Interaction-Driven Dynamics for Collective Behavior: Derivation, Model Hierarchies and Pattern Stability

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Outline

Energy, Gradient and Evolution equation

The heat equation $\rho_t = \Delta\rho$ is a gradient flow:

- $E[\rho] = \frac{1}{2}\int |\nabla\rho|^2$

$$\langle \rho_t, v\rangle_{L^2} = -\left\langle \frac{\delta E}{\delta\rho}, v\right\rangle_{L^2}$$

  See also Allen-Cahn equation $\rho_t = \Delta\rho - \rho^3 + \rho$

- $E[\rho] = \frac{1}{2}\int |\rho|^2$

$$\langle \rho_t, v\rangle_{H^{-1}} = -\left\langle \frac{\delta E}{\delta\rho}, v\right\rangle_{L^2}$$

  See also Cahn-Hilliard equation $\rho_t = \Delta(-\Delta\rho + \rho^3 - \rho)$

- $E[\rho] = \int \rho \log\rho$

$$\langle \rho_t, v\rangle_{\rho} = -\left\langle \frac{\delta E}{\delta\rho}, v\right\rangle_{L^2}$$

  where

$$\langle \rho_t, v\rangle_{\rho} = \int \rho\nabla p_1 \cdot \nabla p_2, \quad -\nabla\cdot(\rho\nabla p_i) = s_i, \ i = 1, 2.$$

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The equation $\rho_t = \nabla \cdot \left(\rho \nabla \frac{\delta E}{\delta \rho} \right)$

a) Heat $\rho_t = \Delta \rho$ or porous medium equation $\rho_t = \Delta \rho^m, (m \neq 1)$

$$E = \int \rho(\log \rho - 1) \quad \text{or} \quad E = \tfrac{m}{m-1} \int \rho^m (m \neq 1)$$

b) Fokker-Planck equation $\rho_t = \Delta \rho + \nabla \cdot (\rho \nabla V)$

$$E = \int \rho(\log \rho - 1) + \tfrac{1}{2} \int \rho V$$

c) Keller-Segel: $\rho_t = \Delta \rho - \nabla \cdot (\rho \nabla c)$, $c = (-\Delta)^{-1} \rho$

$$E = \int \rho(\log \rho - 1) + \tfrac{1}{2} \int \rho (-\Delta)^{-1} \rho$$

d) Granular flow or aggregation equation $\rho_t = \nabla \cdot (\rho \nabla U * \rho)$

$$E = \tfrac{1}{2} \iint U(x-y) \rho(x) \rho(y) \, dy dx$$

e) $\vdots$

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Equation with gradient flow structure

The energy

$$E[\rho] = \underbrace{\int H(\rho)}_{\text{internal energy}} + \underbrace{\int \rho V}_{\text{potential energy}} + \underbrace{\frac{1}{2}\iint U(x-y)\rho(x)\rho(y)}_{\text{interaction energy}}$$

and the equation

$$\rho_t = \nabla \cdot (\rho \nabla (H'(\rho) + V + U * \rho)).$$

The theory:

- Gradient flow
- Optimal transport
- Functional inequalities
- Qualitative behaviours of the equation
- $\vdots$

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Essential features:

- Conservation of the total mass
- Non-negativity of the solution
- The energy (or entropy) $E[\rho]$ is non-increasing:

$$\frac{dE}{dt} = -\int \rho |\nabla \xi|^2, \quad \xi = \frac{\delta E}{\delta \rho} = H'(\rho) + V + U * \rho.$$

- Characterization of steady states:

$$H'(\rho) + V + U * \rho = C, \qquad \text{on supp}\rho.$$

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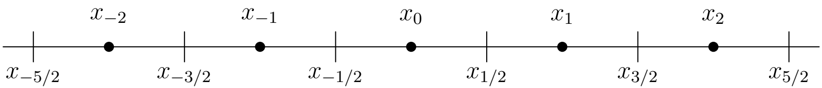
The cell-centred Finite Volume Method in 1D

