

Lagrangian discretizations of compressible fluids with semi-discrete OT

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Joint work with Thomas O. Gallouët and Quentin Mérigot

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→ Focus on convergence towards **smooth solutions**

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- Generalize to complex scenarios: **void** / modelling particle interactions
- Focus on two classes of models:
 - **BAROTROPIC EULER** (conservative)

$$\begin{cases} \partial_t(\rho u) + \nabla \cdot (\rho u \otimes u) + \nabla P(\rho) = 0 \\ \partial_t \rho + \operatorname{div}(\rho u) = 0 \end{cases}$$

- **POROUS MEDIA** (dissipative)

$$\partial_t \rho - \Delta P(\rho) = 0$$

- PRESSURE: depends on density only / defined by $P : [0, +\infty) \rightarrow \mathbb{R}$

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- PRESSURE: depends on density only / defined by $P : [0, +\infty) \rightarrow \mathbb{R}$
- Same physical model in different regimes

1. OVERVIEW

Eulerian setting / High friction limit

- Energy for barotropic Euler on $M \subset \mathbb{R}^d$ (**compact domain**)

$$\mathcal{E}(\rho, u) = \frac{1}{2} \int_M |u|^2 \rho + \mathcal{U}(\rho), \quad \mathcal{U}(\rho) := \int_M U(\rho)$$

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- Thermodynamics:

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BAROTROPIC EULER (non-conservative form)

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DISSIPATIVE LIMIT: $\xi \rightarrow +\infty$

$$\begin{cases} \partial_t u + (u \cdot \nabla) u + \nabla U'(\rho) = -\xi u \\ \partial_t \rho + \operatorname{div}(\rho u) = 0 \end{cases}$$

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- In both cases, density evolves according to **continuity equation**

Lagrangian setting / L^2 structure

- Set $\mathbb{X} := L^2_{\rho_0}(M; \mathbb{R}^d)$. Lagrangian flow $X : [0, T] \rightarrow \mathbb{X}$

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where $\mathcal{F} : D \subset \mathbb{X} \rightarrow \mathbb{R}$

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- Lagrangian counterpart of Wasserstein gradient flow (Otto '01)

Particle discretization

Discrete setting

Given a fixed partition of M , $\mathcal{P}_N = (P_1, \dots, P_N)$,

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- *Smoothed Particle Hydrodynamics* (SPH): $\rho_N^\varepsilon(t) = K_\varepsilon * \rho_N(t)$
 - (+) Flexibility in kernel design \Rightarrow Moment preservation / "high order"
 - (-) Convergence / $U(r) = r^2$ (Franz and Wendland '18)
 - \Rightarrow Choice of kernel is important

L^2 envelope approach

Moreau-Yosida regularization

Given $X_N \in \mathbb{X}_N$, define $\mathcal{F}_\varepsilon : \mathbb{X}_N \rightarrow \mathbb{R}$ by

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- (Leclerc et al. '20) Convergence by direct method for gradient flows:

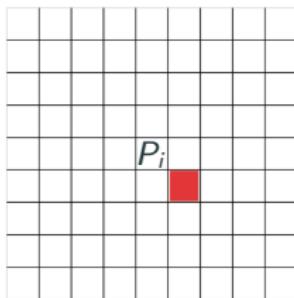
$$\mathcal{U}(\rho) = \int \rho \log \rho, \quad \mathcal{U}(\rho) = \begin{cases} 0 & \text{if } \rho \leq 1 \\ +\infty & \text{otherwise} \end{cases}$$

Regularized flow/density

- Minimum in regularized energy is attained by a minimizer X_N^ε

$$\mathcal{F}_\varepsilon(X_N) = \min_{\sigma \in \mathbb{X}} \frac{\|X_N - \sigma\|_{\mathbb{X}}^2}{2\varepsilon} + \mathcal{F}(\sigma) = \frac{\|X_N - X_N^\varepsilon\|_{\mathbb{X}}^2}{2\varepsilon} + \mathcal{F}(X_N^\varepsilon)$$

- X_N^ε NOT uniquely determined:

