

Geodesic extrapolations and a BDF2 scheme for Wasserstein gradient flows

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Wasserstein gradient flows

PDE formulation

Given $\Omega \subset \mathbb{R}^d$ (convex, bounded), find $\rho : [0, T] \times \Omega \rightarrow \mathbb{R}^+$ solving

$$\partial_t \rho - \operatorname{div} \left(\rho \nabla \frac{\delta \mathcal{E}}{\delta \rho}[\rho] \right) = 0, \\ (\text{IC}) \quad \rho(0, \cdot) = \rho_0, \quad (\text{BC}) \quad \rho \nabla \frac{\delta \mathcal{E}}{\delta \rho}[\rho] \cdot n_{\partial \Omega} = 0$$

where $\mathcal{E} : L^1(\Omega, \mathbb{R}^+) \rightarrow \mathbb{R}$ (energy).

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- Nonlinear diffusion equations (porous media), Fokker-Planck:

$$\mathcal{E}(\rho) = \int_{\Omega} V\rho + \rho \log \rho \quad \Rightarrow \quad \partial_t \rho - \operatorname{div}(\rho \nabla V) - \Delta \rho = 0.$$

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- Numerical challenges: entropy stability (\Rightarrow long time behaviour) / constraints (positivity, density bounds) / **high order discretization**

Wasserstein gradient flows

JKO scheme (Jordan, Kinderlehrer, Otto '98)

Time discretization $t^0 < \dots < t^N$, $\tau = t^{n+1} - t^n$

$$\rho^{n+1} \in \operatorname{argmin}_{\rho \in \mathcal{P}(\Omega)} \frac{W_2^2(\rho^n, \rho)}{2\tau} + \mathcal{E}(\rho) \quad (\text{implicit Euler scheme})$$

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- Numerically: energy decreasing / easier to handle constraints / solution by convex optimization [Benamou, Carlier, Laborde, ..]

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- **JKO alternative:** Variational midpoint rule [Legendre, Turinici '17], Variational BDF2 [Matthes, Plazotta '18]
- High order schemes: *entropy-diminishing Runge-Kutta methods* [Hairer, Lubich '13], nonlinear diffusion [Jüngel, Schuchnigg '17]

The BDF2 scheme in Euclidean space

Euclidean gradient flows: let $F : \mathbb{R}^d \rightarrow \mathbb{R}$ (smooth, convex), $x_0 \in \mathbb{R}^d$,

$$x'(t) = -\nabla F(x(t)), \quad x(0) = x_0.$$

BDF2 scheme: Let $\tau > 0$, given $x_0, x_1 \in \mathbb{R}^d$, for $n \geq 2$ find $x_n \in \mathbb{R}^d$ satisfying

$$\frac{3}{2\tau} \left(x_n - \frac{4}{3}x_{n-1} + \frac{1}{3}x_{n-2} \right) = -\nabla F(x_n).$$

→ *Reformulation as two-stages method:*

$$x_{n-1}^e = x_{n-2} + \frac{4}{3}(x_{n-1} - x_{n-2}), \quad x_n = \operatorname{argmin}_{x \in \mathbb{R}^d} 3 \frac{|x - x_{n-1}^e|^2}{4\tau} + \mathcal{E}(\rho)$$

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This talk: Wasserstein extrapolation → A BDF2 discretization

Wasserstein extrapolations

Geodesics in Wasserstein space

Wasserstein geodesics: $\rho_0, \rho_1 \in \mathcal{P}^{ac}(\Omega)$ $\exists!$ curve $\rho : [0, 1] \rightarrow \mathcal{P}^{ac}(\Omega)$:

$$\rho(0) = \rho_0, \quad \rho(1) = \rho_1, \quad W_2(\rho(t), \rho(s)) = |t - s| W_2(\rho_0, \rho_1),$$

$\forall t, s \in [0, 1]$. Moreover, $\exists \phi : [0, 1] \times \Omega \rightarrow \mathbb{R}$, such that

