Mapping, Transport and Diffusion: Energetic Variational Approaches

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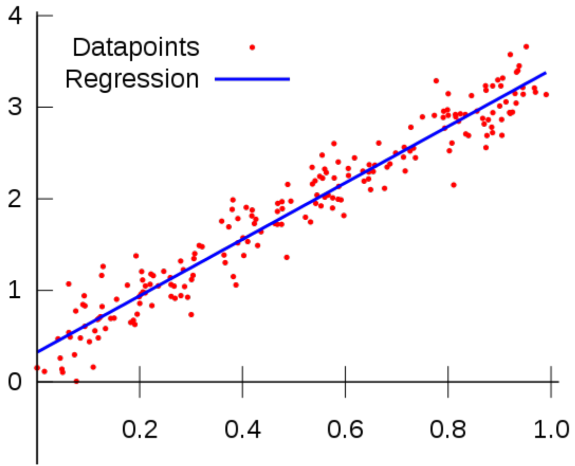
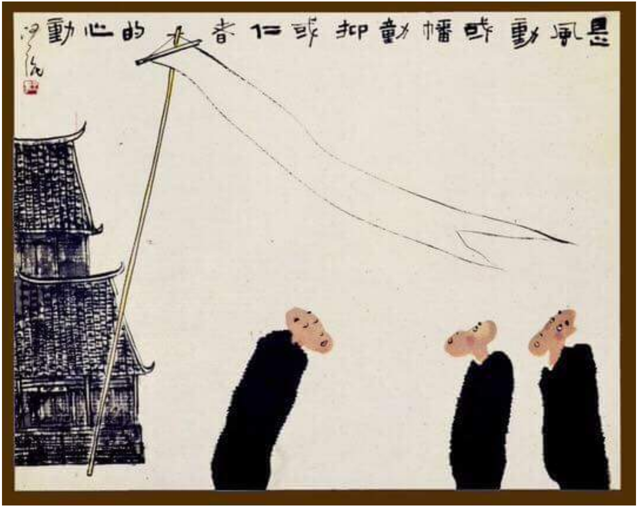


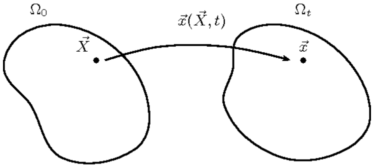
- Find the optimal $y = kx + b$: Variation with respect to $\{k, b\}$.
- For given y_1, y_2 find the the optimal line through (x_1, y_1) and (x_2, y_2): Variation with respect to $\{x_1, x_2\}$.


是風動或幡動抑或仁者的心動

Flow map and kinematic

- Flow map (trajectory) $\mathbf{x}(\mathbf{X},t):\Omega_0\to\Omega$:

$$\mathbf{x}_t = u(\mathbf{x}(\mathbf{X},t),t), \quad \mathbf{x}(\mathbf{X},0)=\mathbf{X}$$



- Deformation gradient:

$$F(\mathbf{X},t)=\frac{\partial\,\mathbf{x}(\mathbf{X},t)}{\partial\,\mathbf{X}} \quad (F_{ij}=\frac{\partial x_i}{\partial X_j})$$

Deformation tensor F carries kinematic/transport information of microstructure, patterns and configurations in complex fluids.

- Scalar transport:

$$\partial_t\phi+\mathbf{u}\cdot\nabla\phi=0 \quad\Longleftrightarrow\quad \phi(\mathbf{x}(\mathbf{X},t),t)=\phi_0(\mathbf{X})$$

- Conserved quantity:

$$\partial_t\phi+\nabla\cdot(\phi\,\mathbf{u})=0 \quad\Longleftrightarrow\quad \phi(\mathbf{x}(\mathbf{X},t),t)=\phi_0(\mathbf{X})/\det F$$

- Vorticity (in 3-D incompressible fluids):

$$\omega_t+\mathbf{u}\cdot\nabla\omega-\omega\cdot\nabla\,\mathbf{u}=0 \quad\Longleftrightarrow\quad \omega(\mathbf{x}(\mathbf{X},t),t)=F\omega_0(\mathbf{X})$$

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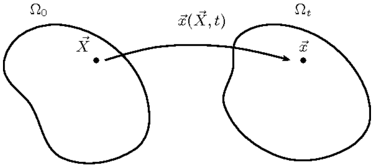