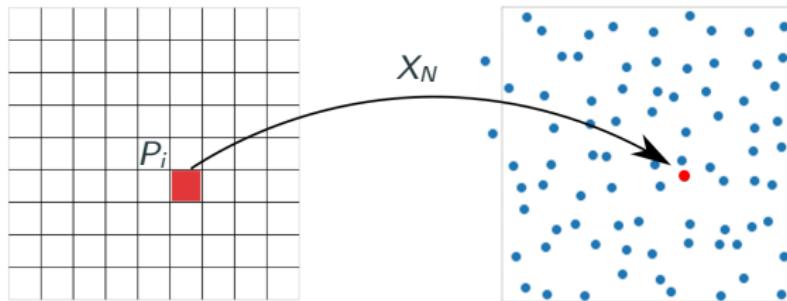


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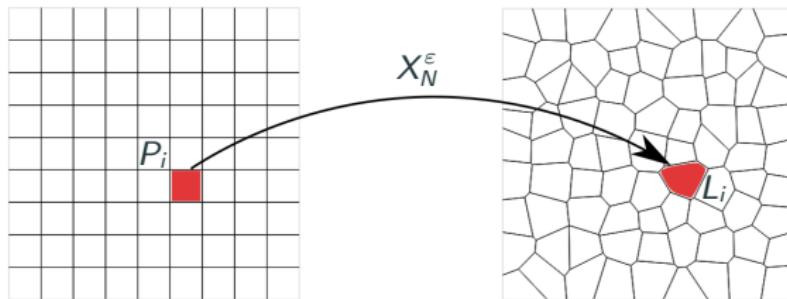


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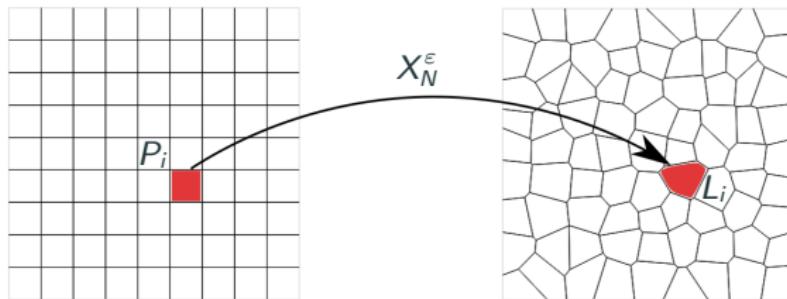


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- $X_N^\varepsilon(P_i) = L_i \leftarrow$ **Laguerre cell** (Voronoi tessellation)
- Regularized density (without convolution):

$$\rho_N^\varepsilon := (X_N^\varepsilon)_\# \rho_0 \quad \Rightarrow \quad \mathcal{U}(\rho_N^\varepsilon) < +\infty$$

Discrete dynamical system (Gradient flow)

- Time/Space-discrete version of $\dot{X} = -\nabla_{\mathbb{X}} \mathcal{F}(X)$

$X_N(t_n) \leftarrow \text{Current state}$

$$X_N^\varepsilon(t_n) \in \operatorname{argmin}_{\sigma \in \mathbb{X}} \frac{\|X_N(t_n) - \sigma\|_{\mathbb{X}}^2}{2\varepsilon} + \mathcal{F}(\sigma)$$

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Potential energy

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Dynamics on $[t_n, t_{n+1})$

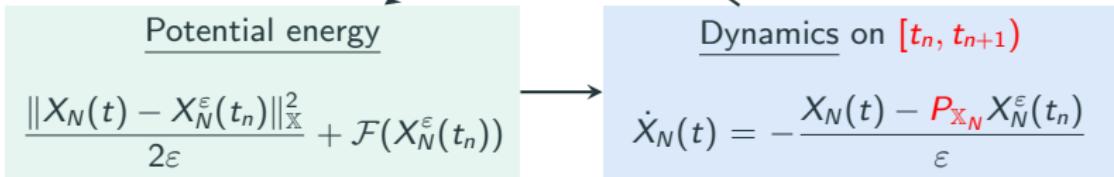
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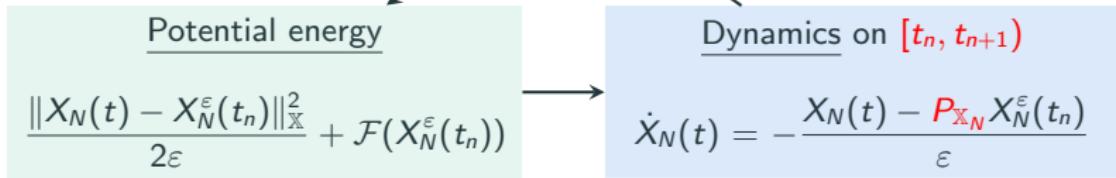


