A variational finite volume scheme for Wasserstein gradient flows

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Wasserstein gradient flows

- domain $\Omega \in \mathbb{R}^d$ convex, bounded open
- energy $\mathcal{E} : L^1(\Omega; \mathbb{R}_+) \to [0, +\infty]$, convex
- $\rho^0 \in L^1(\Omega; \mathbb{R}_+)$, $\mathcal{E}(\rho^0) < +\infty$

$$
\begin{aligned}
\partial_t \varrho - \boldsymbol{\nabla} \cdot \left(\varrho \boldsymbol{\nabla} \tfrac{\delta \mathcal{E}}{\delta \rho}[\varrho]\right) = 0 \quad & \text{in } Q_T = \Omega \times (0, T), \\
\varrho \boldsymbol{\nabla} \tfrac{\delta \mathcal{E}}{\delta \rho}[\varrho] \cdot \boldsymbol{n} = 0 \quad & \text{on } \Sigma_T = \partial\Omega \times (0, T), \\
\varrho(\cdot, 0) = \rho^0 \quad & \text{in } \Omega.
\end{aligned}
$$

JKO scheme

- τ time discretization step

$$\begin{cases} \rho_\tau^0 = \rho^0, \\ \rho_\tau^n \in \operatorname{argmin}_\rho \frac{1}{2\tau} W_2^2(\rho, \rho_\tau^{n-1}) + \mathcal{E}(\rho). \end{cases}$$

dynamical formulation

$$\inf_{\rho, \boldsymbol{v}} \frac{1}{2} \int_{t^{n-1}}^{t^n} \int_\Omega \rho |\boldsymbol{v}|^2 \mathrm{d}\boldsymbol{x} \mathrm{d}t + \mathcal{E}(\rho(t^n)),$$

with the constraints $(\rho \geq 0)$

$$\begin{aligned} \partial_t \rho + \boldsymbol{\nabla} \cdot (\rho \boldsymbol{v}) = 0 \quad & \text{in } \Omega \times (t^{n-1}, t^n), \\ \rho \boldsymbol{v} \cdot \boldsymbol{n} = 0 \quad & \text{on } \partial\Omega \times (t^{n-1}, t^n), \\ \rho(t^{n-1}) = \rho_\tau^{n-1} \quad & \text{in } \Omega. \end{aligned}$$

Inf-Sup problem

- $\boldsymbol{m} = \rho \boldsymbol{v}$
- ϕ is the Lagrange multiplier for the continuity equation

$$\inf_{\rho,\boldsymbol{m}} \sup_{\phi} \int_{t^{n-1}}^{t^n} \int_{\Omega} \frac{|\boldsymbol{m}|^2}{2\rho} \mathrm{d}\boldsymbol{x}\mathrm{d}t + \int_{t^{n-1}}^{t^n} \int_{\Omega} (\rho \partial_t \phi + \boldsymbol{m} \cdot \boldsymbol{\nabla} \phi) \mathrm{d}\boldsymbol{x}\mathrm{d}t$$
$$+ \int_{\Omega} [\phi(t^{n-1})\rho_{\tau}^{n-1} - \phi(t^n)\rho(t^n)]\mathrm{d}\boldsymbol{x} + \mathcal{E}(\rho(t^n)).$$

minimize in $\boldsymbol{m}$, $\boldsymbol{m} = -\rho \boldsymbol{\nabla} \phi$.

$$\sup_{\phi} \inf_{\rho} \int_{t^{n-1}}^{t^n} \int_{\Omega} (\partial_t \phi - \frac{1}{2}|\boldsymbol{\nabla}\phi|^2)\rho \mathrm{d}\boldsymbol{x}\mathrm{d}t$$
$$+ \int_{\Omega} [\phi(t^{n-1})\rho_{\tau}^{n-1} - \phi(t^n)\rho(t^n)]\mathrm{d}\boldsymbol{x} + \mathcal{E}(\rho(t^n)).$$

Dual problem

dual problem

$$\sup_{\phi(t^{n-1})} \int_\Omega \phi(t^{n-1})\rho_\tau^{n-1}\mathrm{d}\boldsymbol{x} + \inf_{\rho(t^n)} \left[\mathcal{E}(\rho(t^n)) - \int_\Omega \phi(t^n)\rho(t^n)\mathrm{d}\boldsymbol{x}\right],$$

subject to the constraints

$$\begin{aligned} -\partial_t\phi + \frac{1}{2}|\boldsymbol{\nabla}\phi|^2 \le 0 &\quad \text{in } \Omega \times (t^{n-1}, t^n), \\ \phi(t^n) \le \frac{\delta\mathcal{E}}{\delta\rho}[\rho(t^n)] &\quad \text{in } \Omega, \\ \phi(t^n) = \frac{\delta\mathcal{E}}{\delta\rho}[\rho(t^n)] &\quad \rho(t^n) \text{ a.e.} \end{aligned}$$

