

Interfacial aspects of biological aggregation

ICMS

Edinburgh

July 17, 2007.

Biological Aggregation



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

- 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

$$V = V_a + V_r$$

$$V_a = \nabla(K * \rho) \quad V_d = -\rho \nabla \rho$$

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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The problem

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

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 (2007)

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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 $-\nabla \cdot (\rho \nabla p_i) = u_i$ 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

Consider $\Omega = \mathbb{R}^n$

$$\begin{aligned}4E &= \int \rho^3 - 2\rho K * \rho dx \\ &= \int \rho^3 - 2\rho^2 dx + \iint (\rho(x) - \rho(y))^2 K(x-y) dx dy \\ &= \iint K(x-y)(\rho(x) - \rho(y))^2 dx dy + \int \rho(1 - \rho)^2 dx\end{aligned}$$

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Modified energy

Consider $\Omega = \mathbb{R}^n$

$$\begin{aligned}4E &= \int \rho^3 - 2\rho K * \rho dx - \int \rho dx \\ &= \int \rho^3 - 2\rho^2 - \rho dx + \iint (\rho(x) - \rho(y))^2 K(x - y) dx dy \\ &= \iint K(x - y) (\rho(x) - \rho(y))^2 dx dy + \int \rho(1 - \rho)^2 dx\end{aligned}$$

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

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Traveling waves

- 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

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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

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

Sharp interface functional

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

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

Gamma Convergence (Alberti and Bellettini)

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

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

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

Sharp interface evolution

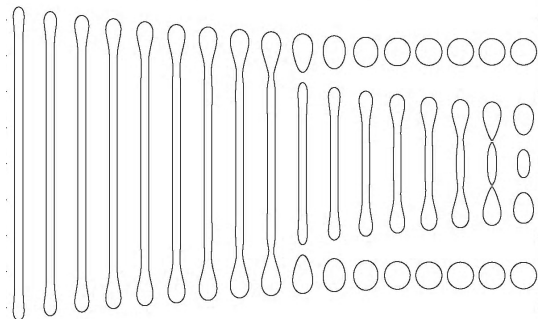
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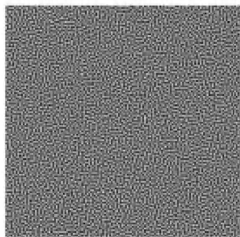
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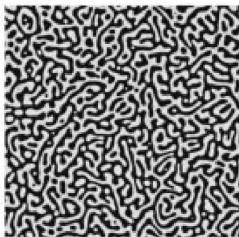


Hele-Shaw dynamics
computed by Glasner
(2002)

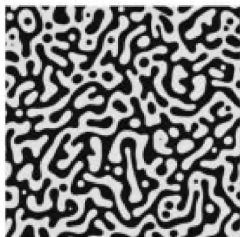
Coarsening behavior in interfacial systems



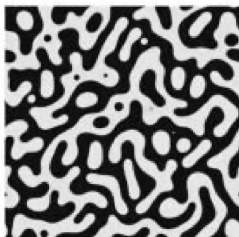
(a)



(b)



(c)



(d)

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

Interfacial evolutions

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Kohn-Otto Framework

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

Interpolation inequality

If \bar{E} small

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

Dissipation relation

For example

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

Upper bound on coarsening rate

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

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

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Coarsening rate: related results

- Kohn and Otto *Upper bounds of coarsening rates in Cahn–Hilliard equations* 2002.
- Kohn and Yan, *Epitaxial growth*
- Kohn and Yan, *Multicomponent phase separation*
- Conti, Niethammer, and Otto *Mullins–Sekerka*
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Dissipation Inequality

We choose L to be the (appropriately averaged) Wasserstein distance to $\bar{\rho}$:

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

Dissipation relation follows from gradient-flow structure:

$$\begin{aligned} \left(\frac{dL}{dt}\right)^2 &= \frac{1}{|\Omega|} \left(\frac{dd_W(\rho, \bar{\rho})}{dt}\right)^2 \\ &\leq \frac{1}{|\Omega|} \langle \rho_t, \rho_t \rangle_\rho \end{aligned}$$

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Interpolation Inequality

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

Need to show

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

- We can assume $K = \frac{1}{\omega_n} \chi_{B(0,1)}$.
- When $\bar{E} \ll 1$ then ρ is interfacial (close to either 0 or 1 on most of Ω)
- To show $L \gtrsim 1$ it suffices to show $\rho * K_l$ is interfacial
- It suffices to show that $\int |\rho - \rho * K_l|$ is small

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Interpolation Inequality (cont.)

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

Good measure of the perimeter

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

Then $\phi(1)$ is a measure of "perimeter density".

Energy bounds the perimeter

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

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

Remark: The bound holds $E = \int W(\rho) + |\nabla \rho|^2$ as well.

Interpolation Inequality (cont.)

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Subadditivity

We have

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

We want

$$\phi(l) = \frac{1}{|\Omega|} \int |\tilde{\rho} - K_l * \tilde{\rho}| \lesssim \frac{1}{4} \quad (2)$$

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 $l \sim 1/\bar{E}$. So $L \gtrsim l \gtrsim 1/\bar{E}$.

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