Discretizing the Fokker-Planck equation with second-order accuracy: a dissipation driven approach

Clément Cancès, Léonard Monsaingeon & Andrea Natale

Inria Université de Lille

5th Gradient Flows face-to-face workshop







The continuous problem

Partial differential equation

$$\begin{cases} \partial_t \rho + \operatorname{div} F = 0 \\ F = -\rho \nabla V - \nabla \rho \end{cases} \qquad \text{in } (0,T)\times\Omega \qquad \text{(FPE)}$$

No-flux boundary condition

$$F \cdot n_{\partial\Omega} = 0 \quad \text{on } (0,T)\times\partial\Omega$$

Initial condition

$$\rho(0,\cdot) = \rho^0 \geq 0 \qquad \text{with} \qquad \mathcal{H}(\rho^0) < +\infty \quad \text{and} \quad M := \int_\Omega \rho^0 > 0.$$

- $\Omega \subset \mathbb{R}^d$ is a bounded convex polyhedral domain
- $T > 0$ is an arbitrary finite time horizon
- $V \in C^2(\overline{\Omega})$ does not depend on time. Gibbs measure $\pi = e^{-V} \geq \pi_\star > 0$.
- $\mathcal{H}(\rho) := \int_\Omega (\rho \log \rho - \rho + 1) \geq 0$ is the Boltzmann (neg-)entropy

Well known facts

Mass conservation

$$\int_\Omega \rho(t) = \int_\Omega \rho^0 = M.$$

Energy and Fisher information

$$\mathcal{E}(\rho) := \mathcal{H}(\rho) + \int_\Omega \rho V, \qquad \mathcal{F}(\rho) = 2\int_\Omega \pi \left| \nabla \sqrt{\frac{\rho}{\pi}} \right|^2$$

EDI characterization of the unique solution

$$\mathcal{E}(\rho)(t) + \int_0^t \left[\int_\Omega \frac{|F|^2}{2\rho} + \mathcal{F}(\rho) \right] \leq \mathcal{E}(\rho^0) \qquad \text{(EDI)}$$

with F satisfying the continuity equation $\partial_t \rho + \operatorname{div} F = 0$.
The curve ρ minimizes the left-hand side for all $0 \leq t \leq T$

What will follow in this talk

Propose a fully discrete approximation that is

- compatible with the gradient flow structure of the Fokker-Planck Equation
- second order accurate in both space and **time**
- provably captures the unique EDI solution
- easy to compute

Time discretizations: preliminaries

Global minimization: Optimal character of the curve ρ solution to (EDI)

$$\rho(T) \in \operatorname*{argmin}_{\rho} \left\{ \mathcal{E}(\rho) + \inf_{\substack{\partial_t \varrho + \operatorname{div} F = 0 \\ \varrho(0) = \rho^{\mathbf{0}} \\ \varrho(T) = \rho}} \int_0^T \left[\int_\Omega \frac{|F|^2}{2\varrho} + \mathcal{F}(\varrho) \right] \right\}$$

Stepwise minimization: Denote by $\overline{\rho}^n = \rho(t^n)$ with ρ being the EDI solution and $0 = t^0 < t^1 < \cdots < t^N = T$, then

$$\overline{\rho}^{n+1} \in \operatorname*{argmin}_{\rho} \left\{ \mathcal{E}(\rho) + \inf_{\substack{\partial_t \varrho + \operatorname{div} F = 0 \\ \varrho(t^n) = \overline{\rho}^n \\ \varrho(t^{n+\mathbf{1}}) = \rho}} \int_{t^n}^{t^{n+\mathbf{1}}} \left[\int_\Omega \frac{|F|^2}{2\varrho} + \mathcal{F}(\varrho) \right] \right\}$$

For the optimal curve ρ

$$F(t) = -\rho(t) \boldsymbol{\nabla} \frac{\delta \mathcal{E}}{\delta \rho}(t) \quad \Longrightarrow \quad \int_\Omega \frac{|F(t)|^2}{2\rho(t)} = \mathcal{F}(\rho(t)), \qquad \forall\, t > 0.$$

The JKO scheme

[Jordan, Kinderlehrer & Otto (1998)]

Uniform time step $\tau = T/N$, $t^n = n\tau$

$$\rho^{n+1} \in \operatorname*{argmin}_{\rho} \left[\frac{1}{2\tau} W_2(\rho, \rho^n)^2 + \mathcal{E}(\rho) \right], \qquad n \geq 0 \qquad \text{(JKO)}$$

- Natural extension to the metric setting of the backward Euler scheme
  $\rightsquigarrow$ first order accuracy
- Benamou-Brenier formula [Benamou & Brenier (2000)]

$$W_2(\rho^{n+1}, \rho^n)^2 = \inf_{\substack{\partial_t \varrho + \operatorname{div} F = 0 \\ \rho^n = \varrho(t^n) \\ \rho^{n+1} = \varrho(t^{n+1})}} \tau \int_{t^n}^{t^{n+1}} \int_\Omega \frac{|F|^2}{\varrho}$$

- Optimality condition in (JKO) is a continuous in time MFG

$$\begin{cases} \partial_t \varrho - \operatorname{div} \varrho \nabla \phi = 0 \\ \partial_t \phi - \frac{1}{2} |\nabla \phi|^2 = 0 \end{cases} \quad \text{and} \quad \begin{cases} \varrho(t^n) = \rho^n \\ \phi(t^{n+1}) = \frac{\delta \mathcal{E}}{\delta \varrho}(\rho^{n+1}) \end{cases}$$

Hard to handle numerically in a Eulerian framework

Stefanelli's Minimizing Movement scheme

[Jüngel, Stefanelli & Trussardi (2020)], [Stefanelli (2022)]

$$\rho^n \in \operatorname*{argmin}_{\rho \in L^1_+(\Omega) \text{ s.t. } \int \rho = M} \left[\frac{1}{2\tau} W_2(\rho, \rho^{n-1})^2 + \tau \mathcal{F}(\rho) + \mathcal{E}(\rho) \right], \qquad n \geq 1 \quad \text{(SMM)}$$

- Closer to (EDI) with the full dissipation
- Rectangle quadrature rule with right endpoint for the Fisher information
  $\rightsquigarrow$ still first order accuracy
- Optimality condition in (SMM) is still a continuous in time MFG

$$\begin{cases} \partial_t \varrho - \operatorname{div} \varrho \nabla \phi = 0 \\ \partial_t \phi - \frac{1}{2} |\nabla \phi|^2 = 0 \end{cases} \quad \text{and} \quad \begin{cases} \varrho(t^{n-1}) = \rho^{n-1} \\ \phi(t^n) = \frac{\delta \mathcal{E}}{\delta \varrho}(\rho^n) + \tau \frac{\delta \mathcal{F}}{\delta \varrho}(\rho^n) \end{cases}$$

Still hard to handle numerically

Second order in time discretizations

Existing methods

- Variational midpoint rule [Legendre & Turinici (2017)]

$$\rho^{n+1} \in \operatorname*{argmin}_{\rho} \left\{ \frac{1}{2\tau} W_2(\rho, \rho^n)^2 + 2\mathcal{E}\left(\frac{\rho + \rho^n}{2}\right) \right\}$$

  - Poorly stable
  - Hard to compute for $d \geq 2$

- Variational BDF2 scheme
  [Matthes, Plazotta (2019)] [Gallouët, Natale & Todeschi (2024)]

$$\rho^{n+1} \in \operatorname*{argmin}_{\rho} \left\{ \frac{1}{\tau} W_2(\rho, \rho^n)^2 - \frac{1}{4\tau} W_2(\rho, \rho^{n-1})^2 + \mathcal{E}(\rho) \right\}$$

  - Non-convex optimization problem
  - Alternative formulation relying on metric extrapolation

  $\rightsquigarrow$ still hard to compute

Going to (really) discrete in time

Discrete curve $(\rho^n)_{0\leq n\leq N}$ with

$$\frac{\rho^{n+1}-\rho^n}{\tau} + \operatorname{div} F^{n+\frac{1}{2}} = 0, \qquad 0 \leq n \leq N-1.$$

Set $h(r) = r\log(r) - r + 1$, then for any $\theta^{n+\frac{1}{2}}$,

$$\begin{aligned}\int_\Omega \frac{\rho^{n+1}-\rho^n}{\tau}\left(h'(\theta^{n+\frac{1}{2}}) + V\right) &= \int_\Omega F^{n+\frac{1}{2}} \cdot \boldsymbol{\nabla}\left(h'(\theta^{n+\frac{1}{2}}) + V\right) \\ &\geq -\int_\Omega \frac{|F^{n+\frac{1}{2}}|^2}{2\theta^{n+\frac{1}{2}}} - \mathcal{F}(\theta^{n+\frac{1}{2}})\end{aligned}$$

