Gradient Flows: Qualitative Properties & Numerical Schemes

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Outline

1. Gradient Flows
   - Models
   - Gradient flows
   - Evolving diffeomorphisms
2. Numerical schemes
   - Explicit/Implicit-in-time discretization
   - Initialization & Full Algorithm
3. 2D Simulations
   - Diffusions
   - Merging
   - Blow-up

Outline

Nonlinear continuity equations

Let us consider a time dependent unknown probability density $\rho(t,\cdot)$ on a domain $\Omega \subset \mathbb{R}^d$, which satisfies the nonlinear continuity equation

$$\partial_t \rho = -\nabla \cdot (\rho u) := \nabla \cdot \left(\rho \nabla \left[U'(\rho) + V + W * \rho \right] \right).$$

- $U : \mathbb{R}^+ \to \mathbb{R}$ denotes the internal energy.
- $V : \mathbb{R}^d \to \mathbb{R}$ is the confining potential.
- $W : \mathbb{R}^d \to \mathbb{R}$ corresponds to an interaction potential.

Nonlinear velocity is given by $u = -\nabla \frac{\delta \mathcal{F}}{\delta \rho}$, where $\mathcal{F}$ denotes the free energy or entropy functional

$$\mathcal{F}(\rho) = \int_{\mathbb{R}^d} U(\rho) dx + \int_{\mathbb{R}^d} V(x)\rho(x) dx + \frac{1}{2} \int_{\mathbb{R}^d \times \mathbb{R}^d} W(x-y)\rho(x)\rho(y) dx dy.$$

Free energy is decreasing along trajectories

$$\frac{d}{dt} \mathcal{F}(\rho)(t) = -\int_{\mathbb{R}^d} \rho(x,t) |u(x,t)|^2 dx.$$

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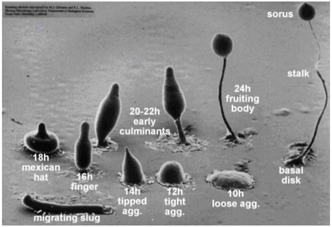
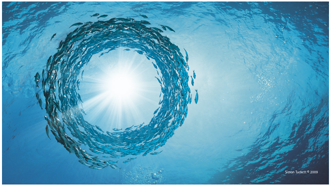
Nonlinear continuity equations

Included models:

- $U(s) = s \log s$, $V = 0$, $W = 0$ heat equation.
- $U(s) = \frac{1}{m-1} s^m$, $V = W = 0$ porous medium ($m > 1$) or fast diffusion ($0 < m < 1$).
- $U(s) = s \log s$, V given, $W = 0$, Fokker Planck equations.
- $U(s) = s \log s$, $V = 0$, W given, Patlak-Keller-Segel model.
- $U = 0$, $V = 0$, $W = \log(-|x|)$ or $W = \frac{1}{2}|x|^2 - \frac{1}{4}|x|^4$ correspond to attraction-(repulsion) potentials in swarming, herding and aggregation models.



(a) Dictyostelium discoideum



(b) Fish school

Outline

Gradient flow formalism[1]

- Solutions ρ can be constructed by the following variational scheme:

$$\rho_{\Delta t}^{n+1} \in \arg\inf_{\rho\in\mathcal{K}} \left\{ \frac{1}{2\Delta t} d_2^2(\rho_{\Delta t}^n, \rho) + \mathcal{F}(\rho) \right\},$$

with $\mathcal{K} = \{\rho \in L_+^1(\mathbb{R}^d) : \int_{\mathbb{R}^d} \rho(x)dx = M, |x|^2\rho \in L^1(\mathbb{R}^d)\}$.

- Quadratic Euclidean Wasserstein distance d_W between two probability measures μ and ν,

$$d_2^2(\mu,\nu) := \inf_{T:\nu=T\#\mu} \int_{\mathbb{R}^d} |x - T(x)|^2 d\mu(x).$$

- Variational scheme corresponds to the time discretization of an abstract gradient flow in the space of probability measures.
- Solutions can be constructed by this variational scheme; naturally preserve positivity and the free-energy decreasing property.