The uniform grid with spacing Δx



and the cell average

$$\overline{\rho}_j(t) = \frac{1}{\Delta x}\int_{x_{j-1/2}}^{x_{j+1/2}} \rho(x,t)\,dx.$$

Fact: for smooth functions,

cell average $\approx$ **evaluation at the cell centre**

$$\Longrightarrow \qquad \overline{\rho}_j(t) \approx \rho(x_j,t), \quad \frac{1}{\Delta x}\int_{x_{j-1/2}}^{x_{j+1/2}} H(\rho(x,t))\,dx \approx H(\overline{\rho}_j(t)), \cdots$$

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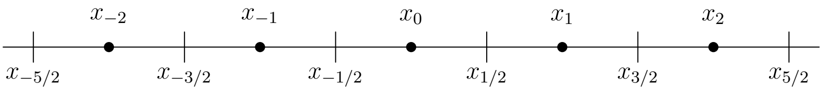

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The cell-centred Finite Volume Method in 1D

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$$\frac{d\overline{\rho}_j(t)}{dt} = \frac{1}{\Delta x}\int_{x_{j-1/2}}^{x_{j+1/2}} \rho_t(x,t)\,dx = -\frac{F_{j+1/2} - F_{j-1/2}}{\Delta x}.$$

The numerical flux $F_{j+1/2}$ is an approximation of $-\rho\xi_x$ at $x_{j+1/2}$.

Non-negativity: "upwind" numerical flux $F_{j+1/2}$+CFL condition.

$$F_{j+1/2} \approx -\rho\Big|_{x_{j+1/2}} \frac{\xi_{j+1} - \xi_j}{\Delta x} := \rho\Big|_{x_{j+1/2}} u_{j+1/2}.$$

with $u_{j+1/2} = -\frac{\xi_{j+1}-\xi_j}{\Delta x}$. Then

$$F_{j+1/2} = \begin{cases} u^+_{j+1/2}\overline{\rho}_j + u^-_{j+1/2}\overline{\rho}_{j+1}, & \text{(first order scheme)}, \\ u^+_{j+1/2}\rho^E_j + u^-_{j+1/2}\rho^W_{j+1}, & \text{(second order scheme)} \end{cases}$$

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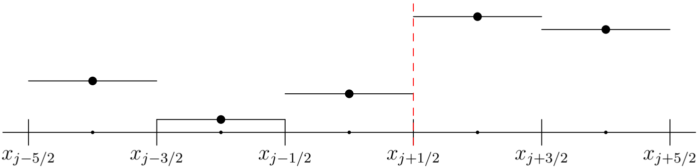
Reconstruction of ρ at $x_{j+1/2}$



Minmod reconstruction: $\tilde{\rho}_j(x) = \overline{\rho}_j + (\rho_x)_j(x - x_j)$

$$(\rho_x)_j = \text{minmod}\left(\theta\,\frac{\overline{\rho}_{j+1} - \overline{\rho}_j}{\Delta x},\ \frac{\overline{\rho}_{j+1} - \overline{\rho}_{j-1}}{2\Delta x},\ \theta\,\frac{\overline{\rho}_j - \overline{\rho}_{j-1}}{\Delta x}\right),$$

where

$$\text{minmod}(z_1, z_2, \ldots) := \begin{cases} \min(z_1, z_2, \ldots), & \text{if } z_i > 0 \quad \forall\ i, \\ \max(z_1, z_2, \ldots), & \text{if } z_i < 0 \quad \forall\ i, \\ 0, & \text{otherwise}, \end{cases}$$

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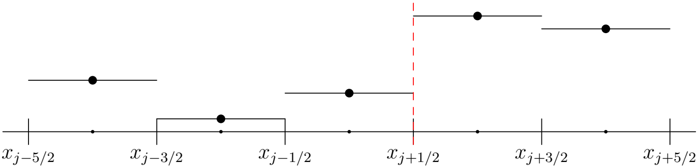