Saddle point

- Monotonicity of the initial value of HJ (second membre – final condition)
- Saturation of the inequalities

Optimality conditions :

$$\partial_t \phi - \frac{1}{2}|\nabla \phi|^2 = 0, \quad \text{in } \Omega \times (t^{n-1}, t^n)$$
$$\partial_t \rho - \nabla \cdot (\rho \nabla \phi) = 0, \quad \text{in } \Omega \times (t^{n-1}, t^n)$$

with

$$\rho(t^{n-1}) = \rho_\tau^{n-1}, \quad \text{in } \Omega$$
$$\phi(t^n) = \frac{\delta \mathcal{E}}{\delta \rho}[\rho(t^n)], \quad \text{in } \Omega$$

weighted H^{-1} distance

dissipation

$$D(\rho;\dot\rho) = \frac{1}{2}\inf_{\boldsymbol{v}}\left(\int_\Omega \rho|\boldsymbol{v}|^2 \mathrm{d}\boldsymbol{x}\right)^{1/2}$$

with the constraints

$$\begin{aligned} \dot\rho + \boldsymbol{\nabla}\cdot(\rho\boldsymbol{v}) = 0 \quad & \text{in } \Omega \\ \rho\boldsymbol{v}\cdot\boldsymbol{n} = 0 \quad & \text{on } \partial\Omega \end{aligned}$$

duality $D(\rho;\xi) = (D^*(\rho;\cdot))^*$

$$D(\rho;\rho-\mu) = \frac{1}{2}\|\rho-\mu\|_{\dot H_\rho^{-1}} = \frac{1}{2}\|\psi\|_{\dot H_\rho^1} = \frac{1}{2}\left(\int_\Omega \rho|\boldsymbol{\nabla}\psi|^2 \mathrm{d}\boldsymbol{x}\right)^{1/2} = D^*(\rho;\psi)$$

with ψ solution to

$$\begin{aligned} \rho - \mu - \boldsymbol{\nabla}\cdot(\rho\boldsymbol{\nabla}\psi) = 0 \quad & \text{in } \Omega, \\ \boldsymbol{\nabla}\psi\cdot\boldsymbol{n} = 0 \quad & \text{on } \partial\Omega. \end{aligned}$$

Linearized inf-sup problem

LJKO scheme

$$\rho_\tau^n \in \operatorname*{argmin}_{\rho \in \mathbb{P}(\Omega)} \frac{1}{2\tau} \left\| \rho - \rho_\tau^{n-1} \right\|^2_{\dot{H}_\rho^{-1}(\Omega)} + \mathcal{E}(\rho), \qquad n \geq 1.$$

Change of variable $(\rho, \psi) \mapsto (\rho, \boldsymbol{m} = -\rho \boldsymbol{\nabla} \psi)$

$$\inf_{\rho, \boldsymbol{m}} \int_\Omega \frac{|\boldsymbol{m}|^2}{2\tau\rho} \mathrm{d}\boldsymbol{x} + \mathcal{E}(\rho), \quad \text{subject to: } \begin{cases} \rho - \rho_\tau^{n-1} + \boldsymbol{\nabla} \cdot \boldsymbol{m} = 0 & \text{in } \Omega, \\ \boldsymbol{m} \cdot \boldsymbol{n} = 0 & \text{on } \partial\Omega. \end{cases}$$

saddle point

$$\inf_{\rho, \boldsymbol{m}} \sup_{\phi} \int_\Omega \frac{|\boldsymbol{m}|^2}{2\tau\rho} \mathrm{d}\boldsymbol{x} - \int_\Omega (\rho - \rho_\tau^{n-1}) \phi \, \mathrm{d}\boldsymbol{x} + \int_\Omega \boldsymbol{m} \cdot \boldsymbol{\nabla} \phi \, \mathrm{d}\boldsymbol{x} + \mathcal{E}(\rho),$$

Linearized optimality conditions

saddle point

$$\sup_{\phi} \int_{\Omega} \rho_{\tau}^{n-1} \phi \, \mathrm{d}\boldsymbol{x} + \inf_{\rho} \int_{\Omega} (-\phi - \frac{\tau}{2} |\boldsymbol{\nabla} \phi|^2) \rho \, \mathrm{d}\boldsymbol{x} + \mathcal{E}(\rho).$$

optimality conditions

$$\phi_{\tau}^{n} + \frac{\tau}{2} |\boldsymbol{\nabla} \phi_{\tau}^{n}|^2 = \frac{\delta \mathcal{E}}{\delta \rho} [\rho_{\tau}^{n}],$$

$$\frac{\rho_{\tau}^{n} - \rho_{\tau}^{n-1}}{\tau} - \nabla \cdot (\rho_{\tau}^{n} \boldsymbol{\nabla} \phi_{\tau}^{n}) = 0,$$

monotonicity of discrete HJ equation $\implies$ saturation constraints

Space discretization

Classicale finite volume mesh (ex: Cartesian grids, Delaunay triangulations or Voronoï tessellations.)