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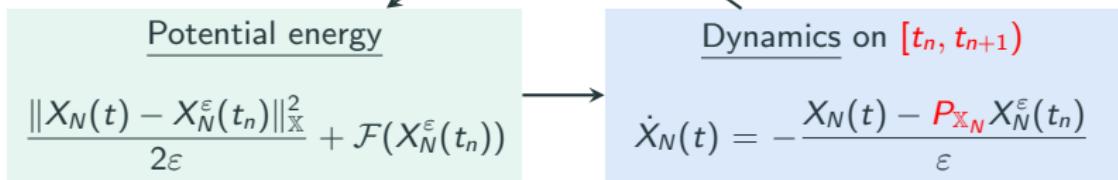
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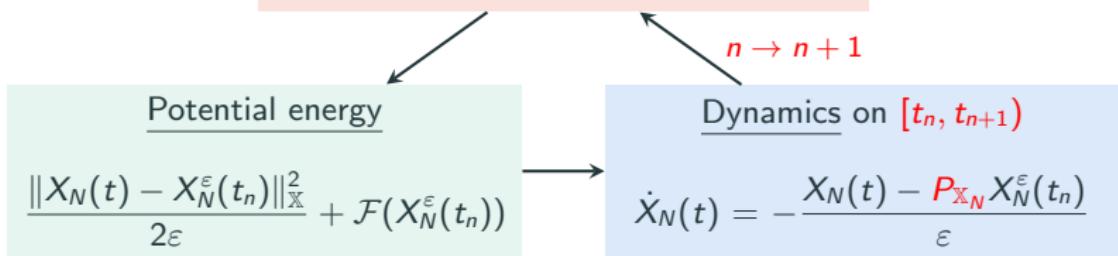
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$$X_N^\varepsilon(t_n) \in \operatorname{argmin}_{\sigma \in \mathbb{X}} \frac{\|X_N(t_n) - \sigma\|_{\mathbb{X}}^2}{2\varepsilon} + \mathcal{F}(\sigma)$$



STABILITY

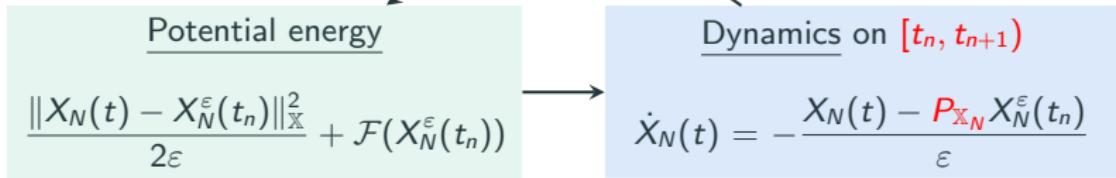
$$\mathcal{F}_\varepsilon(X_N(t_{n+1})) \leq \frac{\|X_N(t_n) - X_N^\varepsilon(t_n)\|_{\mathbb{X}}^2}{2\varepsilon} + \mathcal{F}(X_N^\varepsilon(t_n))$$

Discrete dynamical system (Gradient flow)

- Time/Space-discrete version of $\dot{X} = -\nabla_{\mathbb{X}} \mathcal{F}(X)$

$X_N(t_n) \leftarrow \text{Current state}$

$$X_N^\varepsilon(t_n) \in \operatorname{argmin}_{\sigma \in \mathbb{X}} \frac{\|X_N(t_n) - \sigma\|_{\mathbb{X}}^2}{2\varepsilon} + \mathcal{F}(\sigma)$$



STABILITY

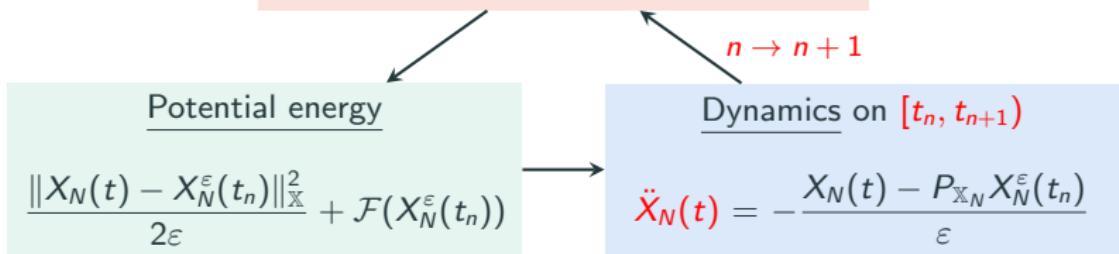
$$\mathcal{F}_\varepsilon(X_N(t_{n+1})) \leq \frac{\|X_N(\textcolor{red}{t_n}) - X_N^\varepsilon(t_n)\|_{\mathbb{X}}^2}{2\varepsilon} + \mathcal{F}(X_N^\varepsilon(t_n)) = \mathcal{F}_\varepsilon(X_N(t_n))$$

Discrete dynamical system (Euler)