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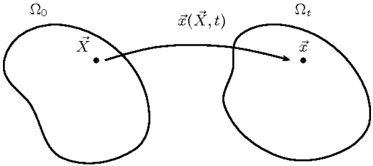

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- Everything interacts with everything else.
- First law of thermodynamics

$$(K \dot{+} U) = \dot{Q} + \dot{W}$$

- Second law of thermodynamics

$$T\dot{S} = \dot{Q} + T\Delta$$

$$\Delta \geq 0$$

- Subtracting (isothermal)

$$\frac{d}{dt}E^{total} = \frac{d}{dt}(K + U - TS) = \dot{W} - T\Delta.$$

EnVarA: Energetic Variational Approaches

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EnVarA: Energetic Variational Approaches [1]

- Energy-dissipation law (from first and second law of thermodynamics)

$$\frac{\mathrm{d}}{\mathrm{d}\,t}(\mathcal{K}+\mathcal{F}) = -2\mathcal{D}$$

- Least Action Principle $\mathcal{A}(\mathbf{x}) = \int_0^T \mathcal{K} - \mathcal{F}\,\mathrm{d}\,t$:

$$\delta\mathcal{A}(\mathbf{x}) = \int_0^T \int_\Omega (\text{force}_{inertial} - \text{force}_{conservation}) \cdot \delta\,\mathbf{x}\,\mathrm{d}\,\mathbf{x}\,\mathrm{d}\,t$$

  $\mathbf{x}$: trajectory if applicable
- Maximum Dissipation Principle

$$\delta\mathcal{D}(\mathbf{x}_t) = \int_\Omega \text{force}_{dissipation} \cdot \mathbf{x}_t\,\mathrm{d}\,\mathbf{x}$$

- Force balance $\text{force}_{inertial} = \text{force}_{conservation} + \text{force}_{dissipation}$:

$$\frac{\delta\mathcal{A}}{\delta\,\mathbf{x}} = \frac{\delta\mathcal{D}}{\delta\,\mathbf{x}_t}$$

[1] Lars Onsager. Reciprocal relations in irreversible processes. i/ii, Physical review, 1931; J W Strutt (L Rayleigh). Some general theorems relating to vibrations. Proceedings of the London Mathematical Society, 1(1):357-368, 1871.

A simple model: Hookean Spring

- Force balance:
$$mx_{tt} + \gamma x_t + kx = 0.$$
- Energy law:
$$\frac{d}{dt}(\frac{1}{2}mx_t^2 + \frac{1}{2}kx^2) = -\gamma x_t^2.$$
- Hamiltonian part of dynamics
  - Least Action Principle
$$\delta \int (\frac{1}{2}mx_t^2 - \frac{1}{2}kx^2)\,dt = \int (-mx_{tt} - kx)\delta x\,dt$$
  - Short time (near initial data) dynamics, transient dynamics.
- Dissipation
  - Maximum Dissipation Principle: $\frac{\partial(\gamma x_t^2)}{\partial x_t} = 2\gamma x_t$.
  - Long time dynamics, near equilibrium, linear response theory.

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- Competitions/couplings between different part of energies.
- Macroscopic hydrodynamics v.s. Micro-structures.
- Interactions vs. Constraints.
- Deterministic v.s. Stochastic.
- Energetics v.s. Kinematics.
- Reversible v.s. Irreversible.
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- Statistical physics: free energy $\mathcal{F}$, non-equilibrium thermodynamics: entropy production Δ.
- Thermal effects can only be introduced through energy.

(Elastic) complex fluids: competitions and couplings

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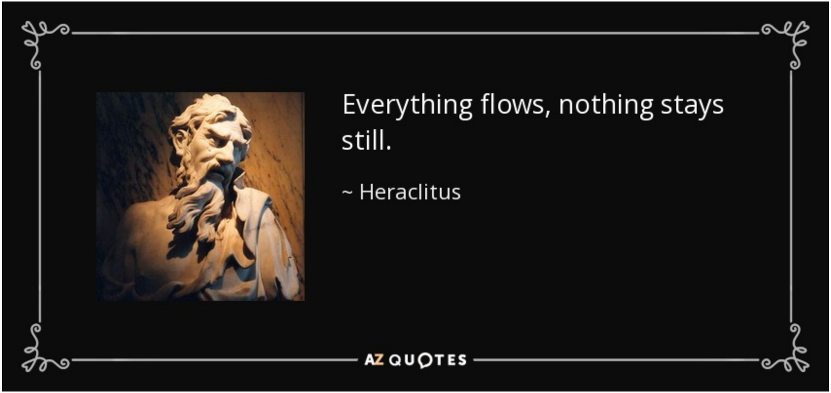
Energetic Variational Approaches in Complex Fluids