[1] Jordan, Kinderlehrer and Otto (1999); Otto (1996, 2001); Ambrosio, Gigli and Savare (2005); Villani(2003).....

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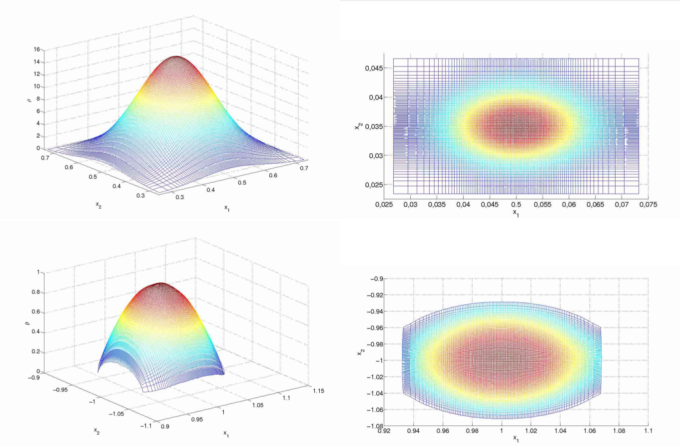
Gradient flow formalism

For a given diffeomorphism $\Phi \in \mathcal{D}$ the corresponding density $\rho \in \mathcal{K}$ is given by

$$\rho = \Phi \# \mathcal{L}^d \llcorner_\Omega \quad \text{which is equivalent to } \rho(\Phi(x)) \det(D\Phi) = 1 \text{ on } \Omega$$

for sufficiently smooth functions.



Gradient flow formalism

- Let Ω and $\tilde{\Omega}$ be smooth, open, bounded and connected subsets of $\mathbb{R}^d$. We denote by $\Phi \in \mathcal{D}$ the set of diffeomorphisms from $\bar{\Omega}$ to $\bar{\tilde{\Omega}}$ (mapping $\partial\Omega$ onto $\partial\tilde{\Omega}$).
- Doing the change of variables by the diffeomorphism $\rho = \Phi \# \mathcal{L}^d$, we get

$$\mathcal{I}(\Phi) = \int_\Omega \Psi(\det D\Phi)dx + \int_\Omega V(\Phi(x))dx + \frac{1}{2}\int_\Omega\int_\Omega W(\Phi(x) - \Phi(y))dxdy.$$

with $\Psi(s) = s\,U(1/s)$ for all $s > 0$.

Classic L^2-gradient flow: Evans, Savin and Gangbo (2004)

$$\Phi^{n+1}_{\Delta t} \in \arg\inf_{\Phi\in\mathcal{D}} \left\{ \frac{1}{2\Delta t}\|\Phi^n_{\Delta t} - \Phi\|^2_{L^2(\Omega)} + \mathcal{I}(\Phi) \right\}$$

converges to solutions of the PDE

$$\begin{aligned}\frac{\partial \Phi}{\partial t} &:= u(t) \star \Phi \\ &= \nabla \cdot [\Psi'(\det D\Phi)(\operatorname{cof} D\Phi)^T] - \nabla V \circ \Phi - \int_\Omega \nabla W(\Phi(x) - \Phi(y))dy,\end{aligned}$$

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Generalization of Gradient flow formalism

Let us denote by $c(x,y) : \mathbb{R}^d \times \mathbb{R}^d \longrightarrow \mathbb{R}^+$ with c is radially symmetric as $c(x,y) = c(x-y) = c(|x-y|)$.