- triplet $\left(\mathcal{T}, \overline{\Sigma}, (\boldsymbol{x}_K)_{K\in\mathcal{T}}\right)$
- cell $K \in \mathcal{T}$ measure $m_K > 0$.
- face $\sigma \in \overline{\Sigma}$ measure $m_\sigma = \mathcal{H}^{d-1}(\sigma) > 0$.
- $K \in \mathcal{T}$, $\overline{\Sigma}_K$ of $\overline{\Sigma}$ such that $\partial K = \bigcup_{\sigma\in\overline{\Sigma}_K} \sigma$, $\bigcup_{K\in\mathcal{T}} \overline{\Sigma}_K = \overline{\Sigma}$.
- cell-centers $(\boldsymbol{x}_K)_{K\in\mathcal{T}}$ orthogonal to $K|L$ face of $K, L \in \mathcal{T}$, same orientation as $\boldsymbol{n}_{KL}$ outward w.r.t. K.
- $\Sigma_{\mathrm{ext}} = \{\sigma \subset \partial\Omega\}$ are not involved (no boundary fluxes)
- $\mathcal{N}_K$ the neighboring cells of K
- $d_\sigma = |\boldsymbol{x}_K - \boldsymbol{x}_L|$, diamond cell Δ_σ,
- measure $m_{\Delta_\sigma} = m_\sigma d_\sigma / d$, transitivity $a_\sigma = m_\sigma / d_\sigma$

Upstream weighted dissipation potentials

$L^2(\mathbb{R}^{\mathcal{T}})$ scalar product

$$\langle \boldsymbol{h}, \boldsymbol{\phi} \rangle_{\mathcal{T}} = \sum_{K \in \mathcal{T}} h_K \phi_K m_K, \qquad \forall \boldsymbol{h} = (h_K)_{K \in \mathcal{T}}, \boldsymbol{\phi} = (\phi_K)_{K \in \mathcal{T}},$$

$\frac{1}{2} \|\phi\|^2_{\dot{H}^1_\rho}$ dissipation,

$$D^*_{\mathcal{T}}(\boldsymbol{\rho}; \boldsymbol{\phi}) = \frac{1}{2} \sum_{\substack{\sigma \in \Sigma \\ \sigma = K|L}} a_\sigma \rho_\sigma \left(\phi_K - \phi_L\right)^2 \geq 0,$$

$$\rho_\sigma = \begin{cases} \rho_K & \text{if } \phi_K > \phi_L, \\ \rho_L & \text{if } \phi_K < \phi_L, \end{cases} \qquad \forall \sigma = K|L \in \Sigma.$$

not symmetric $D^*_{\mathcal{T}}(\boldsymbol{\rho}; \boldsymbol{\phi}) \neq D^*_{\mathcal{T}}(\boldsymbol{\rho}; -\boldsymbol{\phi})$

Upstream weighted dissipation potentials II

$$\mathbb{R}_0^{\mathcal{T}} = \left\{ \boldsymbol{h} = (h_K)_{K\in\mathcal{T}} \in \mathbb{R}^{\mathcal{T}} \;\middle|\; \langle \boldsymbol{h}, \mathbf{1}\rangle_{\mathcal{T}} = 0 \right\}$$

$$\mathbb{F}_{\mathcal{T}} = \left\{ \boldsymbol{F} = (F_{K\sigma}, F_{L\sigma})_{\sigma=K|L\in\boldsymbol{\Sigma}} \in \mathbb{R}^{2\boldsymbol{\Sigma}} \;\middle|\; F_{K\sigma} + F_{L\sigma} = 0 \right\}.$$

discrete dissipation

$$D_{\mathcal{T}}(\boldsymbol{\rho}; \boldsymbol{h}) = \inf_{\boldsymbol{F}} \sum_{\sigma\in\boldsymbol{\Sigma}} \frac{(F_\sigma)^2}{2\rho_\sigma} d_\sigma m_\sigma \geq 0, \qquad \forall \boldsymbol{h} \in \mathbb{R}_0^{\mathcal{T}},$$