- Liquid Crystals: orientational order and partial positional order (with Fang-Hua Lin) Nonparabolic Dissipative Systems Modeling the Flow of Liquid Crys- tals, Communications on Pure and Applied Mathematics, Vol. 48, Issue 5, 501 – 537 (1995)..
- Polymeric Materials and Biomaterials (gels, tissues): microscopic patterns and structures. (with Qiang Du and Yunkyong Hyon) On some PDF based moment closure approxima- tions of micro-macro models for viscoelastic polymeric uids, Journal of Computational and Theoretical Nanoscience (2010)..
- Viscoelastic Materials: macroscopic continuum descriptions. (with Masakazu Endo, Yoshikazu Giga and Dario Gotz) Stability of a two-dimensional Poiseuille-type ow for a viscoelastic uid, Journal of Mathematical Fluid Mechanics (2017)..
- Magneto-hydrodynamics (MHD), electrolyte (EHD), EMHD (with Jinchao Xu and Maximilian Metti) Energetically stable discretizations for charge transport and electrokinetic models, Journal of Computational Physic (2016)..
- Mixtures: internal impurity/hetrogeneity (with Jie Shen) A Phase Field Model for the Mixture of Two Incompressible Fluids and its Approximation by a Fourier-Spectral Method, Physica D, 179, 4, 211–228 (2003)..
- Surface effects, interface effects (with Hao Wu) An Energetic Variational Approach for the Cahn-Hilliard Equation with Dynamic Boundary Conditions: Derivation and Analysis, Archive of Rational Mechanics and Analysis (2018).
- Ionic fluids and ion channels (with Nir Gavish and Bob Eisenberg) Do Bi-Stable Steric Poisson-Nernst-Planck Models Describe Single Channel Gating, Journal of Physical Chemistry B (2018)..


Everything flows, nothing stays still.
~ Heraclitus
AZ QUOTES

$f_t = \gamma \Delta f$ as a gradient flow (Eulerian)

- Energy-dissipation Law (fast descent):

$$\frac{\mathrm{d}}{\mathrm{d}\,t}\int_\Omega \frac{1}{2}|\nabla f|^2\,\mathrm{d}\,\mathbf{x} = -\int_\Omega \frac{1}{\gamma}|f_t|^2\,\mathrm{d}\,\mathbf{x}\,.$$

- $\mathcal{K}=0$, $\mathcal{F}(f)=\int_\Omega \frac{1}{2}|\nabla f|^2\,\mathrm{d}\,\mathbf{x}$, $\mathcal{D}(f_t)=\frac{1}{2\gamma}\int_\Omega |f_t|^2$

$$\frac{\delta \mathcal{D}}{\delta f_t} = -\frac{\delta \int_0^T \mathcal{F}\,\mathrm{d}\,t}{\delta f} \Rightarrow f_t = \gamma \Delta f$$

- Implicit Euler can be derived by

$$\min_{f^{n+1}\text{given } f^n} \int_\Omega \frac{1}{\gamma}\frac{|f^{n+1}-f^n|^2}{2\tau} + \frac{1}{2}|\nabla f^{n+1}|^2\,\mathrm{d}\,\mathbf{x}\,.$$

- Numerical methods in Eulerian coordinate:
  - Easy to deal with / can handle the large deformation
  - Difficult to capture the singularity and track the free boundary

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- In Lagrangian coordinate (search for flow map):

$$\frac{\mathrm{d}}{\mathrm{d}\,t} \int_{\Omega_0} \frac{1}{2} |(\frac{\partial\,\mathbf{x}}{\partial\,\mathbf{X}})^{-\mathrm{T}} \nabla_{\mathbf{X}} f_0|^2 \det \frac{\partial\,\mathbf{x}}{\partial\,\mathbf{X}} \,\mathrm{d}\,\mathbf{X} = - \int_{\Omega_0} \frac{1}{\gamma} |\,\mathbf{x}_t \cdot \nabla f|^2 \det \frac{\partial\,\mathbf{x}}{\partial\,\mathbf{X}} \,\mathrm{d}\,\mathbf{X},$$