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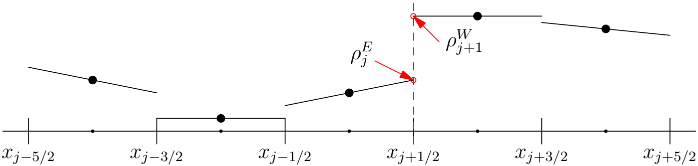
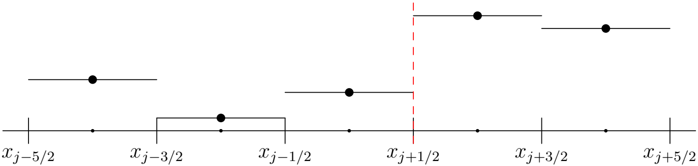


$$\rho_j^E = \overline{\rho}_j + \frac{\Delta x}{2}(\rho_x)_j, \quad \rho_{j+1}^W = \overline{\rho}_{j+1} - \frac{\Delta x}{2}(\rho_x)_{j+1}.$$

Approximation of ξ_j in $F_{j+1/2} \approx -\rho\big|_{x_{j+1/2}} \frac{\xi_{j+1}-\xi_j}{\Delta x} := \rho\big|_{x_{j+1/2}} u_{j+1/2}$

$$\xi = \frac{\delta E}{\delta \rho} = H'(\rho) + V + U * \rho.$$



$$\begin{aligned}
\xi_j \approx \xi|_{x_j} &= H'(\overline{\rho}_j) + V(x_j) + \int U(x_j - y)\rho(y)\,dy \\
&= H'(\overline{\rho}_j) + V(x_j) + \sum_i \overline{\rho}_i \int_{x_{i-1/2}}^{x_{i+1/2}} U(x_j - y)\,dy \\
&= H'(\overline{\rho}_j) + V(x_j) + \sum_i \overline{\rho}_i U_{j-i}
\end{aligned}$$

with $U_j = \int_{x_{j-1/2}}^{x_{j+1/2}} U(y)\,dy.$

Discrete energy

Energy and Discrete energy

$$E[\rho] = \int H(\rho) + \int \rho V + \frac{1}{2} \iint U(x-y)\rho(x)\rho(y).$$

$$E_\Delta[\overline{\rho}] = \Delta x \sum_j \left[H(\overline{\rho}_j) + V_j \overline{\rho}_j + \frac{1}{2} \Delta x \sum_i U_{j-i} \overline{\rho}_i \overline{\rho}_j \right]$$

where $U_j = \int_{x_{j-1/2}}^{x_{j+1/2}} U(y)\,dy$.

Notice that

$$\xi_j = \frac{\partial E_\Delta}{\partial(\overline{\rho}_j \Delta x)} = H'(\overline{\rho}_j) + V(x_j) + \sum_k \overline{\rho}_k U_{j-k}.$$

Discrete energy dissipation

Energy dissipation

$$\frac{d}{dt}E[\rho] = -\int \rho|\nabla\xi|^2.$$

$$\begin{aligned}\frac{d}{dt}E_\Delta(t) = \Delta x \sum_j \xi_j \frac{d\overline{\rho}_j}{dt} &= -\Delta x \sum_j \xi_j \frac{F_{j+\frac{1}{2}} - F_{j-\frac{1}{2}}}{\Delta x} \\ &= -\Delta x \sum_j u_{j+\frac{1}{2}} \left[u^+_{j+\frac{1}{2}}\rho^{\mathrm{E}}_j + u^-_{j+\frac{1}{2}}\rho^{\mathrm{W}}_{j+1}\right] \\ &\leq -\Delta x \sum_j (u_{j+\frac{1}{2}})^2 \min_j(\rho^{\mathrm{E}}_j, \rho^{\mathrm{W}}_{j+1})\end{aligned}$$