Generalized gradient flow

Several authors (Agueh, Ambrosio-Gigli-Savaré, McCann-Puel) proved for different costs that the scheme

$$\rho_{\Delta t}^{n+1} \in \arg\inf_{\rho\in\mathcal{K}_c} \left\{ \Delta t \inf_{\Pi\in\Gamma(\rho_{\Delta t}^n,\, \rho)} \left\{ \int_{\mathbb{R}^d\times\mathbb{R}^d} c\left(\frac{x-y}{\Delta t}\right) d\Pi(x,y) \right\} + \mathcal{F}(\rho) \right\},$$

where $\Gamma(\rho_{\Delta t}^n, \rho)$ is the set of measures in the product space $\mathbb{R}^d \times \mathbb{R}^d$ with marginals $\rho_{\Delta t}^n$ and ρ respectively, is convergent to a solution of the PDE

$$\frac{\partial \rho}{\partial t} = -\nabla\cdot(\rho u_c) := \nabla\cdot\left\{\rho\nabla c^*\left[\nabla\left(U'(\rho) + V + W*\rho\right)\right]\right\},$$

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Generalization of Gradient flow formalism

The p-Laplacian equation and the doubly nonlinear equation.-

$$\frac{\partial \rho}{\partial t} = \nabla \cdot \left[|\nabla \rho^m|^{p-2} \nabla \rho^m \right],$$

with $1 < p < \infty$, $m \geq m_c := \frac{d-p}{d(p-1)}$. The cost is given by $c(x) = |x|^q/q$ with q the conjugate exponent of p and the internal energy given by

$$U(s) = \begin{cases} \dfrac{1}{p-1} s \ln s & \text{if} \quad m = \dfrac{1}{p-1} \\[2ex] \dfrac{ms^\gamma}{\gamma(\gamma-1)}, \ \gamma = m + \dfrac{p-2}{p-1} & \text{if} \quad m \neq \dfrac{1}{p-1}. \end{cases}$$

Generalization of Gradient flow formalism

The relativistic heat equation.-

$$\frac{\partial \rho}{\partial t} = \nabla \cdot \left(\rho \frac{\nabla \rho}{\sqrt{\rho^2 + |\nabla \rho|^2}} \right) = \nabla \cdot \left(\rho \frac{\nabla \log \rho}{\sqrt{1 + |\nabla \log \rho|^2}} \right).$$

Here, the cost function is given by

$$c(x) = \begin{cases} 1 - \sqrt{1 - |x|^2} & \text{if } |x| \leq 1 \\ +\infty & \text{if } |x| > 1. \end{cases},$$

with $c^*(x) = \sqrt{1 + |x|^2} - 1$ and the logarithmic entropy functional.

Lagrangian Coordinates

- PDE for the evolving diffeomorphisms Φ is the Lagrangian coordinate representation of the original Eulerian formulation for ρ, in 1D it is the monotone rearrangement.
- Heat equation

$$\frac{\partial \rho}{\partial t} = \rho_{xx} \quad \Rightarrow \quad \frac{\partial \Phi}{\partial t} = -\frac{\partial}{\partial x}\left(\frac{1}{\Phi_x}\right) = \frac{\Phi_{xx}}{(\Phi_x)^2},$$

- Porous medium equation

$$\frac{\partial \rho}{\partial t} = \partial_{xx}(\rho^m) \quad \Rightarrow \quad \frac{\partial \Phi}{\partial t} = -\frac{\partial}{\partial x}\left(\frac{1}{(\Phi_x)^m}\right) = m\frac{\Phi_{xx}}{(\Phi_x)^{m+1}}.$$

- Relativistic heat equation

$$\rho_t = \left(\rho \frac{\rho_x}{\sqrt{\rho^2 + |\rho_x|^2}}\right)_x \quad \Rightarrow \quad \Phi_t = \left(\frac{\Phi_x}{\sqrt{\Phi^4 + |\Phi_x|^2}}\right)_x.$$