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$\rho_t = \gamma\Delta\rho$ as a diffusion

- Conserved quantity: $\rho_t + \nabla \cdot (\rho\,\mathbf{u}) = 0$.
- Energy-dissipation law ($\mathcal{K} = 0, \mathcal{F} = \int_\Omega \omega(\rho)\,\mathrm{d}\,\mathbf{x}$):

$$\frac{\mathrm{d}}{\mathrm{d}\,t}\int_\Omega \omega(\rho)\,\mathrm{d}\,\mathbf{x} = -\int_\Omega \underbrace{\eta(\rho)|\,\mathbf{u}\,|^2}_{\text{Darcy's Law}}\,\mathrm{d}\,\mathbf{x},$$

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- For ideal gas: $\omega(\rho) = \rho\ln\rho$, $\eta(\rho) = \frac{1}{\gamma}\rho \Rightarrow \rho_t = \gamma\Delta\rho$

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- Discretize the energy-dissipation law by discretizing the flow map

$$\mathbf{x}_h(\mathbf{X}, t) = \sum_{i=1}^{N} \boldsymbol{\xi}_i(t)\phi_i(\mathbf{X})$$

Let $\boldsymbol{\Xi}(t) = (\xi_1^{(1)}(t), \xi_1^{(2)}(t), \ldots, \xi_1^{(d)}(t), \ldots, \xi_N^{(1)}, \xi_N^{(2)}, \ldots, \xi_N^{(d)}) : \mathbb{R} \to \mathbb{R}^{N\times d}$:

- Discrete action function $\mathcal{A}_h(\boldsymbol{\Xi}(t))$
- Discrete dissipation: $\mathcal{D}_h(\boldsymbol{\Xi}(t), \boldsymbol{\Xi}'(t))$
- A discrete Energetic Variational Approach:

$$\frac{\delta \mathcal{D}_h}{\delta \boldsymbol{\Xi}'(t)} = \frac{\delta \mathcal{A}_h}{\delta \boldsymbol{\Xi}(t)},$$

which is a nonlinear ODE system of $\xi_i^{(k)}(t)$.

- Introduce a proper temporal discretization $\Rightarrow$ Numerical scheme

- Numerical approximate the flow map $\mathbf{x}(\mathbf{X}, t)$, $\rho(\mathbf{x}, t)$ is determined by the kinematic relations ($\rho(\mathbf{x}, t) = \rho_0(\mathbf{X}) / \det F$).
- A diffeomorphism $\mathbf{x}(\mathbf{X}, t)$ can be approximated by a piecewise linear map (ReLu). For a given t:

  the deformation matrix F is piecewise constant, so is F^{-1} and $\det F$
- Finite element methods:
  - triangularize the $\Omega_0 \in \mathbb{R}^d$ into some simple finite elements, denote by $\mathcal{T}_h$. which consists of a set of simplexes $\{\tau_e \mid e = 1, \ldots M\}$ and a set of nodal points $\mathcal{N}_h = \{\mathbf{X}_1, \mathbf{X}_2, \ldots, \mathbf{X}_N\}$.
- Discrete flow map:

$$\mathbf{x}_h(\mathbf{X}, t) = \sum_{i=1}^{N} \boldsymbol{\xi}_i(t) \phi_i(\mathbf{X})$$

where $\phi_i(\mathbf{X}) : \mathbb{R}^d \to \mathbb{R}$ is the hat function satisfies $\phi_i(\mathbf{X}_j) = \delta_{ij}$.