Equality case

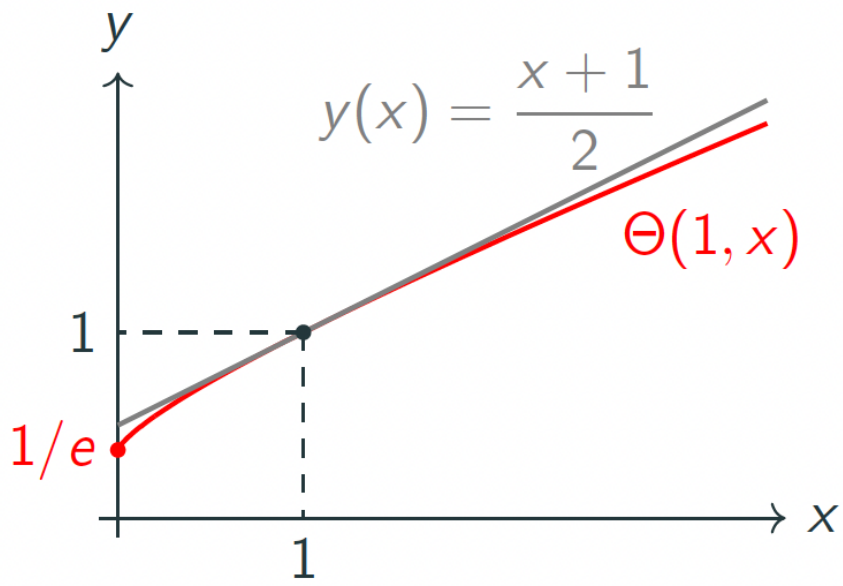
$$F^{n+\frac{1}{2}} = -\theta^{n+\frac{1}{2}}\boldsymbol{\nabla}\left(h'(\theta^{n+\frac{1}{2}}) + V\right) = -\theta^{n+\frac{1}{2}}\boldsymbol{\nabla} V - \boldsymbol{\nabla}\theta^{n+\frac{1}{2}}$$

Nonlinear time average

Entropic mean

$$\Theta(a,b) = (h')^{-1}\left(\frac{h(a)-h(b)}{a-b}\right)$$
$$= \exp\left(\frac{a\log a - b\log b}{a-b} - 1\right)$$

1-homogeneous, jointly concave



$$\theta^{n+\frac{1}{2}} = \Theta(\rho^n, \rho^{n+1}) \quad \Longrightarrow \quad \int_\Omega \frac{\rho^{n+1}-\rho^n}{\tau}\left(h'(\theta^{n+\frac{1}{2}}) + V\right) = \frac{\mathcal{E}(\rho^{n+1}) - \mathcal{E}(\rho^n)}{\tau}$$

Remark: $\theta^{n+\frac{1}{2}}(x)$ is a (pointwise) interpolation between $\rho^n(x)$ and $\rho^{n+1}(x)$
$\rightsquigarrow$ easy to handle numerically

Time semi-discretization

Tentative scheme

$$\begin{cases} \dfrac{\rho^{n+1}-\rho^n}{\tau} + \operatorname{div} F^{n+\frac{1}{2}} = 0 \\ F^{n+\frac{1}{2}} = -\theta^{n+\frac{1}{2}} \nabla V - \nabla \theta^{n+\frac{1}{2}} \\ \theta^{n+\frac{1}{2}} = \Theta(\rho^n, \rho^{n+1}) \end{cases}$$

Energy discrete equality (formal)

$$\mathcal{E}(\rho^{n+1}) + \tau \int_\Omega \frac{|F^{n+\frac{1}{2}}|^2}{2\theta^{n+\frac{1}{2}}} + \tau \mathcal{F}(\theta^{n+\frac{1}{2}}) = \mathcal{E}(\rho^n)$$

- Really semi-discrete
- No metric interpolation
- Full dissipation is captured
- Mid-point rule $\rightsquigarrow$ second order accuracy
- $\times$ Not always solvable

A remark on the Crank-Nicolson scheme

Gradient flow in $\mathbb{R}^d$

$$\dot{u} = -\nabla E(u), \qquad u(0) = u^0 \in \mathbb{R}^d$$

Crank-Nicolson scheme

$$u^{n+1} = u^n - \tau \nabla E\left(\frac{u^n + u^{n+1}}{2}\right), \qquad n \geq 0$$

Extrapolation based equivalent formulation

$$\begin{cases} u^{n+\frac{1}{2}} = u^n - \dfrac{\tau}{2} \nabla E\left(u^{n+\frac{1}{2}}\right) \\ u^{n+1} = 2u^{n+\frac{1}{2}} - u^n \end{cases} \qquad n \geq 0$$

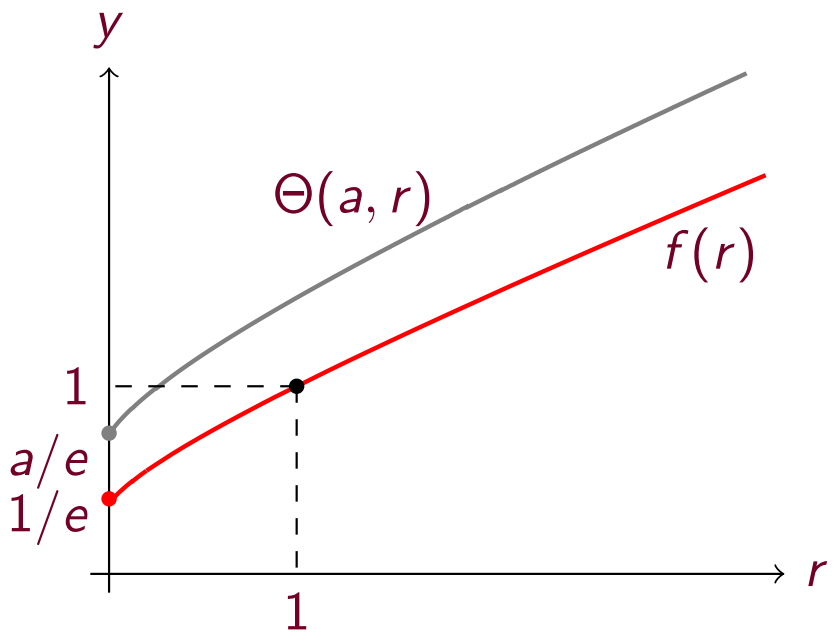
Nonlinear extrapolation operator

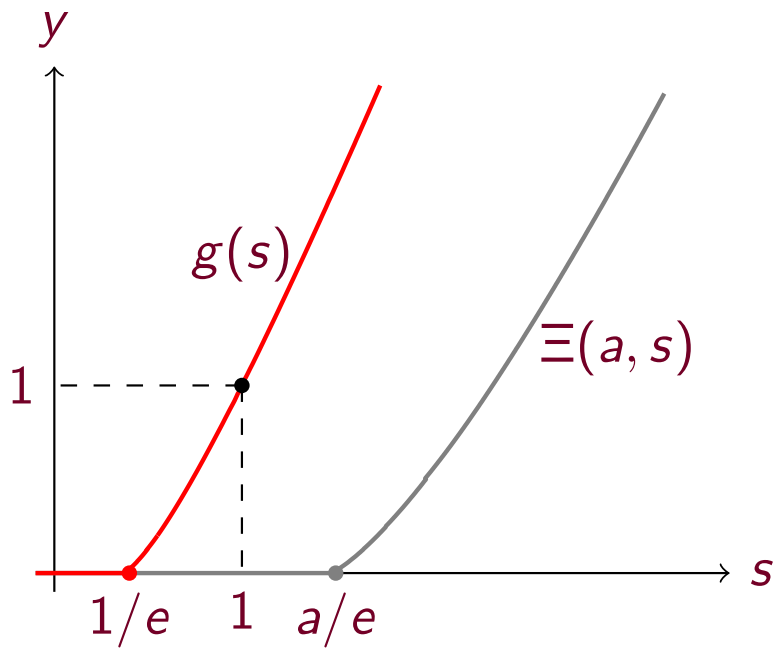
Set $f(r) = \Theta(1, r)$ for $r \geq 0$, then define its generalized inverse g by

$$g(s) := \begin{cases} f^{-1}(s) & \text{if } s > e^{-1} \\ 0 & \text{otherwise} \end{cases}$$

Define the nonlinear extrapolation operator

$$\Xi(a, c) := \begin{cases} a g\left(\frac{c}{a}\right) & \text{if } a > 0 \\ ec & \text{if } a = 0 \end{cases}, \quad c \in \mathbb{R} \ .$$





Extrapolation based semi-discretization in time

Time semi-discretization

$$\begin{cases} \dfrac{\rho^{n+1} - \rho^n}{\tau} + \operatorname{div} F^{n+\frac{1}{2}} = 0 \\ F^{n+\frac{1}{2}} = -\theta^{n+\frac{1}{2}} \nabla V - \nabla \theta^{n+\frac{1}{2}} \qquad n \geq 0 \\ \rho^{n+1} = \Xi(\rho^n, \theta^{n+\frac{1}{2}}) \end{cases}$$

Proposition

Let $(\rho^{n+1}, \theta^{n+\frac{1}{2}})$ *be a solution of the above scheme, then*

$$\mathcal{E}(\rho^{n+1}) + \tau \int_\Omega \frac{|F^{n+\frac{1}{2}}|^2}{2\theta^{n+\frac{1}{2}}} + \tau \mathcal{F}(\theta^{n+\frac{1}{2}}) \leq \mathcal{E}(\rho^n) \qquad (\mathrm{EDI}_\tau)$$

with equality iff $\theta^{n+\frac{1}{2}} \geq \rho^n / e$.