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- Particles travel in straight lines: $\phi(0, \cdot) + \frac{|\cdot|^2}{2}$ is convex,

$$\rho(t) = (t \nabla \phi(0, \cdot) + \operatorname{Id})_{\#} \rho_0 \tag{1}$$

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- Finite existence even if ρ_0, ρ_1 smooth and strictly positive
- Geodesic continuation: let $\alpha > 1$:

$$\alpha \phi(0, \cdot) + \frac{|\cdot|^2}{2} \text{ convex} \Leftrightarrow (1) \text{ is a geodesic up to } t = \alpha$$

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Dissipative extrapolation: A curve $\rho : [0, \alpha] \rightarrow \mathcal{P}(\mathbb{R}^d)$ s.t.

$$\rho(0) = \rho_0, \quad \rho(1) = \rho_1, \quad W_2(\rho(t), \rho(s)) \leq |t - s| W_2(\rho_0, \rho_1),$$

$\forall t, s \in [0, \alpha]$, AND equality if \exists geodesic extension up to $\max(t, s)$

Lagrangian vs Eulerian extrapolation

Lagrangian extrapolation. No collisions / $\text{supp}(\rho(t)) \not\subseteq \Omega$

$$\rho(t) = X(t, \cdot)_\# \rho_0, \quad X(t, \cdot) := t \nabla \phi(0, \cdot) + \text{Id}, \quad \forall t \in [0, \alpha]$$

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Eulerian extrapolation. Find $\rho : [1, \alpha] \rightarrow \mathcal{P}(\Omega)$, $u(t, \cdot) \in L^2(\Omega, \rho(t))$

$$\begin{cases} \partial_t \rho + \text{div}(\rho u) = 0, \\ \partial_t(\rho u) + \text{div}(\rho u \otimes u) = 0, \end{cases} \quad (\text{IC}) \quad \rho(1) = \rho_1, \quad u(1, \cdot) = \nabla \phi(1, \cdot).$$

→ Energy dissipation via *sticky collisions* condition (inelastic)

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→ In 1d [Grenier, Brenier, ..], $\Omega = \mathbb{R}$, $F_0(x) = \rho_0((-\infty, x])$,

$$\tilde{X}(t, x) := [P_K X(t, F_0^{[-1]}(x))] \circ F_0(x) \quad P_K : L^2 \text{ proj. on monotone maps}$$

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→ $d > 1$, existence dissipative measure solutions [Cavalletti et al 19],

“for almost all initial data sticky solns are free flow” [Bianchini, Daneri 21]

Metric extrapolation

Euclidean extrapolation. Let $x_0, x_1 \in \mathbb{R}^d$, $\alpha > 1$ and $\beta = \alpha - 1$.

Extrapolation at time α from x_0 to x_1 :

$$x_\alpha = \operatorname{argmin}_x \alpha|x - x_1|^2 - \beta|x - x_0|^2.$$

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- If $0 < \alpha < 1 \rightarrow$ Wasserstein geodesic/barycenter
- $\alpha > 1 \Rightarrow$ non-convex in Eulerian sense
- 2-convex along generalized geodesics based at ρ_1 [Matthes et al 19]
 \Rightarrow Unique minimizer for any $\rho_0, \rho_1 \in \mathcal{P}(\Omega)$

Relation with geodesic extensions

- Set $\Omega = \mathbb{R}^d$, $\mathcal{P}_2(\mathbb{R}^d)$: prob. measures + finite 2nd moments
- Let $\rho_0, \rho_1 \in \mathcal{P}_2^{ac}(\mathbb{R}^d)$, define for any $\rho \in \mathcal{P}_2(\mathbb{R}^d)$

$$\Phi(\rho) := \frac{W_2^2(\rho, \rho_1)}{2\beta} - \frac{W_2^2(\rho, \rho_0)}{2\alpha}$$

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- Triangular + Young inequality \Rightarrow

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- Dissipative? It holds

$$W_2(\rho_\alpha, \rho_0) \leq \alpha W_2(\rho_1, \rho_0), \quad W_2(\rho_\alpha, \rho_1) \leq \beta W_2(\rho_1, \rho_0)$$

Dual formulation and HJ equation

Problem : $\min_{\rho} \Phi(\rho), \quad \Phi(\rho) := \frac{W_2^2(\rho, \rho_1)}{2\beta} - \frac{W_2^2(\rho, \rho_0)}{2\alpha}$