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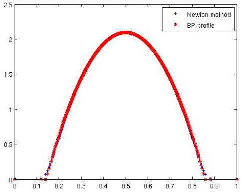
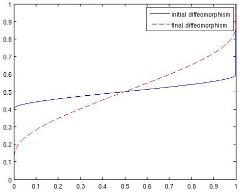
1D Diffusion: Simulations

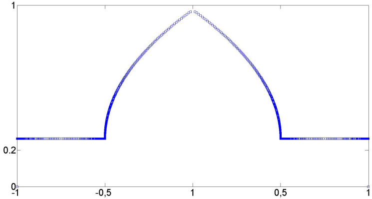
1D simulation of the PME for $m = 2$ and the relativistic equation:

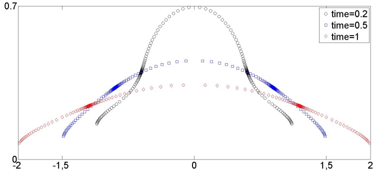


(c) Density ρ

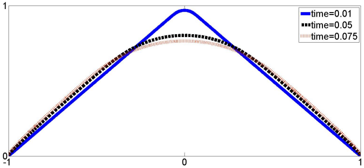


(d) Diffeomorphism Φ





$m \neq 1$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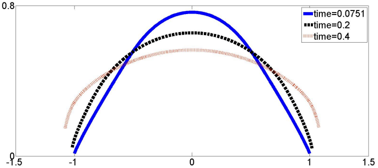
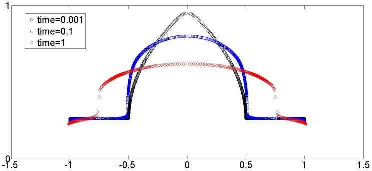
time=0.05
time=0.075
1
0
-1
0
1


time=0.0751
time=0.2
time=0.4
0.8
0
-1.5
-1
0
1
1.5


time=0.001
time=0.1
time=1
1
0
-1.5
-1
-0.5
0
0.5
1
1.5

Why do we make our life so much harder ?

- Automatic mesh adaptation and mesh merging in regions of high density.
- A Dirac Delta corresponds to a degeneration of the transport map - numerically more tractable than blow-up for densities.
- Energy dissipation and positivity.

Entropy Dissipation in a bounded domain for Φ:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{I}(\Phi(t)) = -\int_{\Omega} |u(t) * \Phi|^2 \,\mathrm{d}x - \int_{\partial\Omega} \Psi'(\det D\Phi)\, \eta^T (\operatorname{cof} D\Phi)^T \frac{\partial \Phi}{\partial t}\, \mathrm{d}x$$

from which, we conclude that the natural boundary condition associated to the variational scheme for Φ is:

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Boundary conditions

- BC's in Lagrangian formulation are

$$n^T(\operatorname{cof} D\Phi)^T \frac{\partial \Phi}{\partial t} = (\operatorname{cof} D\Phi) n \cdot \frac{\partial \Phi}{\partial t} = 0.$$

- On the square $\Omega = [-1,1]^2$ these boundary conditions translate to

$$\frac{\partial \Phi_1}{\partial t}\frac{\partial \Phi_2}{\partial x_2} - \frac{\partial \Phi_2}{\partial t}\frac{\partial \Phi_2}{\partial x_1} = 0 \text{ for } x_1 = -1, x_1 = 1$$
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- Consider only diffeomorphisms which map each edge of $\partial\Omega$ to the corresponding one of $\partial\tilde{\Omega}$ without rotation. This reduces to

$$\Phi_1(t,\pm 1) = \pm 1 \qquad \frac{\partial \Phi_2}{\partial t}\frac{\partial \Phi_2}{\partial x_1} = 0 \text{ for } x_1 = \pm 1$$
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Outline

Implicit Euler scheme: Minimization then discretization

$$\frac{\Phi^{n+1}-\Phi^n}{\Delta t} = \nabla\cdot[\Psi'(\det D\Phi^{n+1})(\operatorname{cof} D\Phi^{n+1})^T] + \nabla V\circ\Phi^{n+1} + \int \nabla W(\Phi^{n+1}(x)-\Phi^{n+1}(y))dy$$