- Time/Space-discrete version of $\ddot{\mathbf{X}} = -\nabla_{\mathbb{X}} \mathcal{F}(\mathbf{X})$

$X_N(t_n)$ and $\dot{X}_N(t_n) \leftarrow \underline{\text{Current state}}$

$$X_N^\varepsilon(t_n) \in \operatorname{argmin}_{\sigma \in \mathbb{X}} \frac{\|X_N(t_n) - \sigma\|_{\mathbb{X}}^2}{2\varepsilon} + \mathcal{F}(\sigma)$$



STABILITY

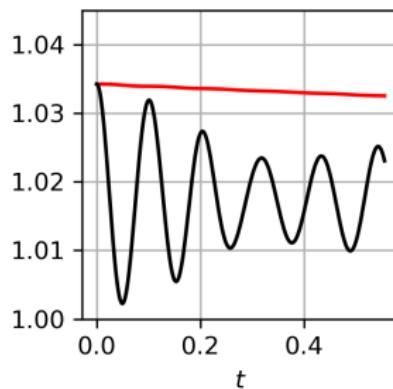
$$\frac{\|\dot{X}_N(t_{n+1})\|_{\mathbb{X}}^2}{2} + \mathcal{F}_\varepsilon(X_N(t_{n+1})) \leq \frac{\|\dot{X}_N(t_n)\|_{\mathbb{X}}^2}{2} + \mathcal{F}_\varepsilon(X_N(t_n))$$

Simulations - Euler / $U(r) = r^2$

INITIAL CONDITIONS

$$M = [-0.5, 0.5]^2, \quad \rho(0, x) = C_0 + C_1 \exp\left(-\frac{|x|^2}{2\sigma^2}\right), \quad u(0, \cdot) = 0$$

POTENTIAL/TOTAL



Simulations - Euler / $U(r) = r^2$

INITIAL CONDITIONS

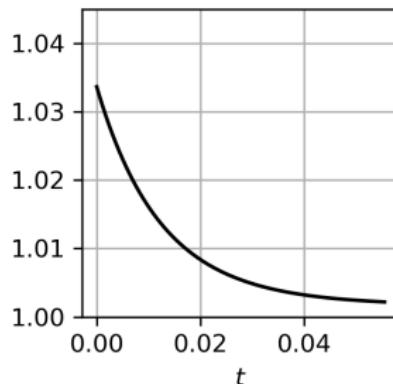
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Simulations - Gradient flow / $U(r) = r^2$

INITIAL CONDITIONS

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POTENTIAL



Simulations - toy dam break

POTENTIAL ENERGY

$$\int_M \rho^2 + g \int_M y \rho \leftarrow \text{Gravity}$$

2. CONVERGENCE

Main results - Euler

- Initial conditions: $X_N(0) = P_{\mathbb{X}_N} \text{Id}$ (Velocity: $\dot{X}_N(0) = u(0, X_N(0))$)
- Initial mesh size: $h_N = \max_i \text{diam}(P_i)$
- Smooth str. convex U , such that $|P''(r)| \leq CU''(r)$

Theorem: Convergence Euler

Hyp.: (ρ, u) strong solution, $u \in C^1(0, T; C^{2,1}(M))$, $\rho_0 \in C^{1,1}(M)$; either $\rho \geq \rho_{min} > 0$ or $|U'''_+(0)| < +\infty$. Then,

$$\|\dot{X}_N(T) - u(T, X_N(T))\|_{\mathbb{X}}^2 + \|X_N(T) - X(T)\|_{\mathbb{X}}^2 \leq C\left(\frac{h_N^2}{\varepsilon} + h_N + \varepsilon + \frac{\tau}{\varepsilon}\right),$$

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- Role of ε : CFL condition $\tau = o(\varepsilon)$ / Scaling $h_N^2 = o(\varepsilon)$
→ Rate 1/2 for optimal choice
- Positivity non necessary as long as $|U_+'''(0)| < +\infty$

Main results - Gradient flow

- Initial conditions: $X_N(0) = P_{\mathbb{X}_N} \text{Id}$ (Velocity: $\dot{X}_N(0) = u(0, X_N(0))$)
- Initial mesh size: $h_N = \max_i \text{diam}(P_i)$
- Smooth str. convex U , such that $|P''(r)| \leq CU''(r)$