Proposition (Dual formulation) Set $C = -\int \frac{|x|^2}{2} (\rho_0 + \rho_1)$, then

$$\min_{\rho} \Phi(\rho) = \inf_{\rho} \left\{ \int u \rho_0 + \int u^* \rho_1 : u \text{ is } \frac{\beta}{\alpha}\text{-convex} \right\} + C \quad (\mathcal{DP})$$

Moreover, $\rho_\alpha = \nabla \left(\alpha u - \beta \frac{|x|^2}{2} \right) \# \rho_0$

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- Toland duality → **Convex dual**: Case $\alpha = \beta = 1$ [Carlier '07]

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- If u Brenier potential $\rho_0 \rightarrow \rho_1$ is β/α -convex

$$\Phi(\rho_\alpha) = -\frac{W^2(\rho_0, \rho_1)}{2} \quad \text{and} \quad \rho_\alpha \text{ is a geodesic extension}$$

Relation with HJ equation

- Geodesic from ρ_0 to ρ_1 : $\exists \phi(0, \cdot) : \mathbb{R}^d \rightarrow \mathbb{R}^d$ (-1)-convex s.t.

$$\begin{cases} \partial_t \rho + \operatorname{div}(\rho \nabla \phi) = 0, \\ \partial_t \phi + \frac{|\nabla \phi|^2}{2} = 0. \end{cases}$$

- Let $u(t, \cdot) = t\phi(0, \cdot) + \frac{|\cdot|^2}{2}$, then $\rho(t) = [\nabla u(t, \cdot)]_\# \rho_0$,

$$\phi(t, x) = \inf_y \phi(0, y) + \frac{|x - y|^2}{2t} \quad (\text{Hopf-Lax formula})$$

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- Geodesic extension via HJ:

$$\rho(t) = [\nabla u(t, \cdot)^{**}]_\# \rho_0$$

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- Geodesic extension via HJ:

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- $\rho(\alpha)$ is the metric extrapolation iff \tilde{u} solves (\mathcal{DP}) :

$$\tilde{u} := \frac{1}{\alpha} \left[\alpha u(1, \cdot) - \beta \frac{|x|^2}{2} \right]^{**} + \frac{\beta}{\alpha} \frac{|x|^2}{2}$$

Relation with pressureless fluids

- $\Omega = \mathbb{R}$, $\mu, \nu \in \mathcal{P}_2(\mathbb{R})$ then

$$W_2(\mu, \nu) = \|F_\mu^{[-1]} - F_\nu^{[-1]}\|_{L^2([0,1])}$$

$$F_\mu : x \rightarrow \mu((-\infty, x]), \quad F_\nu : x \rightarrow \nu((-\infty, x])$$

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Metric extrapolation (1d): $\rho_\alpha = (G_\alpha)_\# dx|_{[0,1]}$ where

$$G_\alpha := \underset{\substack{G \in L^2([0,1], \mathbb{R}) \\ \text{monotone}}}{\operatorname{argmin}} \alpha \|G - F_1^{[-1]}\|_{L^2}^2 - \beta \|G - F_0^{[-1]}\|_{L^2}^2,$$

$$\text{i.e. } G_\alpha = P_K(\alpha F_1^{[-1]} - \beta F_0^{[-1]}), \quad K := \{G \in L^2([0, 1], \mathbb{R}), \text{monot.}\}$$

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- $\Omega = \mathbb{R}$, $\mu, \nu \in \mathcal{P}_2(\mathbb{R})$ then
$$W_2(\mu, \nu) = \|F_\mu^{[-1]} - F_\nu^{[-1]}\|_{L^2([0,1])}$$

$$F_\mu : x \rightarrow \mu((-\infty, x]), \quad F_\nu : x \rightarrow \nu((-\infty, x])$$

Metric extrapolation (1d): $\rho_\alpha = (G_\alpha)_\# dx|_{[0,1]}$ where

$$G_\alpha := \underset{\substack{G \in L^2([0,1], \mathbb{R}) \\ \text{monotone}}}{\operatorname{argmin}} \alpha \|G - F_1^{[-1]}\|_{L^2}^2 - \beta \|G - F_0^{[-1]}\|_{L^2}^2,$$

$$\text{i.e. } G_\alpha = P_K(\alpha F_1^{[-1]} - \beta F_0^{[-1]}), \quad K := \{G \in L^2([0, 1], \mathbb{R}), \text{monot.}\}$$