$\Longrightarrow$ Discrete energy inequality with rate

$$I_\Delta = \Delta x \sum_j (u_{j+\frac{1}{2}})^2 \min_j(\rho^{\mathrm{E}}_j, \rho^{\mathrm{W}}_{j+1}).$$

A few remarks

- CFL condition for the fully discrete scheme:

$$\Delta t \leq \frac{\Delta x}{2} \frac{1}{\max_j u^+_{j+1/2} - u^-_{j+1/2}}.$$

- Strong-stability-preserving ODE solver [1]
- The accuracy of the approximation

$$\int_{x_{i-1/2}}^{x_{i+1/2}} U(x_j - y)\rho(y)\,dy \approx \rho_i \int_{x_{i-1/2}}^{x_{i+1/2}} U(x_j - y)\,dy$$

- Stabilization using diffusion
- Extension to non-uniform or unstructured grid
- Extension to higher (spatial) order
- Extension to DG methods

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Example: Generalized Keller-Segel in 1D

$$\rho_t = \nabla \cdot \left(\rho \nabla (\nu \rho^{m-1} + U * \rho\right), \quad U(x) = |x|^\alpha / \alpha.$$

and

$$E[\rho] = \frac{\nu}{m} \int \rho^m + \frac{1}{\alpha} \iint |x-y|^\alpha \rho(x)\rho(y).$$

Different regimes classified by the mass invariant scaling $\rho \to \lambda^d \rho(\lambda x)$:

- Diffusion-dominated regime: $m > (d-\alpha)/d$
- Balanced regime: $m = (d-\alpha)/d$
- Aggregation-dominated regime: $m < (d-\alpha)/d$

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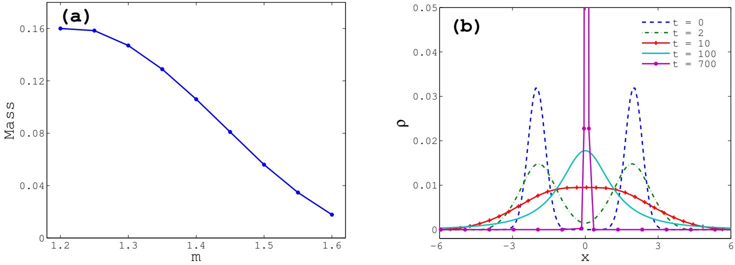

a) The critical mass in the balance regime $m + \alpha = 1$ (in 1D) and $\nu = 1$. **b)** Blowup in the balanced regime when the initial mass is slightly larger than the critical mass.

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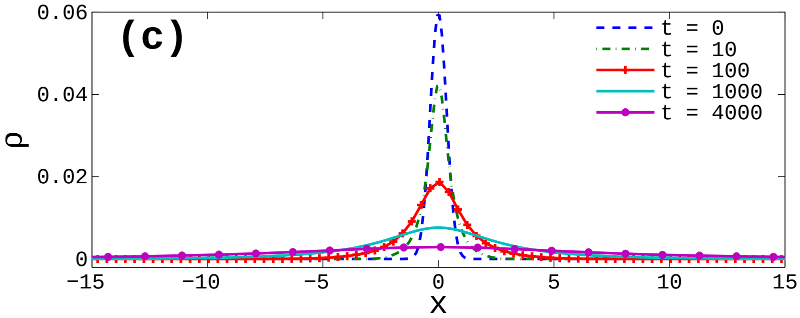
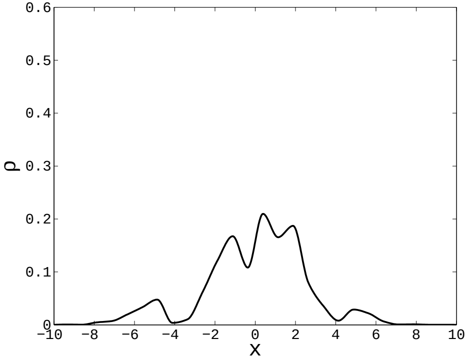


c) Decay to zero in the balance regime when the initial mass is slightly smaller than the critical mass ($m = 1.5$, $M_0 = 0.053 < M_c = 0.055$).