subject to (continuity equation)

$$h_K m_K = \sum_{\sigma\in\boldsymbol{\Sigma}_K} m_\sigma F_{K\sigma}, \qquad \forall K \in \mathcal{T}.$$

$$\frac{(F_\sigma)^2}{2\rho_\sigma} = \begin{cases} 0 & \text{if } F_\sigma = 0 \text{ and } \rho_\sigma = 0, \\ +\infty & \text{if } F_\sigma > 0 \text{ and } \rho_\sigma = 0, \end{cases}$$

upwind choice

$$\rho_\sigma = \rho_K \text{ if } \; F_{K\sigma} > 0, \quad \rho_L \text{ if } \; F_{L\sigma} > 0,$$

Discrete duality

duality

$$D_{\mathcal{T}}(\boldsymbol{\rho}; \boldsymbol{h}) = \sup_{\phi} \langle \boldsymbol{h}, \phi \rangle_{\mathcal{T}} - D^*_{\mathcal{T}}(\boldsymbol{\rho}; \phi), \qquad \forall \boldsymbol{h} \in \mathbb{R}^{\mathcal{T}}_0.$$

$$D_{\mathcal{T}}(\boldsymbol{\rho}; \boldsymbol{h}) = D^*_{\mathcal{T}}(\boldsymbol{\rho}; \phi) = \frac{1}{2} \langle \boldsymbol{h}, \phi \rangle_{\mathcal{T}}.$$

with (identification)

$$h_K m_K = \sum_{\substack{\sigma \in \Sigma_K \\ \sigma = K|L}} a_\sigma \rho_\sigma (\phi_K - \phi_L), \qquad \forall K \in \mathcal{T},$$

or

$$F_{K\sigma} = \rho_\sigma \frac{\phi_K - \phi_L}{d_\sigma}, \qquad \forall \sigma = K|L \in \Sigma.$$

Discrete JKO

$$\mathbb{P}_{\mathcal{T}} = \left\{ \boldsymbol{\rho} \in \mathbb{R}_+^{\mathcal{T}} \;\middle|\; \langle \boldsymbol{\rho}, \mathbf{1} \rangle_{\mathcal{T}} = \langle \boldsymbol{\rho}^0, \mathbf{1} \rangle_{\mathcal{T}} \right\} = (\boldsymbol{\rho}^0 + \mathbb{R}_0^{\mathcal{T}}) \cap \mathbb{R}_+^{\mathcal{T}}.$$

convexity of $\boldsymbol{\rho} \mapsto D_{\mathcal{T}}(\boldsymbol{\rho}; \boldsymbol{\mu} - \boldsymbol{\rho})$

$$D_{\mathcal{T}}(\boldsymbol{\rho}; \boldsymbol{\mu} - \boldsymbol{\rho}) = \sup_{\boldsymbol{\phi}} \langle \boldsymbol{\mu} - \boldsymbol{\rho}, \boldsymbol{\phi} \rangle_{\mathcal{T}} - D_{\mathcal{T}}^*(\boldsymbol{\rho}; \boldsymbol{\phi}).$$

discrete JKO

$$\boldsymbol{\rho}^n \in \underset{\boldsymbol{\rho} \in \mathbb{P}_{\mathcal{T}}}{\operatorname{argmin}} \frac{1}{\tau} D_{\mathcal{T}}(\boldsymbol{\rho}; \boldsymbol{\rho}^{n-1} - \boldsymbol{\rho}) + \mathcal{E}_{\mathcal{T}}(\boldsymbol{\rho}), \qquad n \geq 1.$$

direct existence uniqueness (of $\boldsymbol{\rho}^n$) and energy estimates

Inf-Sup problem

$$\inf_{\boldsymbol{\rho}\in\mathbb{P}_{\mathcal{T}}} \inf_{\boldsymbol{F}} \frac{1}{\tau} \sum_{\sigma\in\Sigma} \frac{(F_\sigma)^2}{2\rho_\sigma} d_\sigma m_\sigma + \mathcal{E}_{\mathcal{T}}(\boldsymbol{\rho}).$$