Theorem: Convergence gradient flow

Hyp.: ρ strong solution, $\rho_0 \in C^{1,1}(M)$ and $u_t := -\nabla U'(\rho_t) \in C^{2,1}$ uniformly on $[0, T]$; either $\rho \geq \rho_{min} > 0$ or $|U_+'''(0)| < +\infty$. Then,

$$\int_0^T \|\dot{X}_N(s) - u(s, X_N(s))\|_{\mathbb{X}}^2 ds + \|X_N(T) - X(T)\|_{\mathbb{X}}^2 \leq C\left(\frac{h_N^2}{\varepsilon} + h_N + \varepsilon + \frac{\tau}{\varepsilon}\right),$$

- Role of ε : CFL condition $\tau = o(\varepsilon)$ / Scaling $h_N^2 = o(\varepsilon)$
→ Rate 1/2 for optimal choice
- Positivity non necessary as long as $|U_+'''(0)| < +\infty$
- Integral of velocity error on left-hand side

Wasserstein distance/semi-discrete OT

Wasserstein distance

Given $\rho, \mu \in \mathcal{P}(M)$, $W_2^2(\mu, \rho) := \inf \left\{ \int_M |T(x) - x|^2 d\rho, T_{\#}\rho = \mu \right\}$

Brenier's theorem: ρ a.c. $\implies T = \nabla \psi$, where ψ is a convex function

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$$L_i := \{x \in M : |x - X_i|^2 - w_i \leq |x - X_j|^2 - w_j \quad \forall i \neq j\}$$

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- Newton's method to solve for w_i (Kitagawa, Mérigot, Thibert '16)

Eulerian view on regularized energy

$$\mathcal{F}_\varepsilon(X_N) = \inf_{\sigma \in X} \frac{\|X_N - \sigma\|_{\mathbb{X}}^2}{2\varepsilon} + \mathcal{U}(\sigma_\# \rho_0) = \inf_{\rho \in \mathcal{P}_{ac}(M)} \frac{W_2^2(\rho_N, \rho)}{2\varepsilon} + \mathcal{U}(\rho)$$

We need it for: COMPUTATIONS / PROOF

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- Let $\nabla\psi$ optimal map from ρ_N^ε to ρ_N
- $\nabla\psi$ defined via Laguerre decomposition $(L_i)_i$ with weights $(w_i)_i$
- ρ_N^ε has an EXPLICIT expression:

$$\rho_N^\varepsilon|_{L_i} = (2\varepsilon U')^{-1}((w_i - |x - X_i|^2) \vee U'(0)),$$

$$\int_{L_i} \rho_N^\varepsilon = \int_{P_i} \rho_0$$

- Weights w_i are determined via a Newton's solve

C++ libraries with Python wrappers **pysdot/sdot** (Hugo Leclerc)

Computing $\nabla_{\mathbb{X}_N} \mathcal{F}_\varepsilon$

DISCRETE SCHEME

$$\ddot{X}_N(t) = -\frac{X_N(t) - P_{\mathbb{X}_N} X_N^\varepsilon(t_n)}{\varepsilon}, \quad X_N^\varepsilon(t_n) \in \operatorname{argmin}_{\sigma \in \mathbb{X}} \frac{\|X_N(t_n) - \sigma\|_{\mathbb{X}}^2}{2\varepsilon} + \mathcal{F}(\sigma)$$

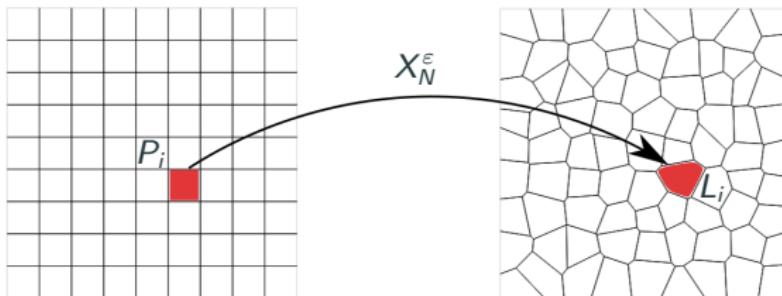
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X_N^ε is ANY map pushing $\rho_0|_{P_i}$ to $\rho_N^\varepsilon|_{L_i}$

$$(P_{\mathbb{X}_N} X_N^\varepsilon) : P_i \rightarrow \text{barycenter}(\rho_N^\varepsilon|_{L_i})$$



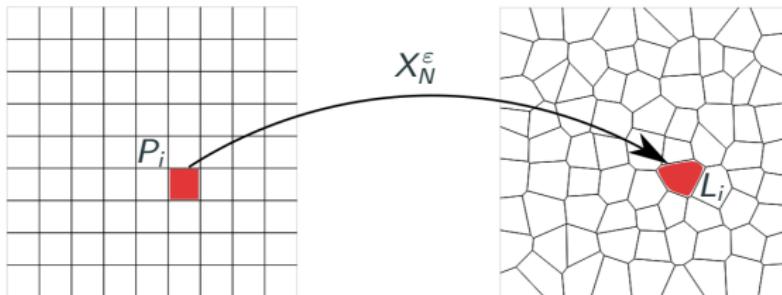
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- Note: $(P_{\mathbb{X}_N} X_N^\varepsilon)$ is UNIQUE (if $X_i \neq X_j$) since so is ρ_N^ε