Admissible tessellation of Ω

[Eymard-Gallouët-Herbin '00]

- $\mathcal{T}$: **primal cells**

$$\bigcup_{K\in\mathcal{T}} \overline{K} = \overline{\Omega}, \qquad K\cap L = \emptyset \text{ if } K \neq L.$$

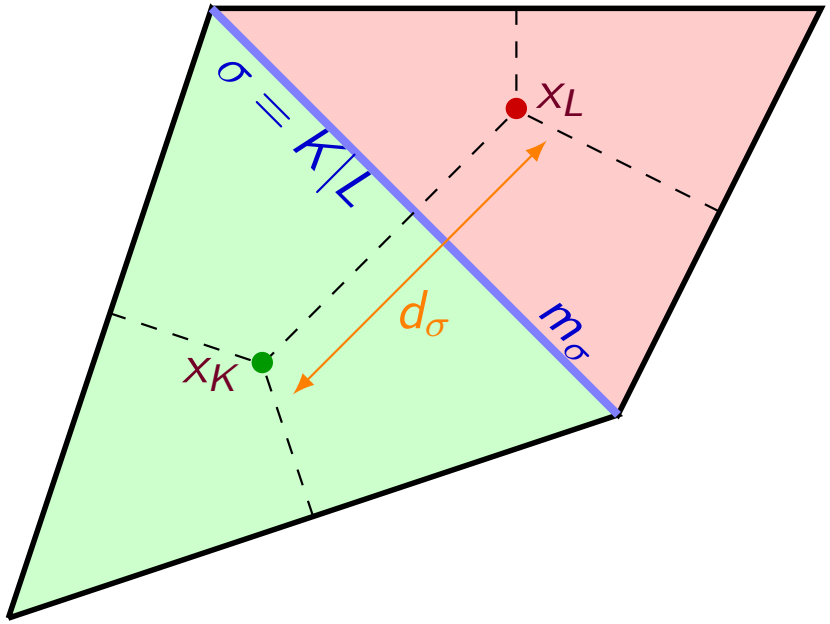
- Σ: **edges / faces**

$$\partial K = \bigcup_{\sigma\in\Sigma_K} \overline{\sigma}, \quad \sigma = K|L \text{ or } \sigma \subset \partial\Omega$$

- $(x_K)_{K\in\mathcal{T}}$: **cell centers**

$$x_K \in K$$

- $(\Delta_\sigma)_{\sigma\in\Sigma}$: **diamond cells**



Orthogonality condition

$$(x_K, x_L) \perp \sigma, \qquad \forall \sigma = K|L \qquad \Longrightarrow \qquad n_{K\sigma} = \frac{x_L - x_K}{d_\sigma}$$

Admissible tessellation of Ω

[Eymard-Gallouët-Herbin '00]

- $\mathcal{T}$: **primal cells**

$$\bigcup_{K\in\mathcal{T}} \overline{K} = \overline{\Omega}, \qquad K\cap L = \emptyset \text{ if } K \neq L.$$

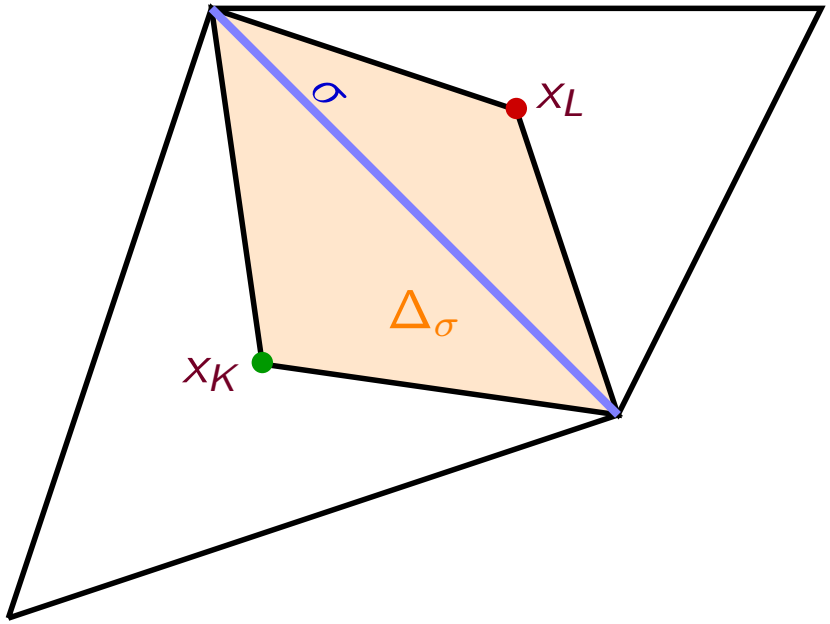
- Σ: **edges / faces**

$$\partial K = \bigcup_{\sigma\in\Sigma_K} \overline{\sigma}, \quad \sigma = K|L \text{ or } \sigma \subset \partial\Omega$$

- $(x_K)_{K\in\mathcal{T}}$: **cell centers**

$$x_K \in K$$

- $(\Delta_\sigma)_{\sigma\in\Sigma}$: **diamond cells**



Orthogonality condition

$$(x_K, x_L) \perp \sigma, \qquad \forall \sigma = K|L \qquad \Longrightarrow \qquad n_{K\sigma} = \frac{x_L - x_K}{d_\sigma}$$

The numerical scheme

Data discretization

- Initial data

$$\rho_K^0 = \frac{1}{m_K} \int_K \rho^0, \qquad K \in \mathcal{T}$$

- External potential and stationary Gibbs measure

$$V_K = V(x_K) \quad \text{and} \quad \pi_K = \pi(x_K) = e^{-V_K}, \qquad K \in \mathcal{T}$$

March in time

- Discrete conservation law

$$\frac{\rho_K^{n+1} - \rho_K^n}{\tau} m_K + \sum_{\sigma \in \Sigma_K} m_\sigma F_{K\sigma}^{n+\frac{1}{2}} = 0, \qquad K \in \mathcal{T}$$

- Local nonlinear extrapolation

$$\rho_K^{n+1} = \Xi(\rho_K^n, \theta_K^{n+\frac{1}{2}}), \qquad K \in \mathcal{T}$$

The numerical scheme (continued)

Discrete fluxes

- No-flux boundary condition:

$$F_{K\sigma}^{n+\frac{1}{2}} = 0 \quad \text{if } \sigma \subset \partial\Omega,$$

- Square-root approximation (SQRA) discrete inner fluxes
  [Lie, Fackeldey & Weber (2013)], [Heida (2018)]

$$F_{K\sigma}^{n+\frac{1}{2}} = \frac{1}{d_\sigma}\pi_\sigma \left(\frac{\theta_K^{n+\frac{1}{2}}}{\pi_K} - \frac{\theta_L^{n+\frac{1}{2}}}{\pi_L} \right) \quad \text{with} \quad \pi_\sigma = \sqrt{\pi_K \pi_L}, \qquad \sigma = K|L \in \Sigma_{\text{int}}$$

The numerical scheme (continued)

Discrete fluxes

- No-flux boundary condition:

$$F_{K\sigma}^{n+\frac{1}{2}} = 0 \quad \text{if } \sigma \subset \partial\Omega,$$

- Square-root approximation (SQRA) discrete inner fluxes
  [Lie, Fackeldey & Weber (2013)], [Heida (2018)]

$$F_{K\sigma}^{n+\frac{1}{2}} = \frac{1}{d_\sigma}\pi_\sigma \left(\frac{\theta_K^{n+\frac{1}{2}}}{\pi_K} - \frac{\theta_L^{n+\frac{1}{2}}}{\pi_L} \right) \quad \text{with} \quad \pi_\sigma = \sqrt{\pi_K \pi_L}, \qquad \sigma = K|L \in \Sigma_{\text{int}}$$

Remarks

- Local conservation property

$$F_{K\sigma}^{n+\frac{1}{2}} + F_{L\sigma}^{n+\frac{1}{2}} = 0, \qquad \sigma = K|L \in \Sigma_{\text{int}}$$