ϕ Lagrange multiplier for

$$m_K(\boldsymbol{\rho}^{n-1} - \boldsymbol{\rho}) = \sum_{\sigma\in\Sigma_K} m_\sigma F_{K\sigma}, \qquad \forall K \in \mathcal{T}.$$

minimize in $F_{K\sigma}$, $F_{K\sigma} = \rho_\sigma \frac{\phi_K - \phi_L}{d_\sigma}$

$$\sup_{\boldsymbol{\phi}} \inf_{\boldsymbol{\rho}\geq\mathbf{0}} \left\langle \boldsymbol{\rho}^{n-1} - \boldsymbol{\rho}, \boldsymbol{\phi} \right\rangle_{\mathcal{T}} - \frac{\tau}{2} \sum_{\substack{\sigma\in\Sigma \\ \sigma=K|L}} a_\sigma \rho_\sigma (\phi_K - \phi_L)^2 + \mathcal{E}_{\mathcal{T}}(\boldsymbol{\rho}).$$

Optimality conditions

$$\sup_{\phi} \inf_{\boldsymbol{\rho} \geq \mathbf{0}} \left\langle \boldsymbol{\rho}^{n-1} - \boldsymbol{\rho}, \boldsymbol{\phi} \right\rangle_{\mathcal{T}} - \frac{\tau}{2} \sum_{\substack{\sigma \in \boldsymbol{\Sigma} \\ \sigma = K|L}} a_\sigma \rho_\sigma (\phi_K - \phi_L)^2 + \mathcal{E}_{\mathcal{T}}(\boldsymbol{\rho}).$$

Unique saddle point

$$m_K \phi_K^n + \frac{\tau}{2} \sum_{\sigma \in \boldsymbol{\Sigma}_K} a_\sigma \left((\phi_K^n - \phi_L^n)^+ \right)^2 = \frac{\partial \mathcal{E}_{\mathcal{T}}}{\partial \rho_K}(\boldsymbol{\rho}^n),$$

$$(\rho_K^n - \rho_K^{n-1}) m_K + \tau \sum_{\sigma \in \boldsymbol{\Sigma}_K} a_\sigma \rho_\sigma^n (\phi_K^n - \phi_L^n) = 0$$

up-winding leads saturation of the constraints

Monotonicity

the inverse of the operator $\phi \mapsto \phi + \frac{\tau}{2}|\boldsymbol{\nabla}\phi|^2$ is monotone.

$$\mathcal{G}_K(\boldsymbol{\phi}) := \phi_K + \frac{\tau}{2m_K} \sum_{\substack{\sigma\in\Sigma_K \\ \sigma=K|L}} a_\sigma \left((\phi_K - \phi_L)^+\right)^2, \qquad \forall K \in \mathcal{T}.$$

min ϕ implies $|\boldsymbol{\nabla}\phi|^2 = 0$

lemma

$\boldsymbol{f} \in \mathbb{R}^{\mathcal{T}}$, there exists a unique solution to $\boldsymbol{\mathcal{G}}(\boldsymbol{\phi}) = \boldsymbol{f}$, and it satisfies

$$\min \boldsymbol{f} \leq \boldsymbol{\phi} \leq \max \boldsymbol{f}.$$

let $\boldsymbol{\phi}, \widetilde{\boldsymbol{\phi}}$ be the solutions corresponding to $\boldsymbol{f}$ and $\widetilde{\boldsymbol{f}}$ then

$$\boldsymbol{f} \geq \widetilde{\boldsymbol{f}} \quad \Longrightarrow \quad \boldsymbol{\phi} \geq \widetilde{\boldsymbol{\phi}}.$$

Proof: $\boldsymbol{f} \geq \widetilde{\boldsymbol{f}}$ let K^* be the cell such that

$$\phi_{K^*} - \tilde{\phi}_{K^*} = \min_{K \in \mathcal{T}} \left(\phi_K - \tilde{\phi}_K \right).$$

$$\phi_{K^*} - \tilde{\phi}_{K^*} \leq \phi_L - \tilde{\phi}_L \implies \phi_{K^*} - \phi_L \leq \tilde{\phi}_{K^*} - \tilde{\phi}_L$$

$$\frac{\tau}{2m_K} \sum_{\substack{\sigma \in \Sigma_{K^*} \\ \sigma = K^*|L}} a_\sigma \left((\phi_{K^*} - \phi_L)^+ \right)^2 \leq \frac{\tau}{2m_K} \sum_{\substack{\sigma \in \Sigma_{K^*} \\ \sigma = K^*|L}} a_\sigma \left((\tilde{\phi}_{K^*} - \tilde{\phi}_L)^+ \right)^2.$$

$\mathcal{G}_{K^*}(\phi) \geq \mathcal{G}_{K^*}(\tilde{\phi})$ yields $\phi_{K^*} \geq \tilde{\phi}_{K^*}$

$$\phi_K \geq \tilde{\phi}_K$$

- uniqueness of the solution ϕ of $\boldsymbol{\mathcal{G}}(\phi) = \boldsymbol{f}$
- maximum principle
- Existence