Example: Aggregation with degenerate diffusion in 1D

$$\rho_t = (\rho(\nu\rho^{m-1})_x)_x + (\rho(U * \rho)_x)_x.$$

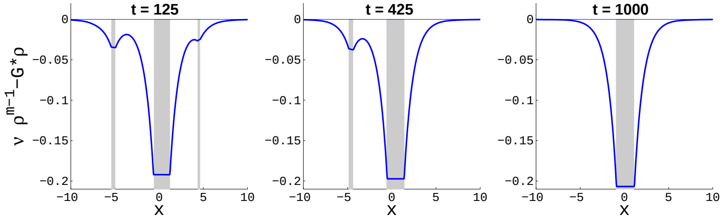


Example: Aggregation with degenerate diffusion in 1D

During the metastable stage, the solution to

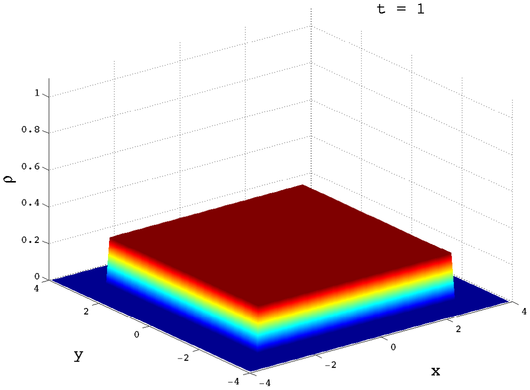
$$\rho_t = (\rho(\nu\rho^{m-1})_x)_x - (\rho(G * \rho)_x)_x$$

is almost steady on the support, or $\xi = \nu\nu\rho^{m-1} - G * \rho$ is close to a constant.



Example: Aggregation with degenerate diffusion in 2D

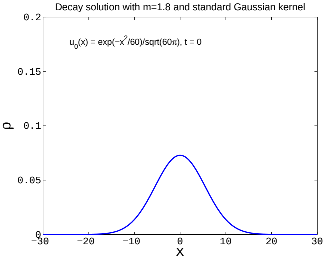
$$\rho_t = \nu \Delta \rho^m - \nabla \cdot (\rho \nabla G * \rho), \quad G(x) = \frac{1}{2\pi} e^{-|x|^2/2}.$$

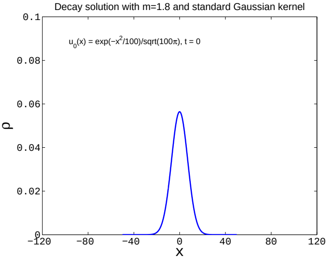


Example: Aggregation with degenerate diffusion in 1D

$$\rho_t = (\rho(\nu\rho^{m-1})_x)_x - (\rho(G*\rho)_x)_x$$

Bifurcation in steady states and decay solutions [2] for $1 < m < 2$:



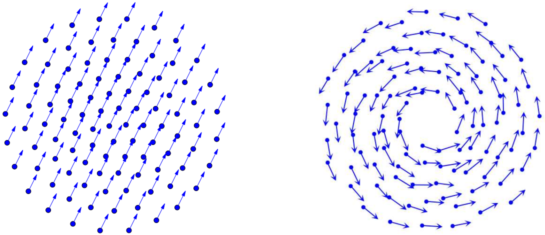


[2] M. Burger, R. Fetecau and Y. Huang, SIAM J. Appl. Dyn. Syst., 2014

Example: Flock and mill density

The particle system:

$$\frac{dx_i}{dt} = v_i \,,$$
$$\frac{dv_i}{dt} = \alpha v_i - \beta v_i |v_i|^2 - \frac{1}{N} \nabla_{x_i} \sum_{j \neq i} U(x_i - x_j) \,.$$