- Exponentially fitted scheme based on flux reformulation

$$F = -\nabla\rho - \rho\nabla V = -\pi\nabla\left(\frac{\rho}{\pi}\right)$$

Well-posedness of the scheme

Proposition

For any $\boldsymbol{\rho}^n \geq 0$ with $\sum_K m_K \rho_K^n > 0$ there exists a unique $\boldsymbol{\theta}^{n+\frac{1}{2}}$ and $\boldsymbol{\rho}^{n+1}$ solution to the scheme. Moreover there holds

$$\theta_K^{n+\frac{1}{2}} > 0, \qquad \rho_K^{n+1} \geq 0, \qquad \sum_{K\in\mathcal{T}} m_K \rho_K^{n+1} = \sum_{K\in\mathcal{T}} m_K \rho_K^n = \int_\Omega \rho^0,$$

and

$$\frac{\rho_K^{n+1} + \rho_K^n}{2} \geq \theta_K^{n+\frac{1}{2}} \geq \min(\rho_K^{n+1}, \rho_K^n)$$

Keypoint of the proof

$$\left(\frac{\theta_K^{n+\frac{1}{2}}}{\pi_K}\right)_K \in \underset{(s_K)_K}{\operatorname{argmin}} \sum_{K\in\mathcal{T}} m_K J_K(s_K) + \sum_{\sigma\in\Sigma_{\mathbf{int}}} \frac{m_\sigma \pi_\sigma}{2 d_\sigma} (s_K - s_L)^2$$

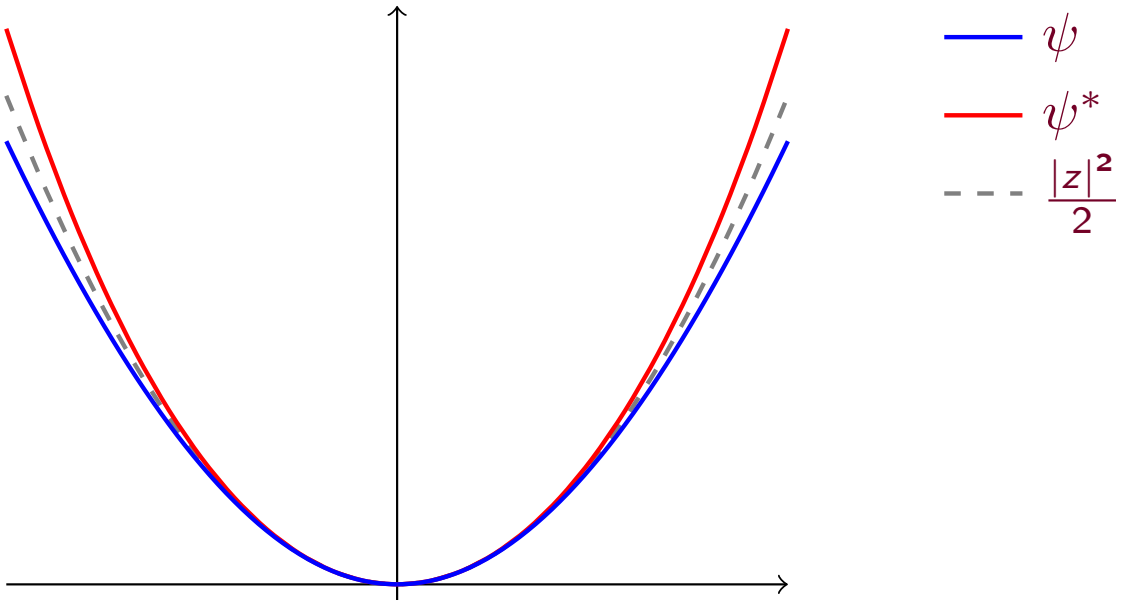
where J_K being the convex antiderivative of $s \mapsto \Xi(\rho_K^n, s\pi_K)$

Cosh-type dissipation potentials

[Peletier, Rossi, Savaré & Tse (2022)], [Peletier & Schlichting (2023)], [CC & Venel (2023)]

$$\psi(z) = 2z \log\left(\frac{z+\sqrt{z^2+4}}{2}\right) - 2\sqrt{4+z^2} + 4$$

$$\psi^*(\xi) = 4(\cosh(\xi/2) - 1)$$



Cosh-type dissipation potentials

[Peletier, Rossi, Savaré & Tse (2022)], [Peletier & Schlichting (2023)], [CC & Venel (2023)]

Geometric mean on the internal edges: $\theta_\sigma^{n+\frac{1}{2}} = \sqrt{\theta_K^{n+\frac{1}{2}} \theta_L^{n+\frac{1}{2}}}$

Discrete Benamou-Brenier functional (jointly convex)

$$\mathcal{D}_\psi(\boldsymbol{\theta}^{n+\frac{1}{2}}, \boldsymbol{F}^{n+\frac{1}{2}}) = \sum_{\sigma \in \Sigma_{\mathbf{int}}} \frac{m_\sigma \theta_\sigma^{n+\frac{1}{2}}}{d_\sigma} \psi\left(\frac{d_\sigma F_\sigma^{n+\frac{1}{2}}}{\theta_\sigma^{n+\frac{1}{2}}} \right) \simeq \frac{1}{2} \int_\Omega \frac{\left| F(t^{n+\frac{1}{2}}) \right|^2}{\rho(t^{n+\frac{1}{2}})}$$

Cosh-type dissipation potentials

[Peletier, Rossi, Savaré & Tse (2022)], [Peletier & Schlichting (2023)], [CC & Venel (2023)]

Geometric mean on the internal edges: $\theta_\sigma^{n+\frac{1}{2}} = \sqrt{\theta_K^{n+\frac{1}{2}} \theta_L^{n+\frac{1}{2}}}$

Discrete Benamou-Brenier functional (jointly convex)

$$\mathcal{D}_\psi(\boldsymbol{\theta}^{n+\frac{1}{2}}, \boldsymbol{F}^{n+\frac{1}{2}}) = \sum_{\sigma \in \Sigma_{\mathbf{int}}} \frac{m_\sigma \theta_\sigma^{n+\frac{1}{2}}}{d_\sigma} \psi\left(\frac{d_\sigma F_\sigma^{n+\frac{1}{2}}}{\theta_\sigma^{n+\frac{1}{2}}} \right) \simeq \frac{1}{2} \int_\Omega \frac{\left| F(t^{n+\frac{1}{2}}) \right|^2}{\rho(t^{n+\frac{1}{2}})}$$

Dual dissipation potential. For $\boldsymbol{F}, \boldsymbol{\xi} \in \mathbb{R}^\Sigma$, set $\langle \boldsymbol{F}, \boldsymbol{\xi} \rangle_\Sigma = \sum_{\sigma \in \Sigma_{\mathbf{int}}} m_\sigma d_\sigma F_\sigma \xi_\sigma$,

$$\mathcal{D}_\psi^*(\boldsymbol{\theta}^{n+\frac{1}{2}}, \boldsymbol{\xi}) = \sup_{\boldsymbol{F} \in \mathbb{R}^\Sigma} \langle \boldsymbol{F}, \boldsymbol{\xi} \rangle_\Sigma - \mathcal{D}_\psi(\boldsymbol{\theta}^{n+\frac{1}{2}}, \boldsymbol{F}) = \sum_{\sigma \in \Sigma_{\mathbf{int}}} \frac{m_\sigma \theta_\sigma^{n+\frac{1}{2}}}{d_\sigma} \psi^*(d_\sigma \xi_\sigma)$$

Cosh-type dissipation potentials

[Peletier, Rossi, Savaré & Tse (2022)], [Peletier & Schlichting (2023)], [CC & Venel (2023)]

Geometric mean on the internal edges: $\theta_\sigma^{n+\frac12} = \sqrt{\theta_K^{n+\frac12}\theta_L^{n+\frac12}}$

Discrete Benamou-Brenier functional (jointly convex)

$$\mathcal{D}_\psi(\boldsymbol{\theta}^{n+\frac12}, \boldsymbol{F}^{n+\frac12}) = \sum_{\sigma\in\Sigma_{\mathbf{int}}} \frac{m_\sigma \theta_\sigma^{n+\frac12}}{d_\sigma} \psi\left(\frac{d_\sigma F_\sigma^{n+\frac12}}{\theta_\sigma^{n+\frac12}}\right) \simeq \frac12 \int_\Omega \frac{\left|F(t^{n+\frac12})\right|^2}{\rho(t^{n+\frac12})}$$

Dual dissipation potential. For $\boldsymbol{F}, \boldsymbol{\xi} \in \mathbb{R}^\Sigma$, set $\langle \boldsymbol{F}, \boldsymbol{\xi}\rangle_\Sigma = \sum_{\sigma\in\Sigma_{\mathbf{int}}} m_\sigma d_\sigma F_\sigma \xi_\sigma$,

$$\mathcal{D}_\psi^*(\boldsymbol{\theta}^{n+\frac12}, \boldsymbol{\xi}) = \sup_{\boldsymbol{F}\in\mathbb{R}^\Sigma} \langle \boldsymbol{F}, \boldsymbol{\xi}\rangle_\Sigma - \mathcal{D}_\psi(\boldsymbol{\theta}^{n+\frac12}, \boldsymbol{F}) = \sum_{\sigma\in\Sigma_{\mathbf{int}}} \frac{m_\sigma \theta_\sigma^{n+\frac12}}{d_\sigma} \psi^*(d_\sigma \xi_\sigma)$$