Saturation of the constraints

the inf-sup rewrites $\sup_{\phi} \inf_{\boldsymbol{\rho} \geq \mathbf{0}}$

$$\left\langle \boldsymbol{\rho}^{n-1} - \boldsymbol{\rho}, \boldsymbol{\phi} \right\rangle_{\mathcal{T}} - \frac{\tau}{2} \sum_{\substack{\sigma \in \Sigma \\ \sigma = K|L}} a_\sigma \rho_\sigma (\phi_K - \phi_L)^2 + \mathcal{E}_{\mathcal{T}}(\boldsymbol{\rho})$$

$$= \mathcal{E}_{\mathcal{T}}(\boldsymbol{\rho}) + \left\langle \boldsymbol{\rho}^{n-1} - \boldsymbol{\rho}, \boldsymbol{\phi} \right\rangle_{\mathcal{T}} - \frac{\tau}{2} \sum_{K} \sum_{\substack{\sigma \in \Sigma_K \\ \sigma = K|L}} a_\sigma \rho_K \left((\phi_K - \phi_L)^+ \right)^2$$

$$= \mathcal{E}_{\mathcal{T}}(\boldsymbol{\rho}) + \left\langle \boldsymbol{\rho}^{n-1}, \boldsymbol{\phi} \right\rangle_{\mathcal{T}} - \langle \boldsymbol{\rho}, \boldsymbol{\mathcal{G}}(\boldsymbol{\phi}) \rangle_{\mathcal{T}} .$$

at $\boldsymbol{\rho}^n$, $\boldsymbol{\phi}^n$ is optimal in

$$\sup_{\boldsymbol{\phi}} \mathcal{E}_{\mathcal{T}}(\boldsymbol{\rho}^n) + \left\langle \boldsymbol{\rho}^{n-1}, \boldsymbol{\phi} \right\rangle_{\mathcal{T}} - \langle \boldsymbol{\rho}^n, \boldsymbol{\mathcal{G}}(\boldsymbol{\phi}) \rangle_{\mathcal{T}} .$$

Energy estimates

direct estimate

$$\mathcal{E}_{\mathcal{T}}(\boldsymbol{\rho}^n) + \frac{1}{\tau} D_{\mathcal{T}}(\boldsymbol{\rho}^n; \boldsymbol{\rho}^{n-1} - \boldsymbol{\rho}^n) \leq \mathcal{E}_{\mathcal{T}}(\boldsymbol{\rho}^{n-1})$$

improved estimate

$$\mathcal{E}_{\mathcal{T}}(\boldsymbol{\rho}^n) + \tau D^*_{\mathcal{T}}(\boldsymbol{\rho}^n; \boldsymbol{\phi}^n) + \tau D^*_{\mathcal{T}}\left(\check{\boldsymbol{\rho}}^n; \check{\boldsymbol{\phi}}^n\right) \leq \mathcal{E}_{\mathcal{T}}(\boldsymbol{\rho}^{n-1}),$$

$\check{\boldsymbol{\rho}}^n$ solution of classical backward Euler

$$(\check{\rho}^n_K - \rho^{n-1}_K) m_K + \tau \sum_{\sigma \in \Sigma_K} a_\sigma \check{\rho}^n_\sigma (\check{\phi}^n_K - \check{\phi}^n_L) = 0, \qquad \check{\phi}^n_K = \frac{1}{m_K} \frac{\partial \mathcal{E}_{\mathcal{T}}}{\partial \rho_K}(\check{\boldsymbol{\rho}}^n)$$

Convergence

$$m_K \phi_K^n + \frac{\tau}{2} \sum_{\sigma \in \Sigma_K} a_\sigma \big((\phi_K^n - \phi_L^n)^+ \big)^2 = \frac{\partial \mathcal{E}_\mathcal{T}}{\partial \rho_K}(\boldsymbol{\rho}^n),$$

$$(\rho_K^n - \rho_K^{n-1}) m_K + \tau \sum_{\sigma \in \Sigma_K} a_\sigma \rho_\sigma^n (\phi_K^n - \phi_L^n) = 0$$

- weak solution of $\partial_t \varrho - \boldsymbol{\nabla} \cdot (\varrho \boldsymbol{\nabla} \frac{\delta \mathcal{E}}{\delta \rho}[\varrho]) = 0$
- Fokker-Planck, non linear diffusion without drift

$$\mathcal{E}_\mathcal{T}(\boldsymbol{\rho}) = \sum_{K \in \mathcal{T}} m_K \left[\rho_K \log \frac{\rho_K}{e^{-V_K}} - \rho_K + e^{-V_K} \right]$$