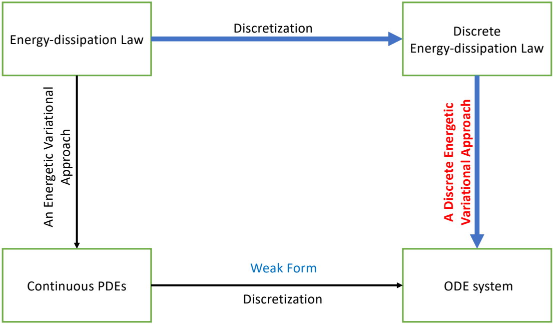
- Ω_0 is taken to be the compact support of $\rho_0(X)$ for the PME.
- $\mathbf{X}_i$ can be viewed as "particles".
- $\boldsymbol{\xi}_i(t)$ can be viewed as the coordinate in Ω_t.
- We fixed $\mathbf{X}_i$ in the current approach. But $\mathbf{X}_i$ can also be a variable.
- Admissible set F_{ad}^h:

$$F_{ad}^h = \left\{ \mathbf{x}_h(\mathbf{X}, t) = \sum_{i=0}^{N+1} \boldsymbol{\xi}_i(t)\phi_i(\mathbf{X}) \mid \det F_e > 0 \right\}.$$

  Nonnegativity of $\rho(\mathbf{x}, t)$ is naturally preserved.
- Minimizing movement scheme: $\boldsymbol{\Xi}^{n+1} := \text{argmin}_{\boldsymbol{\Xi} \in F_{ad}^{\boldsymbol{\Xi}}} J(\boldsymbol{\Xi})$

$$J(\boldsymbol{\Xi}) = \frac{1}{2\tau} \mathsf{D}_n^*(\boldsymbol{\Xi} - \boldsymbol{\Xi}^{\boldsymbol{n}}) \cdot (\boldsymbol{\Xi} - \boldsymbol{\Xi}^{\boldsymbol{n}}) + E(\boldsymbol{\Xi}),$$

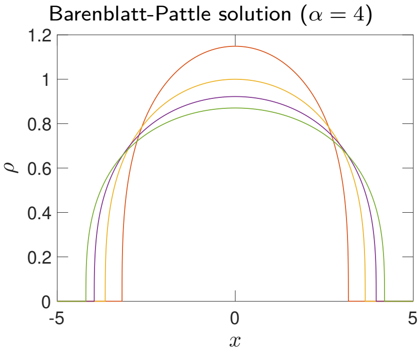
A discrete Energetic Variational Approach

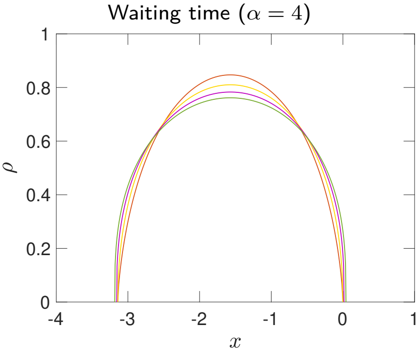


- The two approaches may give us different numerical schemes (non-commute).
- The nonlinear ODE system can be realized as specific weak forms (filters).

Nonlinear Diffusion: Porous Medium $f_t = \Delta f^\alpha$

- Porous medium equation (PME) is a typical example of nonlinear diffusion
- Properties of the PME
  - Finite speed of propagation
  - Waiting time phenomena
  - Lack of regularity near the free boundary





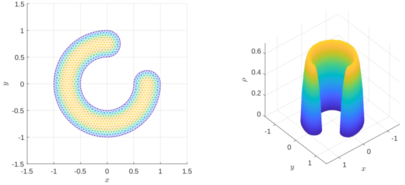
- Porous Medium Equations are examples of nonlinear diffusion.
- Derive different numerical schemes by different energy-dissiption laws.
- Energy-dissipation law 1 (commonly used):

$$\frac{\mathrm{d}}{\mathrm{d}\,t}\int_\Omega \frac{1}{\alpha-1}\rho^\alpha \,\mathrm{d}\,\mathbf{x} = -\int_\Omega \rho|\,\mathbf{u}\,|^2\,\mathrm{d}\,\mathbf{x},$$

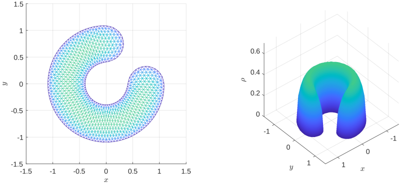
- Energy-dissipation law 2 (equivalent to the PME on its compact support for $\alpha > 2$, good for free boundary)

$$\frac{\mathrm{d}}{\mathrm{d}\,t}\int_\Omega \frac{\alpha}{(\alpha-1)(\alpha-2)}\rho^{\alpha-1}\,\mathrm{d}\,\mathbf{x} = -\int_\Omega |\,\mathbf{u}\,|^2\,\mathrm{d}\,\mathbf{x},$$