- Convex formulation / Equivalent to sticky pressureless model
- For $t \geq 1$, equivalent to gradient flow [Natili, Savaré '09]:

$$\mathcal{E}(t, \rho) = -\frac{W_2^2(\rho, \rho_0)}{2t}, \quad (\text{IC}) : \rho(1, \cdot) = \rho_1.$$

- Not true for $d > 1$! Counterexample for $d = 2$

A BDF2 scheme in
Wasserstein space

Time discretization and dissipation

- Let $\mathcal{E}(\rho) : \mathcal{P}(\mathbb{R}^d) \rightarrow \mathbb{R}$ convex l.s.c., $\mathcal{E}(\rho) = +\infty$ if ρ not a.c. $d\rho|_\Omega$
- $E_\alpha : [\mathcal{P}_2^{ac}(\mathbb{R}^d)]^2 \rightarrow \mathcal{P}_2(\mathbb{R}^d)$ is an α -extrapolation:

$$W_2(\mu, E_\alpha(\mu, \nu)) \leq \alpha W_2(\mu, \nu), \quad W_2(\nu, E_\alpha(\mu, \nu)) \leq \beta W_2(\mu, \nu).$$

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Time discretization. Let $0 = t_0 < \dots < t_N = T$ uniform partition, $\tau = t_{n+1} - t_n$. Given $\rho_0, \rho_1 \in \mathcal{P}^{ac}(\Omega)$, define $\rho_n \in \mathcal{P}^{ac}(\Omega)$ by

$$\begin{cases} \rho_{n-1}^e = E_\alpha(\rho_{n-2}, \rho_{n-1}) \\ \rho_{n+1} \in \underset{\rho \in \mathcal{P}(\mathbb{R}^d)}{\operatorname{argmin}} \frac{W_2^2(\rho, \rho_{n-1}^e)}{2(1-\beta)\tau} + \mathcal{E}(\rho) \end{cases} \quad \text{for } 2 \leq n < N$$

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Dissipation inequality. Dissipative extrapolation implies:

$$\frac{1-\beta}{\tau} W_2^2(\rho^n, \rho^{n-1}) + \mathcal{E}(\rho^n) \leq \frac{\beta}{\tau} W_2^2(\rho^{n-1}, \rho^{n-2}) + \mathcal{E}(\rho^{n-1})$$

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Dissipation inequality. Dissipative extrapolation implies:

$$\beta < \frac{1}{2} \quad \Rightarrow \quad \boxed{\sum_{n=0}^{N-1} \frac{W_2^2(\rho_n, \rho_{n+1})}{2\tau} \leq \frac{C(\rho_0, \rho_1, \mathcal{E})}{(1-2\beta)}} \quad (\text{compactness})$$

Convergence to Fokker-Plank eq.

Fokker-Planck model. Let $V : \Omega \rightarrow \mathbb{R}$ be Lipschitz, define

$$\mathcal{E}(\rho) = \begin{cases} \int_{\Omega} \rho \log \rho + \int_{\Omega} V \rho & \text{if } \rho \text{ a.c. with respect to } dx|_{\Omega} \\ +\infty & \text{otherwise} \end{cases}$$

Wasserstein gradient flow \rightarrow

$$\boxed{\partial_t \rho - \operatorname{div}(\rho \nabla V) - \Delta \rho = 0} \quad (FP)$$

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Wasserstein gradient flow \rightarrow $\partial_t \rho - \operatorname{div}(\rho \nabla V) - \Delta \rho = 0$ (FP)

Consistency assumption. For all $\varphi \in C_c^\infty(\Omega)$, $\exists C_\varphi > 0$:

$$\left| \int_{\Omega} \varphi(E_{\alpha}(\mu, \nu) - (\alpha\nu - \beta\mu)) \right| \leq C_\varphi W_2^2(\mu, \nu) \quad \forall \text{ a.c. } \mu, \nu \in \mathcal{P}(\Omega)$$

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Theorem. Discrete solution $t \mapsto \rho_{\tau}(t)$ converges in W_2 to an a.c. curve $t \mapsto \rho(t)$ s.t. $\rho(0) = \rho_0$, and satisfying (FP) in distributional sense.