- Conforming finite element discretization

$$\begin{aligned} F(\Phi^{n+1},\varphi) = \frac{1}{\Delta t}\int_\Omega(\Phi^{n+1}-\Phi^n)\varphi(x)dx - \int \nabla V(\Phi^{n+1})\varphi(x)dx \\ - \int_\Omega\left[\int_\Omega \nabla W(\Phi^{n+1}(x)-\Phi^{n+1}(y))dy\right]\varphi(x)dx \\ + \int_\Omega \Psi'(\det D\Phi^{n+1})(\operatorname{cof} D\Phi^{n+1})^T\nabla\varphi(x)dx. \end{aligned}$$

- One can use the lowest order H^1 conforming finite elements, i.e.

$$\Phi(x_1,x_2) = \sum_k \begin{pmatrix}\Phi_k^1\\ \Phi_k^2\end{pmatrix}\varphi_k(x_1,x_2).$$

(work in preparation with Ranetbauer and Wolfram - locals!, wait for next week)

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- Full discretization by finite differences and quadrature formulas for the derivatives and integral for interactions, (C.-Moll, SISC 2009).
- To avoid problems at the boundaries with approximation with second derivatives, we need to be careful.

Let us consider a discretization $\Phi_{i,j}$ on a uniform symmetric cartesian grid $\Omega = [-1,1]^2$ of Φ with mesh sizes $\Delta x = \Delta x_1 = \Delta x_2 = 2/N$. Let us introduce the following notations

$$(D^{\leftarrow}\Phi)_{i,j} = \frac{1}{\Delta x}(\Phi_{i,j}-\Phi_{i-1,j}) \;,\; (D^{\rightarrow}\Phi)_{i,j} = \frac{1}{\Delta x}(\Phi_{i+1,j}-\Phi_{i,j})$$

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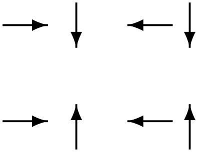

Figure : Schematic representation of the order of derivatives approximation.

Since for compactly supported densities, we have $\det(D\Phi) \to +\infty$ at the boundary, we impose that

$$\Psi'(\det D\Phi)\frac{\partial \Phi_2}{\partial x_2} = 0 \text{ for } x_1 = \pm 1 ,$$

which reflects that $\Psi'(+\infty) = 0$.
Let us remark that the condition $\Psi'(\infty) = 0$ is equivalent to $f(0+) = 0$ with $f(s) = U(s) - sU'(s)$, and the nonlinear diffusion term is originally $\Delta f(\rho)$.

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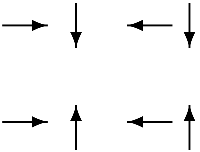

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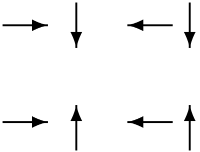

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Explicit schemes: Further comments

- We use explicit Euler if diffusive terms are present if not we use explicit 4th order RK schemes since the resulting approximation is a large ODE couple system, we see degeneracy of the long time asymptotics otherwise.
- The reported spatial discretization of the 2nd order terms leads to a CFL condition of the type

$$\|\Psi'(\det D\Phi)\|_{L^\infty} \frac{\Delta t}{\Delta x^2} \leq \frac{1}{2}\,.$$

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Outline

Calculating the initial diffeomorphism

Rectangular mesh: diffeomorphism can be constructed by subsequently solving two one-dimensional Monge-Kantorovich problems in x_1 and x_2 direction, (Angenenet-Haker-Tannebaum).