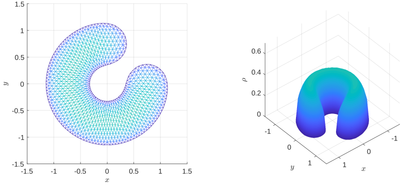
Porous Medium Equation ($\alpha = 3$): Complex Support



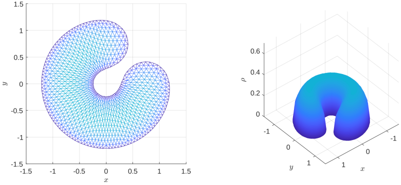
$t = 0.0$



$t = 0.05$

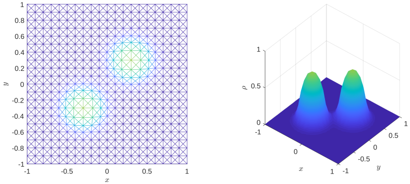


$t = 0.1$

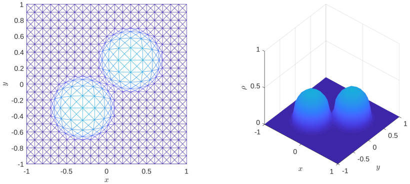


$t = 0.2$

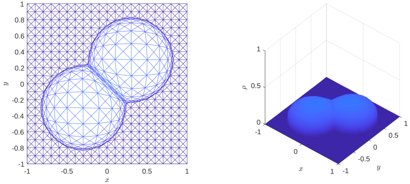
$$\rho_0(X,Y) = e^{-20((X-0.3)^2+(Y-0.3)^2)} + e^{-20((X+0.3)^2+(Y+0.3)^2)} + 0.001$$



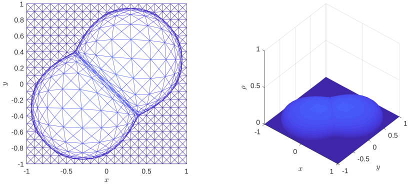
$t = 0.01$



$t = 0.1$

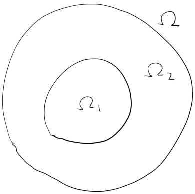


$t = 1$



$t = 5$

- Mixture: fluid 1 + fluid 2



Label:

$$\phi(x,t) = \begin{cases} 1 & \text{fluid 1} \\ -1 & \text{fluid 2} \end{cases}$$

- Mixture energy:

$$\mathcal{F}[\phi, \nabla\phi] = \int_\Omega \frac{1}{2}|\nabla\phi|^2 + G(\phi)\,\mathrm{d}\,x$$

  - Ginzburg-Landau:

$$G(\phi) = \frac{1}{4\epsilon^2}(\phi^2 - 1)^2$$

  - philic v.s phobic by ϵ
  - $\epsilon \to 0$: $\phi \to \pm 1$

- Allen-Cahn equation:

$$\phi_t = -(\Delta\phi - G'(\phi))$$

  - Energy-dissipation Law:

$$\frac{d}{dt}\int_\Omega \frac{1}{2}|\nabla\phi|^2 + G(\phi)dx = -\int_\Omega |\phi_t|^2 dx$$

  - $\epsilon \to 0$: Motion by mean curvature

- Cahn-Hilliard equation:

$$\phi_t = -\nabla \cdot (\nabla(\Delta\phi - G'(\phi)))$$

  - Energy-dissipation Law:

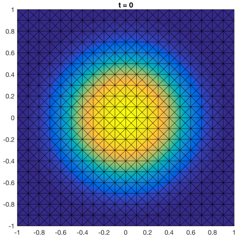
$$\frac{d}{dt}\int_\Omega \frac{1}{2}|\nabla\phi|^2 + G(\phi)dx = -\int_\Omega |\nabla(\Delta\phi - G'(\phi))|^2 dx$$

- Kinematic: $\phi_t + \mathbf{u} \cdot \nabla \phi = 0$
- Energy-dissipation Law (Allen-Cahn):