Discrete Fisher information. $\phi_K^{n+\frac12} = \log \frac{\theta_K^{n+\frac12}}{\pi_K}$ and $(\nabla_\Sigma \boldsymbol{\phi}^{n+\frac12})_{K\sigma} = \frac{\phi_L^{n+\frac12} - \phi_K^{n+\frac12}}{d_\sigma}$

$$\mathcal{F}_\psi(\boldsymbol{\theta}^{n+\frac12}) = \mathcal{D}_\psi^*\left(\boldsymbol{\theta}^{n+\frac12}, \nabla_\Sigma \boldsymbol{\phi}^{n+\frac12}\right) = 2 \sum_{\sigma\in\Sigma_{\mathbf{int}}} \frac{m_\sigma \pi_\sigma}{d_\sigma} \left| \sqrt{\frac{\theta_K^{n+\frac12}}{\pi_K}} - \sqrt{\frac{\theta_L^{n+\frac12}}{\pi_L}} \right|^2$$

Discrete energy dissipation inequality

Flux reformulation

$$F_{K\sigma}^{n+\frac{1}{2}} = \frac{1}{d_\sigma}\pi_\sigma\left(\frac{\theta_K^{n+\frac{1}{2}}}{\pi_K} - \frac{\theta_L^{n+\frac{1}{2}}}{\pi_L}\right) = \frac{2}{d_\sigma}\theta_\sigma^{n+\frac{1}{2}}\sinh\left(\frac{\phi_K^{n+\frac{1}{2}} - \phi_L^{n+\frac{1}{2}}}{2}\right)$$

Young-Fenchel equality

$$\langle \boldsymbol{F}^{n+\frac{1}{2}}, \nabla_\Sigma \phi^{n+\frac{1}{2}}\rangle_\Sigma = -\mathcal{D}_\psi(\boldsymbol{\theta}^{n+\frac{1}{2}}, \boldsymbol{F}^{n+\frac{1}{2}}) - \mathcal{F}_\psi(\boldsymbol{\theta}^{n+\frac{1}{2}}) \qquad \text{(YF)}$$

Discrete energy dissipation inequality

Flux reformulation

$$F_{K\sigma}^{n+\frac{1}{2}} = \frac{1}{d_\sigma}\pi_\sigma\left(\frac{\theta_K^{n+\frac{1}{2}}}{\pi_K} - \frac{\theta_L^{n+\frac{1}{2}}}{\pi_L}\right) = \frac{2}{d_\sigma}\theta_\sigma^{n+\frac{1}{2}}\sinh\left(\frac{\phi_K^{n+\frac{1}{2}} - \phi_L^{n+\frac{1}{2}}}{2}\right)$$

Young-Fenchel equality

$$\langle \boldsymbol{F}^{n+\frac{1}{2}}, \nabla_\Sigma \phi^{n+\frac{1}{2}}\rangle_\Sigma = -\mathcal{D}_\psi(\boldsymbol{\theta}^{n+\frac{1}{2}}, \boldsymbol{F}^{n+\frac{1}{2}}) - \mathcal{F}_\psi(\boldsymbol{\theta}^{n+\frac{1}{2}}) \qquad \text{(YF)}$$

Discrete EDI

Set

$$\mathcal{E}_\mathcal{T}(\boldsymbol{\rho}^n) = \sum_{K\in\mathcal{T}} m_K(h(\rho_K^n) + \rho_K^n V_K), \qquad n \geq 0,$$

then

$$\mathcal{E}_\mathcal{T}(\boldsymbol{\rho}^{n+1}) - \mathcal{E}_\mathcal{T}(\boldsymbol{\rho}^n) + \tau\left(\mathcal{D}_\psi(\boldsymbol{\theta}^{n+\frac{1}{2}}, \boldsymbol{F}^{n+\frac{1}{2}}) + \mathcal{F}_\psi(\boldsymbol{\theta}^{n+\frac{1}{2}})\right) \leq 0$$

Approximate solutions

- Cell-centered density reconstructions

$$\rho_{\mathcal{T},\tau}(t,x) = \rho_K^{n+1}, \quad \theta_{\mathcal{T},\tau}(t,x) = \theta_K^{n+1/2} \quad \text{for a.e. } x \in K, \ t \in (t^n, t^{n+1}]$$

- Edge-based density reconstruction

$$\theta_{\Sigma,\tau}(t,x) = \theta_\sigma^{n+1/2} \quad \text{for a.e. } x \in \Delta_\sigma, \ t \in (t^n, t^{n+1}]$$

where

$$\theta_\sigma^{n+1/2} = \begin{cases} \sqrt{\theta_K^{n+1/2}\theta_L^{n+1/2}} & \text{if } \sigma = K|L \\ \theta_K^{n+1/2} & \text{if } \sigma = \partial K \cap \partial\Omega \end{cases}$$

- Inflated one-directional flux [Chainais-Hillairet, Liu & Peng (2003)]

$$F_{\Sigma,\tau}(t,x) = d\, F_{K\sigma}^{n+1/2} n_{K\sigma} \quad \text{for a.e. } x \in \Delta_\sigma, \ t \in (t^n, t^{n+1}]$$

Sequence of meshes

- Let $(\mathcal{T}_m, \Sigma_m, (x_K)_{K\in\mathcal{T}_m})_{m\geq 0}$ be a sequence of admissible meshes such that

$$h_m = \max_{K\in\mathcal{T}_m} \mathrm{diam}(K) \underset{m\to+\infty}{\longrightarrow} 0$$

  and such that there exist $\zeta > 0$ such that

$$\sum_{\sigma\in\Sigma_K} \frac{m_\sigma d_\sigma}{2d} \leq \zeta m_K \quad \text{and} \quad \zeta^{-1}\,\mathrm{dist}(x_K, K) \leq \mathrm{diam}(K) \leq \zeta \min_{\sigma\in\Sigma_K} d_\sigma\,, \quad \forall\, K \in \mathcal{T}_m$$

- Let $(N_m)_{m\geq 0}$ be such that $N_m \to +\infty$, so that $\tau_m \to 0$.

Remark: We remove the subscript m and denote by $h, \tau \to 0$ the limit $m \to +\infty$

Compactness properties of the approximate solutions

- From the control of the free energy

$$\mathcal{H}_{\mathcal{T}}(\rho_{\mathcal{T},\tau}(t^n)) \leq C_T, \qquad \mathcal{H}_{\mathcal{T}}(\theta_{\mathcal{T},\tau}(t^n)) \leq C_T, \qquad n \geq 0$$

whence

$$\rho_{\mathcal{T},\tau} \underset{h,\tau\to 0}{\longrightarrow} \rho \quad \text{and} \quad \theta_{\mathcal{T},\tau} \underset{h,\tau\to 0}{\longrightarrow} \theta \qquad \text{weakly in } L^1(Q_T)$$

$$\rho_{\mathcal{T},\tau}(T) \underset{h,\tau\to 0}{\longrightarrow} \rho^T \qquad \text{weakly in } L^1(\Omega)$$

- From the control of the dissipation potential

$$\sum_{n=0}^{N-1} \tau \mathcal{D}_\psi(\boldsymbol{\theta}^{n+\frac{1}{2}}, \boldsymbol{F}^{n+\frac{1}{2}}) \leq C \quad \Longrightarrow \quad F_{\Sigma,\tau} \underset{h,\tau\to 0}{\longrightarrow} F \qquad \text{weakly in } L^1(Q_T)^d$$

Compactness properties of the approximate solutions

- From the control of the free energy

$$\mathcal{H}_{\mathcal{T}}(\rho_{\mathcal{T},\tau}(t^n)) \leq C_T, \qquad \mathcal{H}_{\mathcal{T}}(\theta_{\mathcal{T},\tau}(t^n)) \leq C_T, \qquad n \geq 0$$

whence

$$\rho_{\mathcal{T},\tau} \underset{h,\tau\to 0}{\longrightarrow} \rho \quad \text{and} \quad \theta_{\mathcal{T},\tau} \underset{h,\tau\to 0}{\longrightarrow} \theta \qquad \text{weakly in } L^1(Q_T)$$

$$\rho_{\mathcal{T},\tau}(T) \underset{h,\tau\to 0}{\longrightarrow} \rho^T \qquad \text{weakly in } L^1(\Omega)$$