Modulated energy: Euclidean setting

- Dynamical system on \mathbb{R}^n : find $Y : [0, T] \rightarrow \mathbb{R}^n$ solving

$$\ddot{Y}(t) = -\nabla F(Y(t)), \quad Y(0) = Y_0, \quad \dot{Y}(0) = \dot{Y}_0$$

where $F : \mathbb{R}^n \rightarrow \mathbb{R}$ is **CONVEX**

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- Energy convex function on state space (\dot{Y}, Y)

$$\frac{|\dot{Y}|^2}{2} + F(Y)$$

- Modulated energy (relative entropy): $Y, Z : [0, T] \rightarrow \mathbb{R}^d$

$$F(t, Y|Z) = F(Y(t)) - F(Z(t)) - \nabla F(Z(t)) \cdot (Y(t) - Z(t))$$

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- Stability estimate $\frac{d}{dt} E(t, Y|Z) \leq CE(t, Y|Z)$ hinges on bounding

$$\nabla F(t, Y|Z) = \nabla F(Y(t)) - \nabla F(Z(t)) - \nabla^2 F(Z(t)) \cdot (Y(t) - Z(t))$$

Modulated energy: Lagrangian setting

Potential Energy in Lagrangian variables

Let $X : M \rightarrow M$ be a smooth map

$$\mathcal{F}(X) = \mathcal{U}(X_{\#}\rho_0) = \int_M U\left(\frac{\rho_0}{\det \nabla X}\right) \det \nabla X$$

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- $M = [0, 1]$, $\mathcal{F} : D \subset \mathbb{X} \rightarrow \mathbb{R}$, D str. increasing maps, CONVEX iff

$$\lambda \mapsto U\left(\frac{c}{\lambda}\right)\lambda \quad \text{is convex}$$

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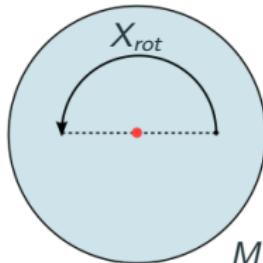
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- \mathcal{F} NOT convex in general: $M = B(1) \subset \mathbb{R}^2$ unit ball



$$X_{rot}(x) = R_{\pi} \cdot x$$

$$X_{\alpha} = \alpha \text{Id} + (1-\alpha)X_{rot}, \quad \alpha \in [0, 1]$$

$$X_{1/2}(x) = 0, \quad \forall x \in M$$

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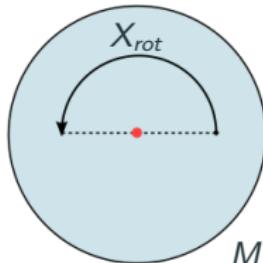
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- \mathcal{F} may be convex only along specific directions
→ *geodesic convexity*: restrict to $X = \nabla \psi$ with ψ convex

Modulated energy: Eulerian setting

Total Energy in Eulerian variables

$$(\rho, m) \mapsto \int_M \frac{|m|^2}{2\rho} + \mathcal{U}(\rho) \quad \text{where } m = \rho u \text{ (momentum)}$$

Modulated energy: Eulerian setting

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- Convex function of (ρ, m) (1-homogeneous + strictly convex)
- Relative kinetic energy

$$\mathcal{K}((\rho, m)|(\bar{\rho}, \bar{m})) = \frac{1}{2} \int_M |u - \bar{u}|^2 \rho$$

- Relative potential energy

$$\mathcal{U}(\rho|\bar{\rho}) = \int_M U(\rho) - U(\bar{\rho}) - U'(\bar{\rho})(\rho - \bar{\rho})$$

Modulated energy: Eulerian setting

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- “ $\nabla F(t, Y|Z)$ ” ? By integration by parts, only need to control

$$\boxed{\int_M |P(\rho|\bar{\rho})| \leq C \mathcal{U}(\rho|\bar{\rho})} \quad P(\rho|\bar{\rho}) = P(\rho) - P(\bar{\rho}) - P'(\bar{\rho})(\rho - \bar{\rho})$$

Satisfied if $|P''(r)| \leq C U''(r)$

- Classical (Dafermos, DiPerna)/ Generalizations!