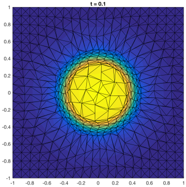
$$\frac{d}{dt} \int_{\Omega} \frac{1}{2} |\nabla \phi|^2 + G(\phi) dx = - \int_{\Omega} |\, \mathbf{u} \cdot \nabla \phi|^2 dx$$

- Governing equation:

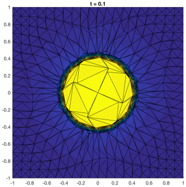
$$(\nabla \phi \otimes \nabla \phi) \, \mathbf{u} = -\nabla \cdot \left(\nabla \phi \otimes \nabla \phi - (\frac{1}{2} |\nabla \phi|^2 + G(\phi)) \mathrm{I} \right)$$



Initial



$\frac{1}{4\epsilon^2} = 100$



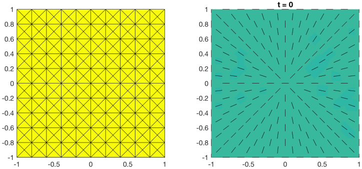
$\frac{1}{4\epsilon^2} = 1000$

Gradient Flow: LC confined in a square

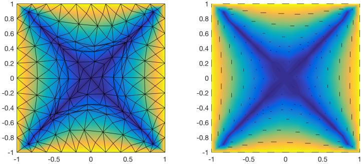
- Well-Order-Reconstruction Solution (WORS)
- 2D Q-tensor: $\mathrm{Q} = \begin{pmatrix} d_1 & d_2 \\ d_2 & -d_1 \end{pmatrix}$
- Energy-dissipation law:

$$\frac{\mathrm{d}}{\mathrm{d}\,t} \int_{\Omega} \frac{1}{2} |\nabla \mathrm{d}\,|^2 + \frac{1}{4\epsilon^2} (1 - |\,\mathrm{d}\,|^2)^2 \,\mathrm{d}\,\mathbf{x} \quad = - \int_{\Omega} \frac{1}{\gamma} |\,\mathrm{d}_t\,|^2 \,\mathrm{d}\,\mathbf{x}$$

- Hybrid with Eulerian solver to update the value of d in each node.



Initial



WORS

- The goal: to minimize the relative entropy (Kullback–Leibler divergence KL divergence) to a target distribution $\rho^*(\mathbf{x}) = \frac{1}{Z}e^{-V(\mathbf{x})}$

$$KL(\rho||\rho^*) = \int \rho(\mathbf{x}) \ln\left(\frac{\rho(\mathbf{x})}{\rho^*(\mathbf{x})}\right) \mathrm{d}\,\mathbf{x}$$
$$= \int \rho(\mathbf{x}) \ln \rho(\mathbf{x}) + V(\mathbf{x})\rho(\mathbf{x}) \,\mathrm{d}\,\mathbf{x} + \text{constant.}$$

- Continous energy-dissiption law

$$\frac{\mathrm{d}}{\mathrm{d}\,t}\int_\Omega \rho(\mathbf{x}) \ln \rho(\mathbf{x}) + V(\mathbf{x})\rho(\mathbf{x}) \,\mathrm{d}\,\mathbf{x} = -\int_\Omega \rho|\,\mathbf{u}\,|^2 \,\mathrm{d}\,\mathbf{x}$$

- A minimizer of $KL(\rho||\rho^*)$ can found by solving the Fokker-Planck equation:

$$\partial_t \rho = \nabla \cdot (\nabla \rho + \nabla V \rho)$$

- Rènyi entropy: Porous Media Euation.

- The goal: to minimize the relative entropy (Kullback–Leibler divergence KL divergence) to a target distribution $\rho^*(\mathbf{x}) = \frac{1}{Z}e^{-V(\mathbf{x})}$

$$
\begin{aligned}
KL(\rho||\rho^*) &= \int \rho(\mathbf{x}) \ln\left(\frac{\rho(\mathbf{x})}{\rho^*(\mathbf{x})}\right) \mathrm{d}\,\mathbf{x} \\
&= \int \rho(\mathbf{x}) \ln \rho(\mathbf{x}) + V(\mathbf{x})\rho(\mathbf{x}) \,\mathrm{d}\,\mathbf{x} + \text{constant.}
\end{aligned}
$$