- Consistency assumption needed for “ $\partial_t \rho$ ”
- Verified for Lagrangian / Eulerian / metric extrapolations

Convergence in the EVI sense

EVI formulation. Let $\mathcal{E} : \mathcal{P}(\Omega) \rightarrow \mathbb{R}$ λ -geodesically convex, then $t \mapsto \rho(t)$ is a solution in EVI sense iff $\forall \nu \in \mathcal{P}(\Omega)$ and $\forall t \in (0, T)$

$$\frac{d}{dt} \frac{1}{2} W_2^2(\rho(t), \nu) \leq \mathcal{E}(\nu) - \mathcal{E}(\varrho(t)) - \frac{\lambda}{2} W_2^2(\varrho(t), \nu), \quad (EVI)$$

- EVI formulation \rightarrow general energies (singular interaction kernels,..)

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Theorem. *For the metric extrap., discrete solution $t \mapsto \rho_\tau(t)$ converges in W_2 to an a.c. curve $t \mapsto \rho(t)$ s.t. $\rho(0) = \rho_0$, and satisfying (EVI).*

- **Key property:** Given $\rho_0, \rho_1 \in \mathcal{P}(\Omega)$

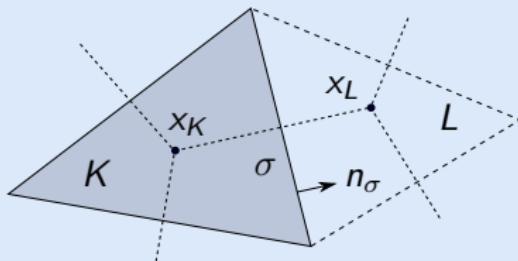
$$\rho_\alpha = \operatorname{argmin}_{\rho \in \mathcal{P}(\Omega)} \Phi(\rho) \quad \Phi(\rho) := \frac{W_2^2(\rho, \rho_1)}{2\beta} - \frac{W_2^2(\rho, \rho_0)}{2\alpha}$$

$$\boxed{\Phi(\rho_\alpha) + \frac{W_2^2(\rho, \rho_\alpha)}{2\alpha\beta} \leq \Phi(\rho) \quad \forall \rho \in \mathcal{P}(\Omega)}$$

Space discretization and numerics

Finite volume discretization

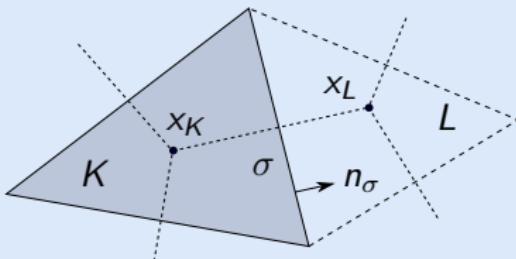
Admissible TPFA triangulation (ex. Delaunay)



$K \in \mathcal{T}$ control volumes, x_K cell centers, $\sigma \in \Sigma$ internal edges

Finite volume discretization

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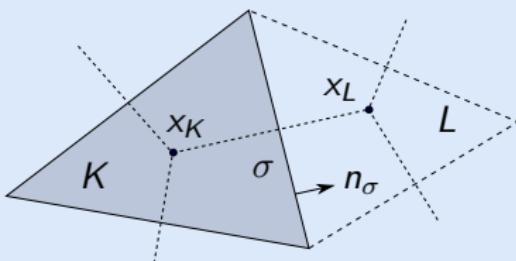


$K \in \mathcal{T}$ control volumes, x_K cell centers, $\sigma \in \Sigma$ internal edges

- $\rho = (\rho_K)_K \in \mathbb{P}_{\mathcal{T}}$, where $\rho_K \approx \rho(x_K)$
- $\phi = (\phi_K)_K \in \mathbb{P}_{\mathcal{T}}$, where $\phi_K \approx \phi(x_K)$

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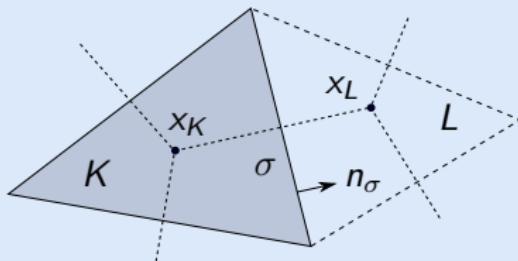


