|}} d(\overline{\rho}(t), a). \tag{1}$$

Remark on local energy

Energy bounds the perimeter

$$\phi(1) \lesssim \overline{E}$$

$$\int |\tilde{\rho} - K * \tilde{\rho}| \lesssim \int W(\rho) + |\nabla \rho|^2 dx$$