- Continous energy-dissiption law

$$
\frac{\mathrm{d}}{\mathrm{d}\,t}\int_\Omega \rho(\mathbf{x}) \ln \rho(\mathbf{x}) + V(\mathbf{x})\rho(\mathbf{x}) \,\mathrm{d}\,\mathbf{x} = -\int_\Omega \rho|\,\mathbf{u}\,|^2 \,\mathrm{d}\,\mathbf{x}
$$

- A minimizer of $KL(\rho||\rho^*)$ can found by solving the Fokker-Planck equation:

$$
\partial_t \rho = \nabla \cdot (\nabla \rho + \nabla V \rho)
$$

  - Rènyi entropy: Porous Media Euation.

- Particle approximation (empirical measure): $\rho(\mathbf{x}, t) \approx \frac{1}{N} \sum_{i=1}^{N} \delta(\mathbf{x} - \mathbf{x}_i(t))$.
- $\{x_i(0)\}_{i=1}^{N}$ are sampled from a prior distribution $\rho_0(\mathbf{x})$.
- $\dot{\mathbf{x}}_i(t)$ can be determined by a semi-discrete energy-dissipation law:

$$\frac{\mathrm{d}}{\mathrm{d}\,t}\left(\frac{1}{N}\left(\sum_{i=1}^{N}(\ln\left(\frac{1}{N}\sum_{j=1}^{N}K(x_i - x_j)\right) + V(x_i)\right)\right) = -\frac{1}{N}\sum_{i=1}^{N}|\dot{x}_i|^2$$

  $K(x - y)$ is an approximation to $\delta(x - y)$.
- A discrete energetic approach:

$$\dot{\mathbf{x}}_i(t) = -\left(\frac{2\sum_{j=1}^{N}\nabla K(\mathbf{x}_i - \mathbf{x}_j)}{\sum_{j=1}^{N}K(\mathbf{x}_i - \mathbf{x}_j)} + \nabla V(\mathbf{x}_i)\right).$$

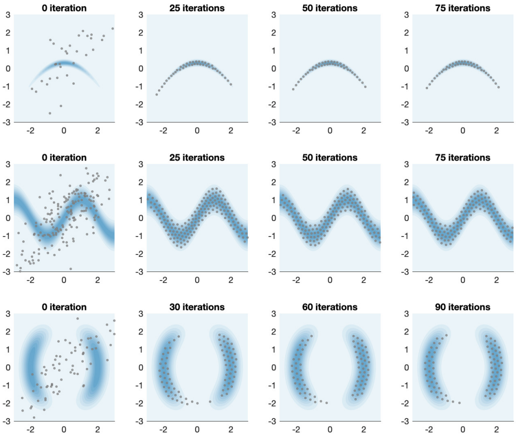
- Solve by an implicit Euler scheme.

Sample from three unnormalized 2-D distributions $\rho^*(\mathbf{x}) \propto \exp\{-V(\mathbf{x})\}$

$$V(\mathbf{x}) = \frac{1}{200}x_1^2 + \frac{1}{2}(x_2 + 0.03x_1^2 - 3)^2$$

$$V(\mathbf{x}) = \frac{1}{2}\left[\frac{x_2 - \sin\frac{\pi x_1}{2}}{0.4}\right]^2$$

$$V(\mathbf{x}) = \frac{1}{2}\left(\frac{||\mathbf{x}||_2 - 2}{0.4}\right)^2 + \log\left(e^{-\frac{1}{2}[\frac{x_1-2}{0.6}]^2} + e^{-\frac{1}{2}[\frac{x_1+2}{0.6}]^2}\right)$$



Summary

- We proposed a general framework to derive an efficient structure-preserving numerical scheme for a large class of partial differential equations by a discrete energetic variational approach, which can be adopted to a large class of partial differential equations with energy-dissipation law, such as nonlinear diffusion equations, phase-field equations, and equations for liquid crystals.
- Numerical experiments demonstrate the accuracy of our numerical method as well as its ability in tracking the free boundary for the PME.
- A detailed numerical analysis is needed for such type of methods.
- Limitations: Large deformation / topological change / velocity vanish ($\rho_0(X) = 0$ in the PME)
- Improvements: Local remeshing / reinitialisation (hybrid with Eulerian solver)

Thank you!