Discrete modulated energy

- Recall discrete dynamical system for $t \in [t_n, t_{n+1})$

$$\ddot{X}_N(t) = -\frac{X_N(t) - P_{\mathbb{X}_N} X_N^\varepsilon(t_n)}{\varepsilon},$$

$$\text{TOTAL ENERGY} \rightarrow \frac{\|\dot{X}_N(t)\|_{\mathbb{X}}^2}{2} + \frac{\|X_N(t) - X_N^\varepsilon(t_n)\|_{\mathbb{X}}^2}{2\varepsilon} + \mathcal{U}(\rho_N^\varepsilon(t_n))$$

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- Both are discretizations of Eulerian relative energies

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- KINETIC ENERGY $\rightarrow \frac{1}{2} \|\dot{X}_N(t) - u(t, X_N(t))\|_{\mathbb{X}}^2$
- POTENTIAL ENERGY $\rightarrow \frac{\|X_N(t) - X_N^\varepsilon(t_n)\|_{\mathbb{X}}^2}{2\varepsilon} + \mathcal{U}(\rho_N^\varepsilon(t_n)|\rho(t))$

- Both are discretizations of Eulerian relative energies
- Need to extend (ρ, u) outside M to account for $\text{supp}(\rho_N) \not\subseteq M$
 \rightarrow Construct **bounded** extension such that $\partial_t \rho + \text{div}(\rho u) = 0$ on $\mathbb{R}^d \setminus M$.

Discrete modulated energy

- Recall discrete dynamical system for $t \in [t_n, t_{n+1})$

$$\ddot{X}_N(t) = -\frac{X_N(t) - P_{\mathbb{X}_N} X_N^\varepsilon(t_n)}{\varepsilon},$$

$$\text{TOTAL ENERGY} \rightarrow \frac{\|\dot{X}_N(t)\|_{\mathbb{X}}^2}{2} + \frac{\|X_N(t) - X_N^\varepsilon(t_n)\|_{\mathbb{X}}^2}{2\varepsilon} + \mathcal{U}(\rho_N^\varepsilon(t_n))$$

- KINETIC ENERGY $\rightarrow \frac{1}{2} \|\dot{X}_N(t) - u(t, X_N(t))\|_{\mathbb{X}}^2$
- POTENTIAL ENERGY $\rightarrow \frac{\|X_N(t) - X_N^\varepsilon(t_n)\|_{\mathbb{X}}^2}{2\varepsilon} + \mathcal{U}(\rho_N^\varepsilon(t_n)|\rho(t))$

- Both are discretizations of Eulerian relative energies
- Need to extend (ρ, u) outside M to account for $\text{supp}(\rho_N) \not\subseteq M$
→ Construct **bounded** extension such that $\partial_t \rho + \text{div}(\rho u) = 0$ on $\mathbb{R}^d \setminus M$.
- **Gradient flow:** consider only potential part
→ relative kinetic energy appears with “GOOD SIGN”

Back to main results

- Initial conditions: $X_N(0) = P_{\mathbb{X}_N} \text{Id}$ (Velocity: $\dot{X}_N(0) = u(0, X_N(0))$)
- Initial mesh size: $h_N = \max_i \text{diam}(P_i)$
- Smooth str. convex U , such that $|P''(r)| \leq CU''(r)$

Theorem: Convergence Euler

Hyp.: (ρ, u) strong solution, $u \in C^1(0, T; C^{2,1}(M))$, $\rho_0 \in C^{1,1}(M)$; either $\rho \geq \rho_{min} > 0$ or $|U'''_+(0)| < +\infty$. Then,

$$\|\dot{X}_N(T) - u(T, X_N(T))\|_{\mathbb{X}}^2 + \|X_N(T) - X(T)\|_{\mathbb{X}}^2 \leq C\left(\frac{h_N^2}{\varepsilon} + h_N + \varepsilon + \frac{\tau}{\varepsilon}\right),$$

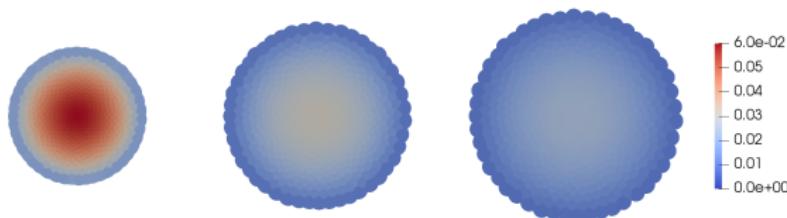
Theorem: Convergence gradient flow

Hyp.: ρ strong solution, $\rho_0 \in C^{1,1}(M)$ and $\nabla U'(\rho_t) \in C^{2,1}$ uniformly on $[0, T]$; either $\rho \geq \rho_{min} > 0$ or $|U'''_+(0)| < +\infty$. Then,

$$\int_0^T \|\dot{X}_N(s) - u(s, X_N(s))\|_{\mathbb{X}}^2 ds + \|X_N(T) - X(T)\|_{\mathbb{X}}^2 \leq C\left(\frac{h_N^2}{\varepsilon} + h_N + \varepsilon + \frac{\tau}{\varepsilon}\right),$$

