

Challenges in Modeling Polycrystalline Materials

Variational Problems in spaces of measures

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Outline



- Some issues in materials modeling
- Proposed framework – variational problems in spaces of measures
- Optimization problems for **special parameterized measures**

Canonical example

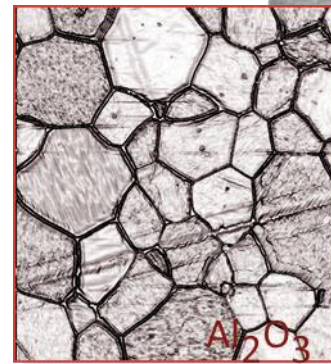
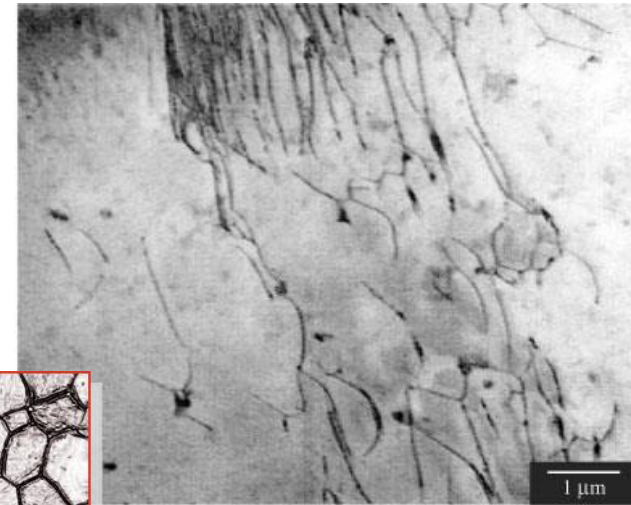
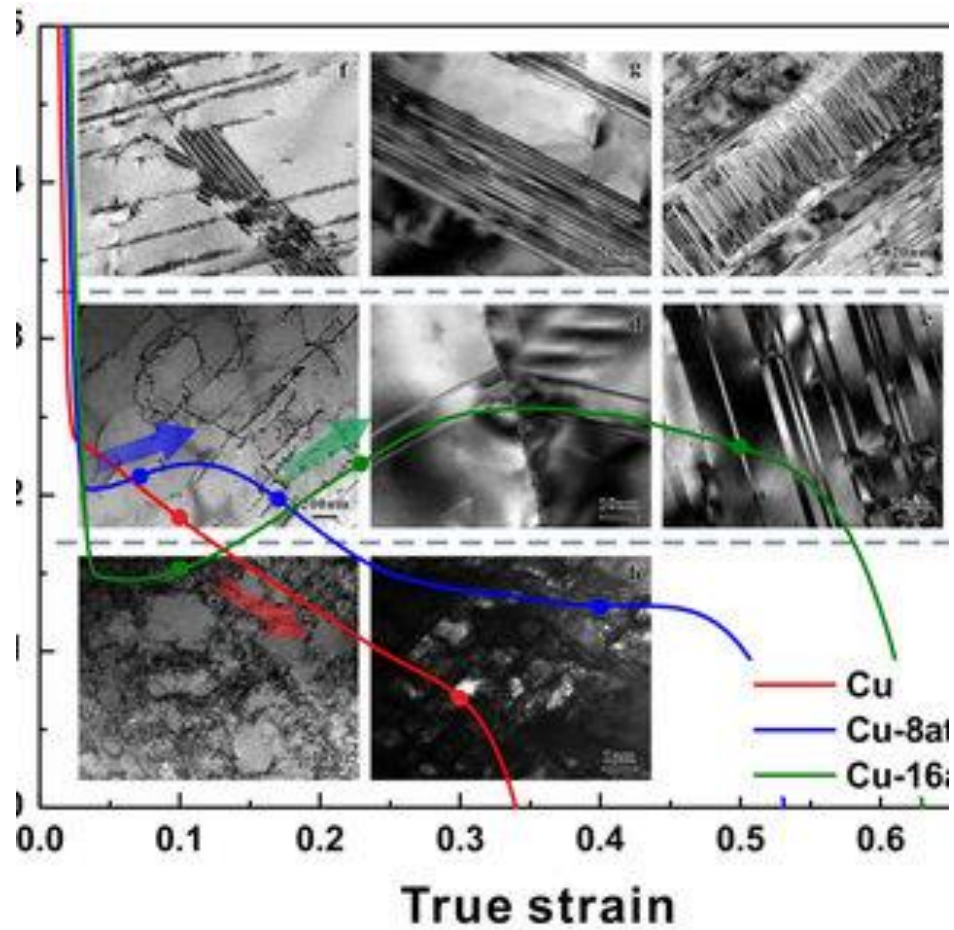
General Theory – existence results