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- $\mathbf{m} = (m_\sigma)_\sigma \in \mathbb{F}_\Sigma$, where $m_\sigma \approx m \cdot n_\sigma$ on σ
- Discrete divergence $\text{div}_{\mathcal{T}} : \mathbb{F}_\Sigma \rightarrow \mathbb{P}_{\mathcal{T}}$ and gradient $\nabla_\Sigma := \text{div}_{\mathcal{T}}^*$

$$[\text{div}_{\mathcal{T}} \mathbf{m}]_K = \sum_{\sigma \in \partial K} m_\sigma (n_\sigma \cdot n_{\partial K}) \frac{|\sigma|}{|K|}$$

Fully discrete scheme

LJKO step [Cancès et al '20]: Given ρ_e^n find ϕ^{n+1} and ρ^{n+1} :

$$\begin{cases} \rho^{n+1} - \rho_e^n + \tau \operatorname{div}_{\mathcal{T}}(R_{\Sigma}(\frac{\rho^{n+1} + \rho_e^n}{2}) \odot \nabla_{\Sigma} \phi^n) = 0, \\ \frac{\delta \mathcal{E}}{\delta \rho}(\rho^{n+1}) - \phi^{n+1} + \frac{\tau}{2} R_{\Sigma}^*(\nabla_{\Sigma} \phi^{n+1})^2 = 0 \end{cases}$$

→ Optimality conditions discrete version of JKO

→ $\phi_{n+1} \approx \phi(1/2, \cdot)$ optimal potential $\rho_n^e \rightarrow \rho_{n+1}$

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Extrapolation step → HJ equation: Given ρ^n , ϕ^n find ρ_e^n and ϕ_e^n :

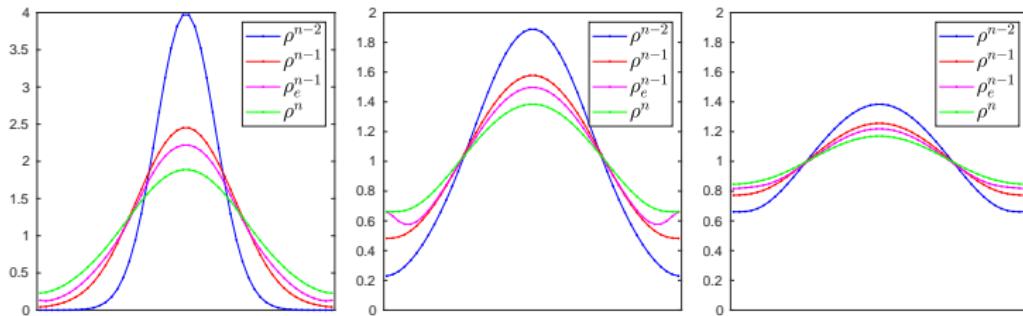
$$\begin{cases} \phi_e^n - \phi^n + \frac{\tau(1+2\beta)}{4} R_{\Sigma}^*(\nabla_{\Sigma} \phi^n)^2 = 0 \\ \rho_e^n - \rho^n + \beta \tau \operatorname{div}_{\mathcal{T}}(R_{\Sigma}(\frac{\rho^n + \rho_e^n}{2}) \odot \nabla_{\Sigma} \phi_e^n) = 0, \end{cases}$$

→ Continuity equation via optimization → positivity

Numerics

$$\mathcal{E}(\rho) = \int_{\Omega} V\rho + \rho \log \rho \quad \Rightarrow \quad \partial_t \rho - \operatorname{div}(\rho \nabla V) - \Delta \rho = 0$$

Density evolution for the BDF2 scheme ($d = 1$)



Numerics

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Convergence test for the BDF2 scheme ($d = 2$)

h_m	τ_m	ϵ_m	rate
0.100	0.050	2.217e-02	/
0.050	0.025	7.016e-03	1.660
0.025	0.013	2.044e-03	1.779
0.013	0.006	5.653e-04	1.854
0.006	0.003	1.508e-04	1.906
0.003	0.002	3.933e-05	1.939

Outlook

Summary

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- Main ingredient: different (related) notions of extrapolation
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Thank you!