- From the control of the dissipation potential

$$\sum_{n=0}^{N-1} \tau \mathcal{D}_\psi(\boldsymbol{\theta}^{n+\frac{1}{2}}, \boldsymbol{F}^{n+\frac{1}{2}}) \leq C \quad \Longrightarrow \quad F_{\Sigma,\tau} \underset{h,\tau\to 0}{\longrightarrow} F \qquad \text{weakly in } L^1(Q_T)^d$$

Conservation law (weak form)

$$\int_\Omega \rho^T \varphi(T) - \int_\Omega \rho^0 \varphi(0) - \iint_{Q_T} F \cdot \boldsymbol{\nabla} \varphi = 0, \qquad \forall\, \varphi \in C^\infty(\overline{Q}_T)$$

Convergence in the distributional sense

Proposition

Assume that

$$\frac{\tau}{\min_{\sigma\in\Sigma} d_\sigma} \underset{\tau,h\to 0}{\longrightarrow} 0, \tag{CFL}$$

then both reconstructions of the density share the same limit ρ*:*

$$\|\theta_{\mathcal{T},\tau} - \rho_{\mathcal{T},\tau}\|_{L^1(Q_T)} \underset{\tau,h\to 0}{\longrightarrow} 0.$$

Moreover, $\boldsymbol{\nabla}\rho \in L^1(Q_T)$ *and* $F = -\boldsymbol{\nabla}\rho - \rho\boldsymbol{\nabla}V$*.*

Corollary

The limit ρ *solves* (FPE) *in the distributional sense.*

Convergence in the distributional sense

Proposition

Assume that

$$\frac{\tau}{\min_{\sigma\in\Sigma} d_\sigma} \underset{\tau,h\to 0}{\longrightarrow} 0, \tag{CFL}$$

then both reconstructions of the density share the same limit ρ*:*

$$\|\theta_{\mathcal{T},\tau} - \rho_{\mathcal{T},\tau}\|_{L^1(Q_T)} \underset{\tau,h\to 0}{\longrightarrow} 0.$$

Moreover, $\boldsymbol{\nabla}\rho \in L^1(Q_T)$ *and* $F = -\boldsymbol{\nabla}\rho - \rho\boldsymbol{\nabla}V$*.*

Corollary

The limit ρ *solves* (FPE) *in the distributional sense.*

Remark: One can further show that

$$\rho_{\mathcal{T},\tau} \underset{\tau,h\to 0}{\longrightarrow} \rho \quad \text{in } L^1(Q_T).$$

Additional assumption: asymptotic isotropy

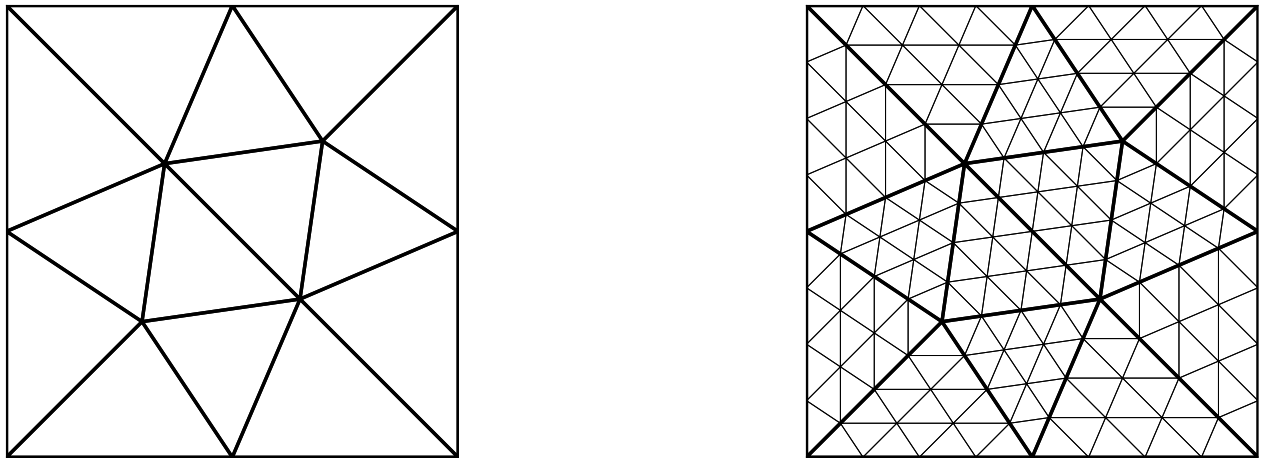
[Eymard, Gallouët & Herbin (2010)], [Gladbach, Kopfer & Maas (2020)]

(Iso) There exists a subset $\mathcal{T}_{\rm iso} \subset \mathcal{T}$ and a nonnegative $\epsilon_{\mathcal{T}} \to 0$ as $h \to 0$, such that

$$(1-\epsilon_{\mathcal{T}})|v|^2 \leq \frac{1}{2m_K} \sum_{\sigma \in \overline{\Sigma}_K} m_\sigma d_\sigma (v \cdot n_{K\sigma})^2 \leq (1+\epsilon_{\mathcal{T}})|v|^2, \quad \forall\, K \in \mathcal{T}_{\rm iso}. \forall\, v \in \mathbb{R}^d$$

Moreover, denoting $\Omega_{\rm iso} := \bigcup \{K\,;\, K \in \mathcal{T}_{\rm iso}\}$ we have

$$\lim_{h \to 0} \text{meas}(\Omega \setminus \Omega_{\rm iso}) = 0$$



Refinement by subdivision [Droniou & Nataraj (2018)]

Energy dissipation principle convergence

[Forkert, Maas & Portinale (2022)], [Heinze, Mielke & Stephan (2025)]

$$\mathcal{E}_\mathcal{T}(\boldsymbol{\rho}^N) + \sum_{n=0}^{N-1} \tau \left(\mathcal{D}_\psi(\boldsymbol{\theta}^{n+\frac{1}{2}}, \boldsymbol{F}^{n+\frac{1}{2}}) + \mathcal{F}_\psi(\boldsymbol{\theta}^{n+\frac{1}{2}}) \right) \leq \mathcal{E}_\mathcal{T}(\boldsymbol{\rho}^0) \qquad (\mathrm{EDI}_{\mathcal{T},\tau})$$

- $\mathcal{E}_\mathcal{T}(\boldsymbol{\rho}^0) \to \mathcal{E}(\rho^0)$ as $h \to 0$
- Lower semi-continuity of the convex energy

$$\mathcal{E}(\rho(T)) \leq \liminf_{h,\tau \to 0} \mathcal{E}_\mathcal{T}(\boldsymbol{\rho}^N)$$

- Γ-lim inf of the jointly convex dissipation potential

$$\iint_{Q_T} \frac{|F|^2}{2\rho} \overset{\text{(Iso)}}{\leq} \liminf_{h,\tau \to 0} \sum_{n=0}^{N-1} \tau \mathcal{D}_\psi(\boldsymbol{\theta}^{n+\frac{1}{2}}, \boldsymbol{F}^{n+\frac{1}{2}})$$

- Γ-lim inf of the convex Fisher infomation

$$\int_0^T \mathcal{F}(\rho) \leq \liminf_{h,\tau \to 0} \sum_{n=0}^{N-1} \tau \mathcal{F}_\psi(\boldsymbol{\theta}^{n+\frac{1}{2}})$$

Energy dissipation principle convergence

[Forkert, Maas & Portinale (2022)], [Heinze, Mielke & Stephan (2025)]

$$\Longrightarrow \quad \mathcal{E}_\mathcal{T}(\rho(T)) + \iint_{Q_T} \frac{|F|^2}{2\rho} + \int_0^T \mathcal{F}(\rho) \leq \mathcal{E}(\rho^0) \qquad \text{(EDI)}$$

- $\mathcal{E}_\mathcal{T}(\boldsymbol{\rho}^0) \to \mathcal{E}(\rho^0)$ as $h \to 0$
- Lower semi-continuity of the convex energy

$$\mathcal{E}(\rho(T)) \leq \liminf_{h,\tau\to 0} \mathcal{E}_\mathcal{T}(\boldsymbol{\rho}^N)$$

- Γ-lim inf of the jointly convex dissipation potential

$$\iint_{Q_T} \frac{|F|^2}{2\rho} \overset{\text{(Iso)}}{\leq} \liminf_{h,\tau\to 0} \sum_{n=0}^{N-1} \tau \mathcal{D}_\psi(\boldsymbol{\theta}^{n+\frac{1}{2}}, \boldsymbol{F}^{n+\frac{1}{2}})$$

- Γ-lim inf of the convex Fisher infomation

$$\int_0^T \mathcal{F}(\rho) \leq \liminf_{h,\tau\to 0} \sum_{n=0}^{N-1} \tau \mathcal{F}_\psi(\boldsymbol{\theta}^{n+\frac{1}{2}})$$