- difficulty : $\frac{\tau}{2} |\boldsymbol{\nabla} \phi|^2 \to 0$ everywhere

Numerical simulations

Newton method $\boldsymbol{u}^{n,k+1} = \boldsymbol{u}^{n,k} + \boldsymbol{d}^k$, $\boldsymbol{d}^k = (\boldsymbol{d}^k_\phi, \boldsymbol{d}^k_\rho)$

$$\boldsymbol{J}^k \boldsymbol{d}^k = \begin{bmatrix} \boldsymbol{J}^k_{\phi,\phi} & \boldsymbol{J}^k_{\phi,\rho} \\ \boldsymbol{J}^k_{\rho,\phi} & \boldsymbol{J}^k_{\rho,\rho} \end{bmatrix} \begin{bmatrix} \boldsymbol{d}^k_\phi \\ \boldsymbol{d}^k_\rho \end{bmatrix} = \begin{bmatrix} \boldsymbol{f}^k_\phi \\ \boldsymbol{f}^k_\rho \end{bmatrix}.$$

$\boldsymbol{f}^k_\phi$ and $\boldsymbol{f}^k_\rho$: discrete HJ and continuity equations at $\boldsymbol{u}^{n,k}$. when $\boldsymbol{J}^k_{\rho,\rho}$ diagonal, Schur complement.

$$\left[\boldsymbol{J}^k_{\phi,\phi} - \boldsymbol{J}^k_{\phi,\rho} (\boldsymbol{J}^k_{\rho,\rho})^{-1} \boldsymbol{J}^k_{\rho,\phi}\right] \boldsymbol{d}^k_\phi = \boldsymbol{f}^k_\phi - \boldsymbol{J}^k_{\phi,\rho} (\boldsymbol{J}^k_{\rho,\rho})^{-1} \boldsymbol{f}^k_\rho,$$

and $\boldsymbol{d}^k_\rho = (\boldsymbol{J}^k_{\rho,\rho})^{-1} (\boldsymbol{f}^k_\rho - \boldsymbol{J}^k_{\rho,\phi} \boldsymbol{d}^k_\phi)$.

Numerical simulations, test cases

Stable and efficient for more energies

- Fokker-planck (gravity)

$$\mathcal{E}(\rho) = \int_\Omega [\rho \log \frac{\rho}{e^{-V}} - \rho + e^{-V}] \mathrm{d}\boldsymbol{x}.$$

$$\partial_t \varrho = \Delta \varrho + \nabla \cdot (\varrho \nabla V) \quad \text{in } Q_T, \tag{1}$$

  with no-flux boundary conditions and initial condition.

- null zone: Porous medium

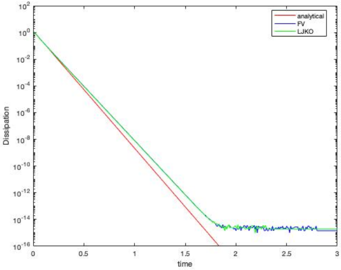
$$\mathcal{E}(\rho) = \int_\Omega \frac{1}{m-1} \rho^m + \rho V,$$

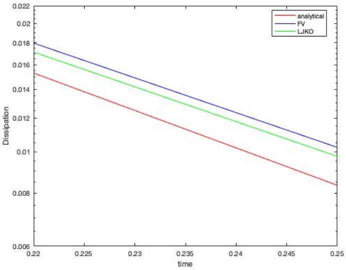
$$\partial_t \rho = \Delta \rho^m + \boldsymbol{\nabla} \cdot (\rho \boldsymbol{\nabla} V),$$

- System : salinity intrusion

Fokker-planck (gravity)