Numerical rates - Gradient flow

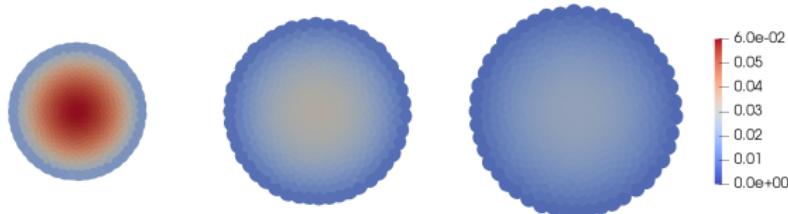
- $\varepsilon = \sqrt{\tau} = 1/\sqrt{N} \implies$ order 1/2
- Porous medium equation / $U(r) = r^2$
- Diffusion of Barenblatt profile: $\rho(t, x) = \frac{1}{\sqrt{t}} \left(C^2 - \frac{1}{16\sqrt{t}} |x|^2 \right)_+$



$1/\sqrt{N}$	ΔX	rate	$\Delta \mathcal{U}$	rate
1.25e-01	4.70e-02	-	1.66e-02	-
6.25e-02	2.78e-02	7.60e-01	9.37e-03	8.23e-01
3.12e-02	1.54e-02	8.48e-01	5.11e-03	8.74e-01
1.56e-02	8.22e-03	9.09e-01	2.72e-03	9.12e-01

Numerical rates - Euler

- $\varepsilon = \sqrt{\tau} = 1/\sqrt{N} \implies$ order 1/2
- Shallow water equations / $U(r) = r^2$
- Diffusion of Barenblatt profile: $\rho(t, x) = \frac{1}{\sqrt{\lambda(t)}} \left(C^2 - \frac{1}{16\sqrt{\lambda(t)}} |x|^2 \right)_+$



$1/\sqrt{N}$	ΔX	rate	$\Delta \mathcal{E}$	rate
1.67e-01	5.33e-02	-	2.76e-02	-
8.33e-02	3.35e-02	6.71e-01	2.00e-02	4.67e-01
4.17e-02	2.04e-02	7.17e-01	1.27e-02	6.51e-01
2.08e-02	1.14e-02	8.39e-01	7.36e-03	7.89e-01

Summary and Perspectives

MAIN POINTS

- Lagrangian scheme → Exploit dynamical system formulation
- Structural link gradient flow/Euler preserved
- **No convexity** for Lagrangian potential \mathcal{F}
- Modulated energy → Exploit convexity in Eulerian setting

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- Lagrangian scheme → Exploit dynamical system formulation
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OPEN ISSUES

- Restriction on h_N , τ , ε unavoidable?
- Alternatives to Moreau-Yosida regularization?
- Convergence in non smooth-setting?
- Generalizations (Euler-Korteweg, Euler-Poisson theory)..

Thank you!

Convergence to non-smooth solutions

MAIN QUESTIONS

- Can we prove existence of limit $X_N \rightarrow X^*$ as $N \rightarrow +\infty$ and $\tau \rightarrow 0$?
 - Do the equations of motion pass to the limit?
-
- **Key property:** Ensure that $\sum_n \frac{W_2^2(\rho_N(t_n), \rho_N^\varepsilon(t_n))}{2\varepsilon} \tau \rightarrow 0$

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- **Key problem:** gradient of potential is projected on \mathbb{X}_N in dynamics
- Gradient flow case: we can show this if

$$\sum_n \frac{\|X_N^\varepsilon(t_n) - P_{\mathbb{X}_N} X_N^\varepsilon(t_n)\|_{\mathbb{X}}^2}{2\varepsilon} \tau \rightarrow 0$$

- This measure ANISOTROPY of Laguerre cells $L_i = X_N^\varepsilon(t_n)(P_i)$

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- This measure ANISOTROPY of Laguerre cells $L_i = X_N^\varepsilon(t_n)(P_i)$
- (Leclerc et al. '20) 1d case for entropy and crowd motion/time-continuous
→ Proof generalizes to our time-discrete setting