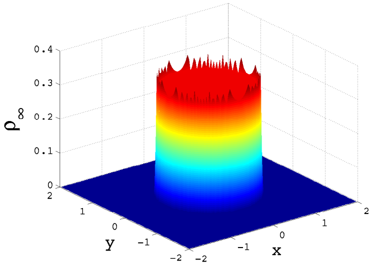


Equation for the flock or mill pattern:

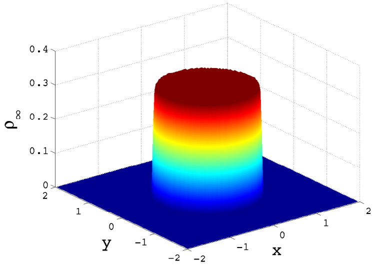
$$\rho_t = \nabla \cdot (\rho \nabla U * \rho) \qquad \rho_t = \nabla \cdot \left(\rho \nabla \left(U * \rho - \frac{\alpha}{\beta} \ln |x| \right) \right)$$

Example: Flock density with degenerate diffusion

$$\rho_t = \nabla \cdot (\rho \nabla U * \rho) + \epsilon \nabla \cdot (\rho \nabla \rho), \quad U(x) = |x|^2/2 - \ln |x|.$$



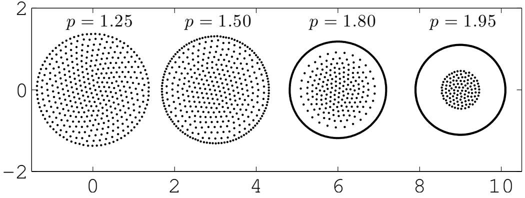
$\epsilon = 0$

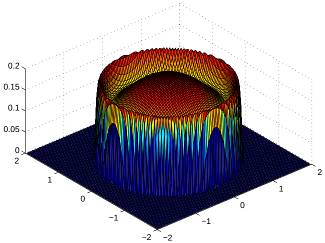


$\epsilon = 0.4(\Delta x^2 + \Delta y^2)$

Example: Flock density

$$U(r) = Ce^{-(r/\ell)^p/p} - e^{-r^p/p}, \quad C = 10/9, \ell = 3/4.$$





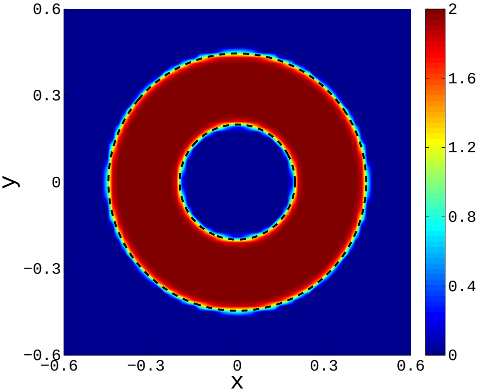
$$\rho_t = \nabla \cdot (\rho \nabla U * \rho) + \epsilon \nabla \cdot (\rho \nabla \rho),$$

$$p = 1.25, \epsilon = 0.4(\Delta x^2 + \Delta y^2).$$

Example: Mill density

$$\rho_t = \nabla \cdot \left(\rho \nabla \left(U * \rho - \frac{\alpha}{\beta} \ln |x|\right)\right) + \epsilon \nabla \cdot (\rho \nabla \rho),$$

$$U(x) = |x|^2/2 - \ln |x|, \quad \epsilon = 0.4(\Delta x^2 + \Delta y^2)$$



Conclusions

- Γ-convergence techniques are a good tool to produce accurate deterministic particle schemes for aggregation-diffusion problems.
- Finite volume schemes preserving the entropy decreasing character can be used to understand numerically many interesting features of the evolutions.
- References:
  1. C.-Chertock-Huang (CCP 2014).
  2. C.-Huang-Patacchini-Wolansky (in preparation).
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