Numerical results

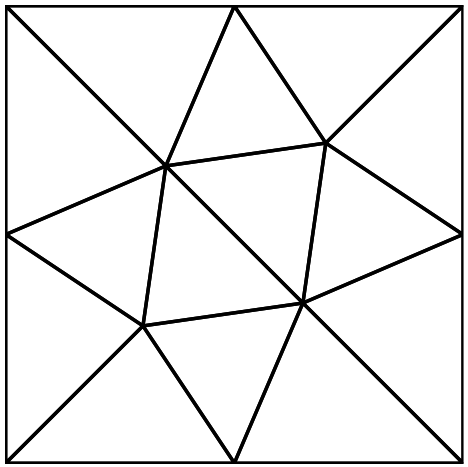
Test case 1: analytical solution

- Data: $\Omega = (0,1)^2$ and $V(x_1, x_2) = -x_1$
- Exact solution:

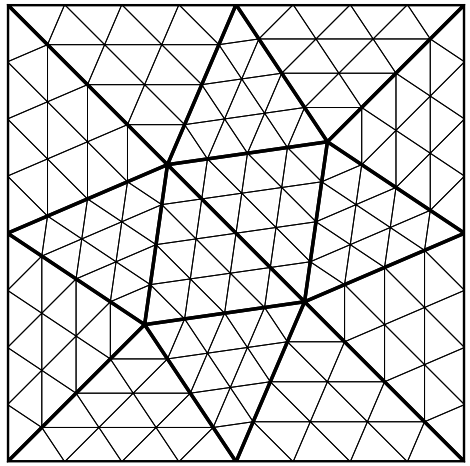
$$\rho(t,(x_1,x_2)) = e^{-(\pi^2+\frac{1}{4})t+\frac{x_1}{2}}\left(\pi\cos(\pi x_1)+\frac{1}{2}\sin(\pi x_1)\right)+\pi e^{x_1-\frac{1}{2}}$$

- Mesh refinement strategies :

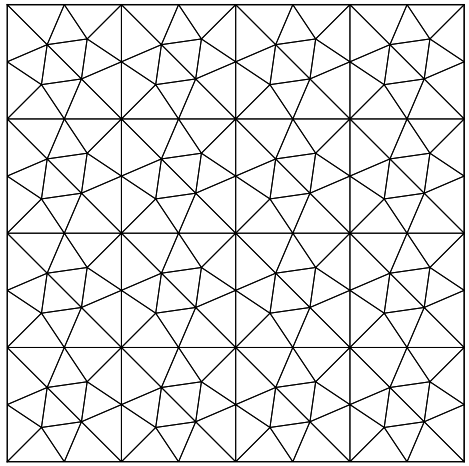
$$h_{m+1} = h_m/2, \quad h_0 = 0.306, \qquad \tau_{m+1} = \tau_m/2, \quad \tau_0 = 0.025$$