Triangular mesh: No natural ordering !
The Monge-Ampère equation gives the optimal transportation plan $T = T(x)$: unique minimizing map is the gradient of a convex function u, i.e. $T_0 = \nabla\varphi$, which satisfies the MA equation

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Numerical simulations

Numerical solver:

1. Given an initial density $\rho_0 = \rho_0(x)$ calculate the corresponding initial diffeomorphism by either determining the solution of the Monge Ampere equation or by succesive 1D transport maps.
2. Map the optimal transportation plan to the initial diffeomorphism $\Phi_0(x) = T_0$.
3. Apply the explicit-in-time discretization for $\Phi = \Phi(x, t)$.
4. Reconstruct the corresponding density $\rho = \rho(x, t)$ via

$$\rho(\Phi(x, t), t) \det(D\Phi(x, t)) = 1.$$

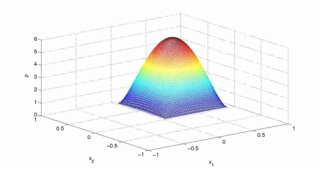
Outline

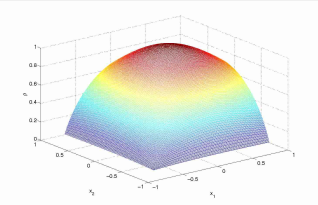
Linear Fokker-Planck Equation

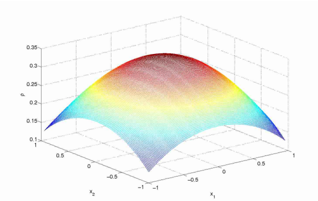
Linear Diffusion:

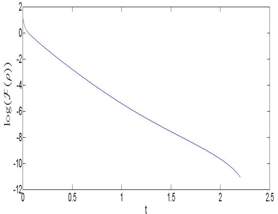
Starting with parabola initial data and with $U(s) = s\log s$, $V = |x|^2/2$ and $W = 0$:

$$\partial_t \rho = \nabla \cdot (\nabla \rho + x\rho)\,.$$







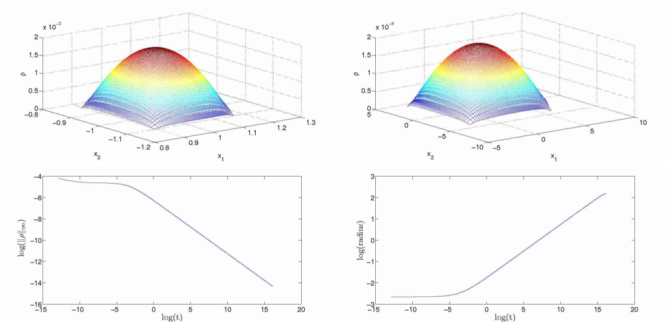


NonLinear Diffusion

Porous Medium Equation:

Starting with parabola initial data and with $U(s) = s/2$, $V = W = 0$:

$$\partial_t \rho = \nabla \cdot \left(\nabla \rho^2 + x\rho \right).$$



Outline

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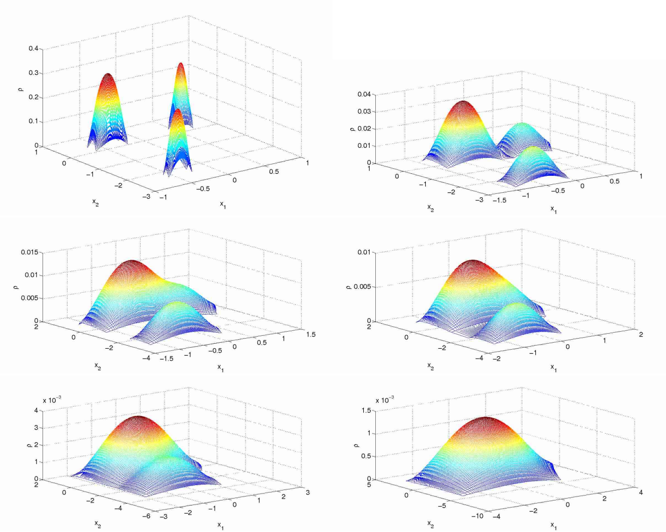
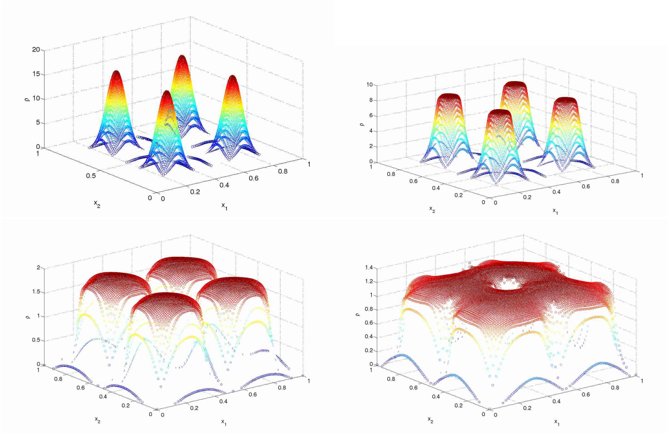