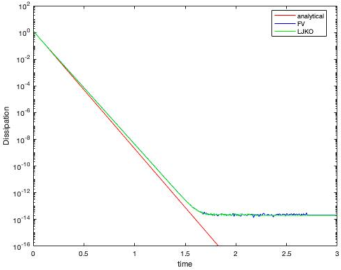
$T = 3, \tau = 0.01, h = 0.1493$

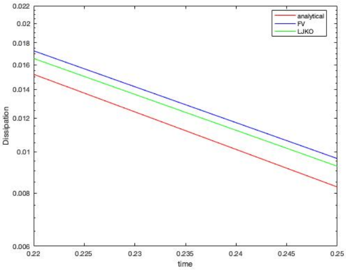




Fokker-planck (gravity) II

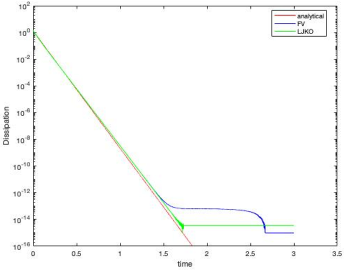
$T = 3, \tau = 0.0063, h = 0.0373$

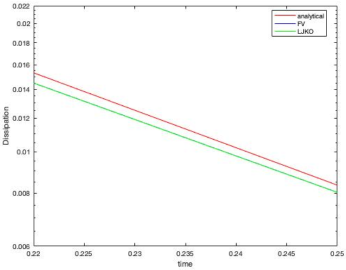




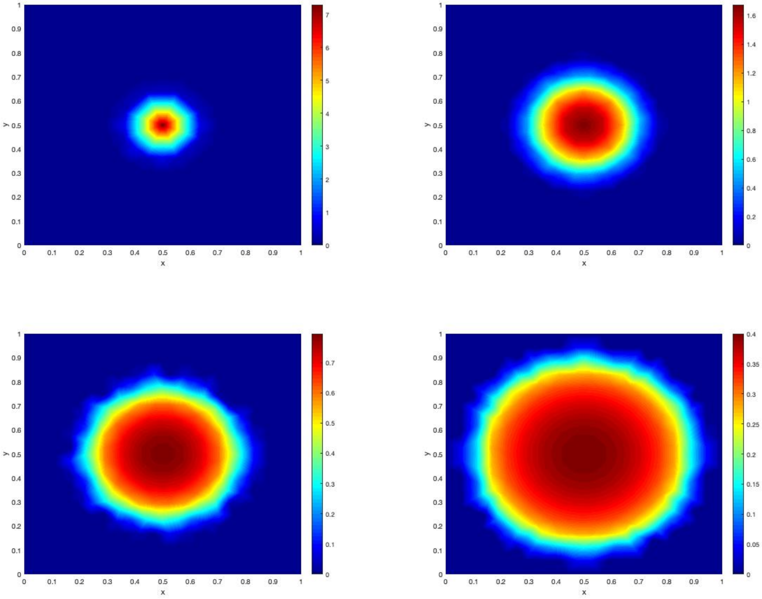
Fokker-planck (gravity) III

$T = 3, \tau = 0.0001, h = 0.1493$





Porous medium



Salinity intrusion

$$\begin{cases} \partial_t f - \nabla \cdot (\nu f \nabla (f + g + b)) = 0 & \text{in } \Omega \times (0, T) \\ \partial_t g - \nabla \cdot (g \nabla (\nu f + g + b)) = 0 & \text{in } \Omega \times (0, T) \end{cases}$$

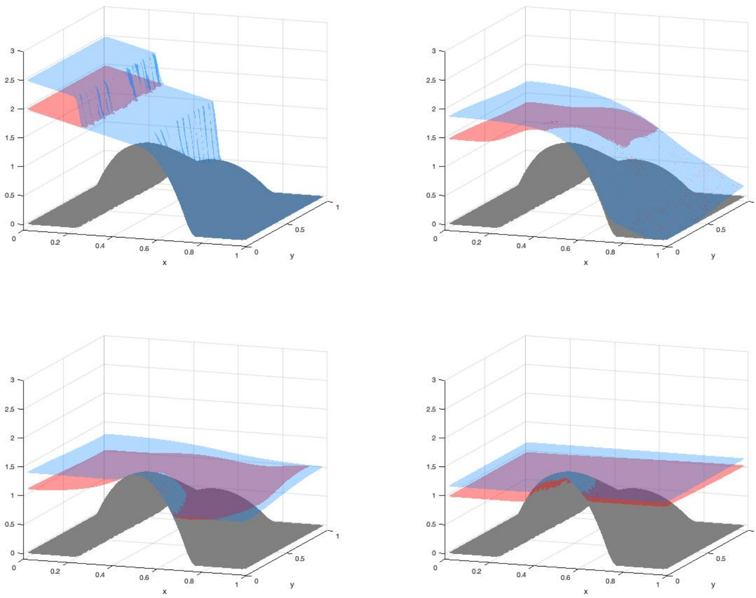
with no-flux boundary conditions

$$\nabla f \cdot \boldsymbol{n} = \nabla g \cdot \boldsymbol{n} = 0 \quad \text{on } \partial\Omega \times (0, T),$$

$\nu = \frac{\rho_f}{\rho_s}$ is the ratio between the constant mass density of the fresh and salt water. Wasserstein gradient flow with respect to the energy

$$\mathcal{E}(f, g) = \int_\Omega \left(\frac{\nu}{2}(f + g + b)^2 + \frac{1 - \nu}{2}(g + b)^2 \right) \mathrm{d}\boldsymbol{x}.$$

Salinity intrusion



Thank you for listening!