Coarsest mesh

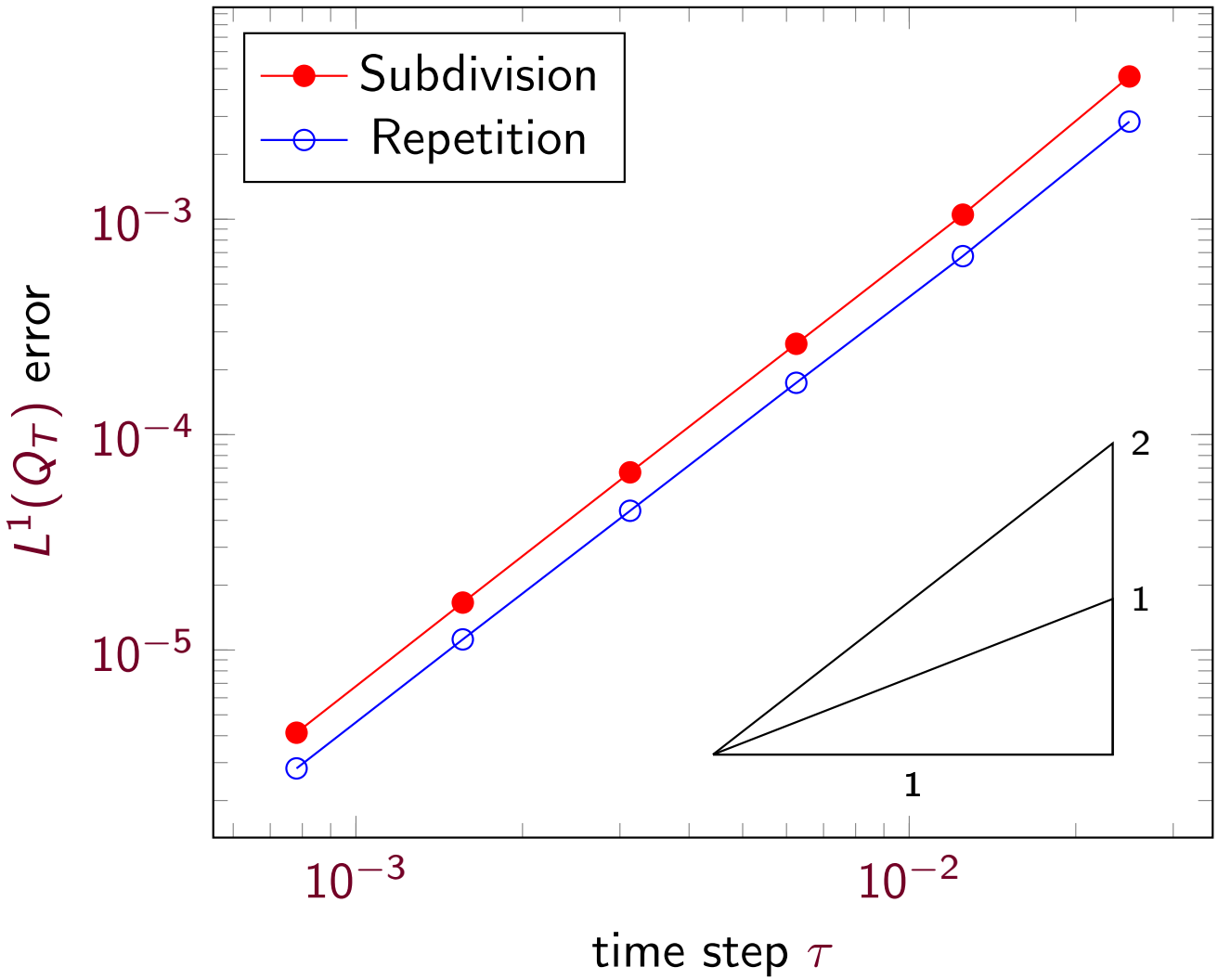


Refinement by subdivision



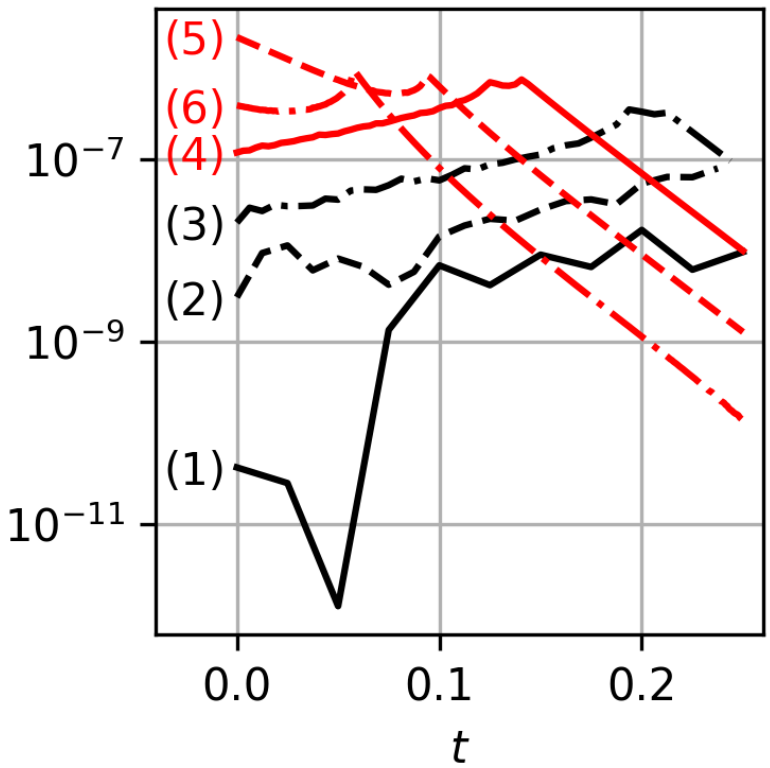
Refinement by repetition

Convergence w.r.t the discretization parameters

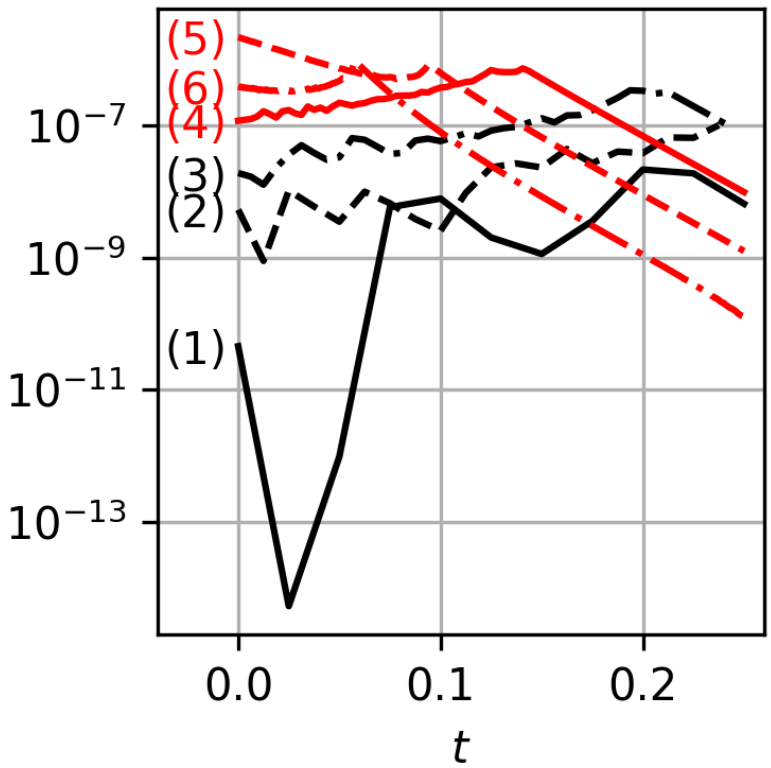


Entropy release

$$\Delta(t^n) = \frac{1}{\tau}\Big[\mathcal{E}_{\mathcal{T}}(\boldsymbol{\rho}^n) - \mathcal{E}_{\mathcal{T}}(\boldsymbol{\rho}^{n+1})) - \mathcal{D}_{\psi}(\boldsymbol{\theta}^{n+1/2}) - \mathcal{D}_{\psi^*}(\boldsymbol{\theta}^{n+1/2})\Big]$$



refinement by subdivision



refinement by repetition

Numerical results

Test case 2: stiff potential

- Data: $\Omega = (-\frac{1}{2}, \frac{1}{2})$ and

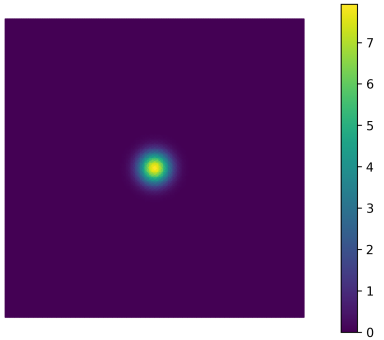
$$V(r\cos\alpha, r\sin\alpha) = 5(1 - \exp(-r^2/\sigma^2))(1 - \cos^6(20r - \alpha))$$

$$\rho^0(r\cos\alpha, r\sin\alpha) = \frac{1}{\sqrt{2\pi}\sigma} \exp(-r^2/\sigma^2)$$

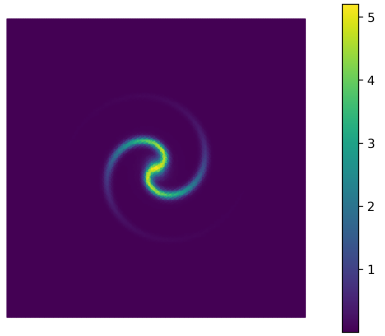
with $\sigma = 10^{-2} \ll 1$.

Numerical results

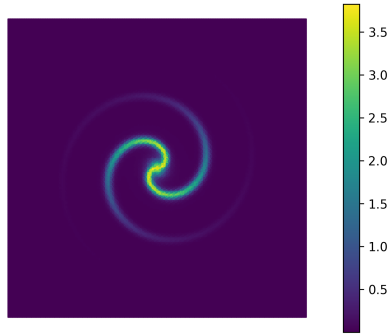
Test case 2: stiff potential



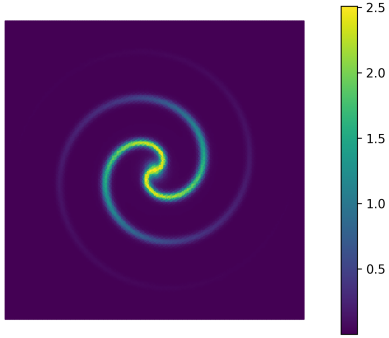
$t = 0$



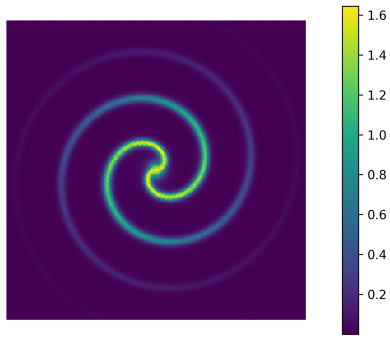
$t = 1.2 \cdot 10^{-2}$



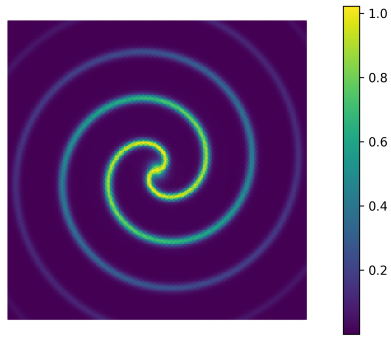
$t = 2.5 \cdot 10^{-2}$



$t = 5 \cdot 10^{-2}$



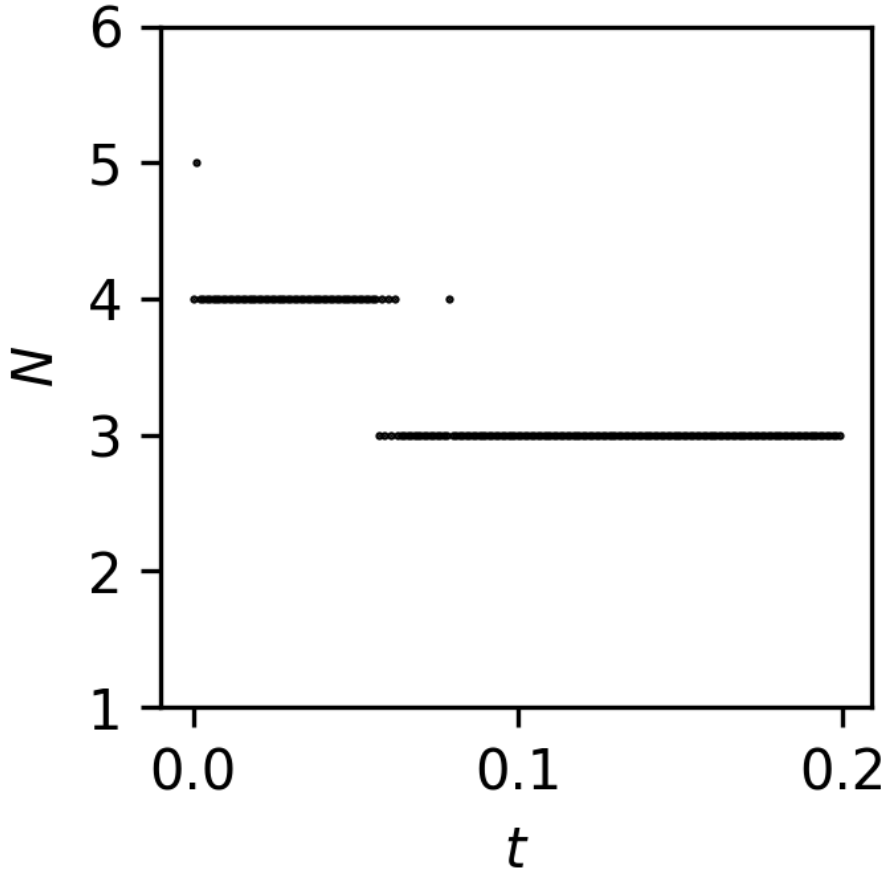
$t = 10^{-1}$



$t = 2 \cdot 10^{-1}$

Numerical results

Test case 2: stiff potential



Number of Newton-Raphson iterations

Conclusion and prospects

Conclusion

- Provably convergent second order in space-time discretization for Fokker-Planck equation
- Scheme designed to capture *de Giorgi*'s functional with second order accuracy
- A cheap local (but nonlinear) extrapolation makes the scheme computationally effective

Prospects

- Scharfetter-Gummel scheme instead of SQRA?
  [Hraivorontska, Schlichting & Tse (2024)]
- Extension to models with cross-diffusion and self-consistent electric drift
  [Burger, Schlake & Wolfram (2012)], [CC, Herda & Massimini (2024)]

Thank you for your attention!