Relativistic Heat Equation

Flux-Limited Diffusion:

$$\frac{\partial \rho}{\partial t} = \nabla \cdot \left(\rho \frac{\nabla \rho}{\sqrt{\rho^2 + |\nabla \rho|^2}} \right) = \nabla \cdot \left(\rho \frac{\nabla \log \rho}{\sqrt{1 + |\nabla \log \rho|^2}} \right).$$



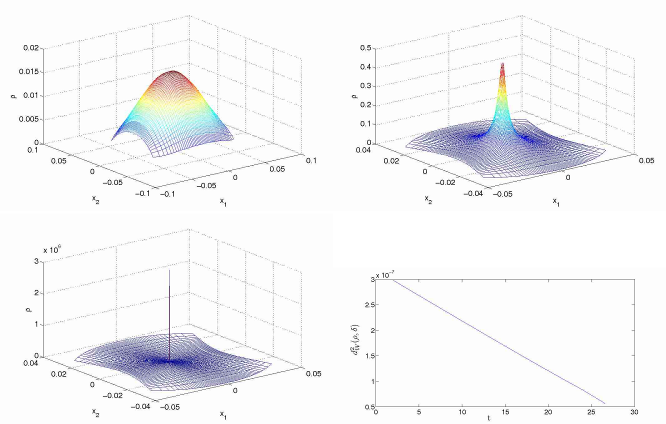
Outline

Swarming Model

Aggregation Equation:

Starting with parabola initial data and with $U(s) = 0$, $V = 0$, and $W(x) = -e^{-|x|}$:

$$\partial_t \rho = \nabla \cdot [(\nabla W * \rho)\rho] .$$



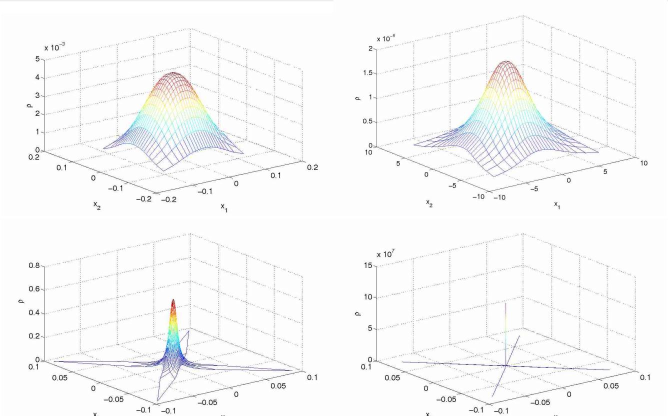
Chemotaxis Model

PKS Equation:

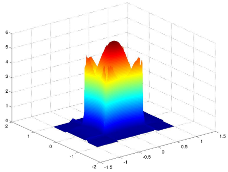
Starting with parabola initial data and with $U(s) = s \log s$, $V = 0$, and $W(x) = \frac{\chi}{2\pi} \log |x|$:

$$\partial_t \rho = \nabla \cdot [\nabla \rho + (\nabla W * \rho)\rho] .$$

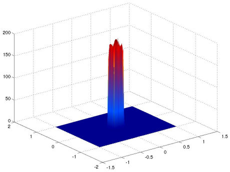
top right $\chi = 7\pi$ at $t = 500$, bottom left $\chi = 9\pi$ at $t = 0.025$, bottom right $\chi = 9\pi$ at $t = 0.02586440688$.



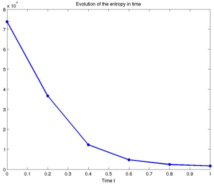
Attraction: $W(x) = \frac{1}{2}|x|^2$



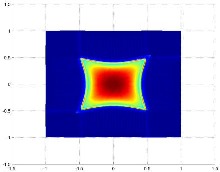
(a) $t = 0.2$



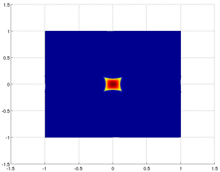
(b) $t = 0.8$



(c) Entropy

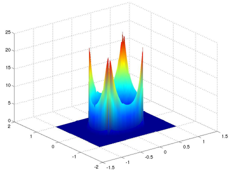


(d) $t = 0.2$

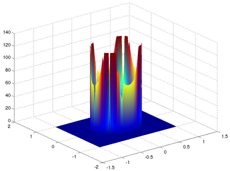


(e) $t = 0.8$

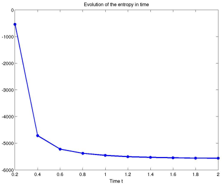
Attraction-repulsion: $W(x) = -\frac{1}{2}|x|^2 + \frac{1}{4}|x|^4$



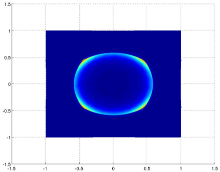
(f) $t = 0.8$



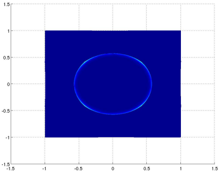
(g) $t = 1.4$



(h) Entropy

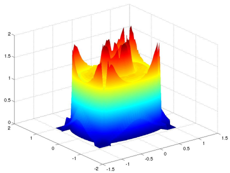


(i) $t = 0.8$

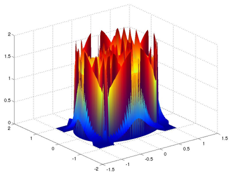


(j) $t = 1.4$

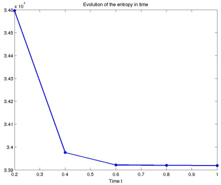
Attraction-repulsion: $W(x) = \frac{1}{2}|x|^2 - \ln(|x|)$, $V(x) = -\frac{1}{4}\ln(|x|)$



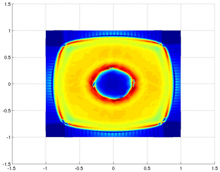
(k) $t = 0.4$



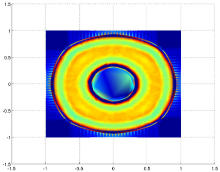
(l) $t = 1$



(m) Entropy



(n) $t = 0.4$



(o) $t = 1$

Conclusions

- The gradient flow interpretation induces a natural Lagrangian particle method on a grid or moving mesh method.
- It is a good solution to track accurately blow-up time and profiles and degenerate diffusion problems.
- It allows for merging of densities and finding stationary states for competing attractive-repulsive effects.
- Further improvements needs to be done to reconstruct better the density and to approximate the evolution of the diffeomorphisms with higher order accuracy.
- References:
  1. C.-Moll (SISC 2009), C.-Caselles-Moll (PLMS 2013).
  2. C.-Ranetbauer-Wolfram (work in preparation)

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