- Homogenization problems
- Variational Evolution Equations for **special parameterized measures**

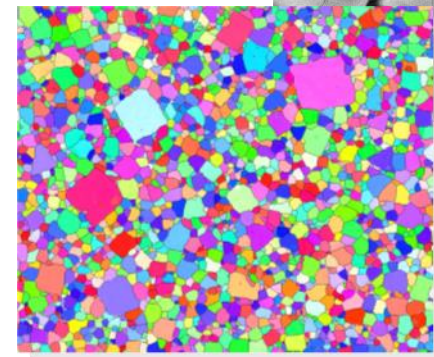
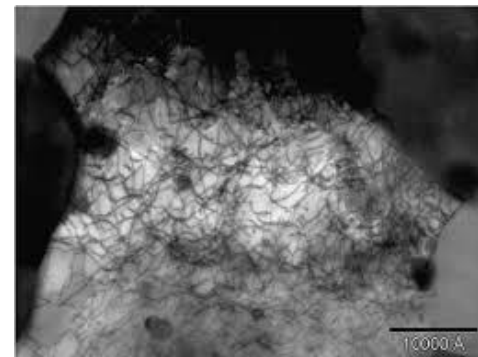
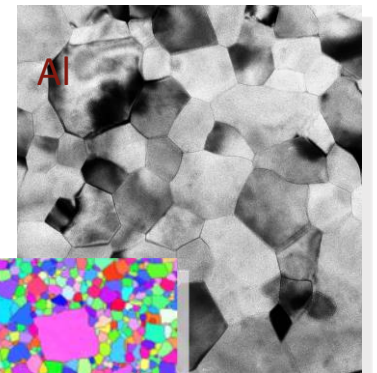


Defects

Points, lines, surfaces



TEM of annealed steel.



Modeling using measures

Examples of measures in materials description:

pairwise interatomic displacements

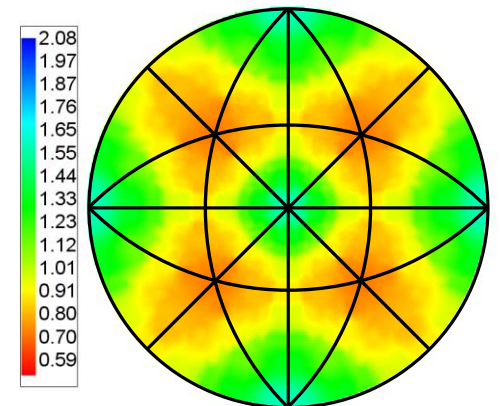
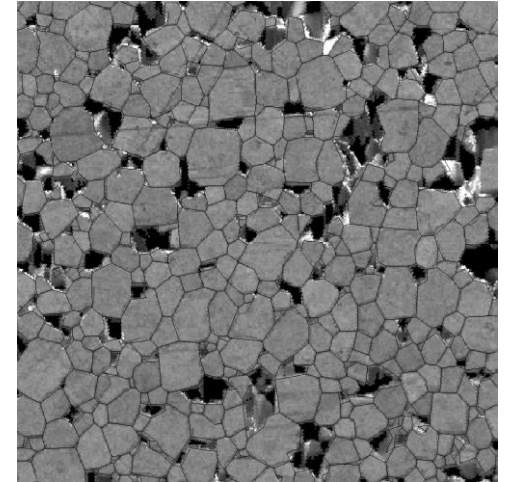
grain size distribution

grain boundary character (GBCD)

lattice orientation distribution

...

Want a measure to describe microscopic properties
at each macroscopic point → Young measures



GBCD: (Rohrer)

DiPerna Measure-Valued Solutions

$$f(x, u_n(x))dx \xrightarrow{*} \int_{\mathbb{R}^n} f(x, \eta) d\nu_x(\eta) dx + \int_{S^{n-1}} f^\infty(x, \beta) d\nu_x^\infty(\beta) \lambda$$

Generalized Young measures $(\nu_x, \lambda, \nu_x^\infty)$

Describe oscillations and concentration

- The moments of the measure satisfy the PDE in the sense of distributions
- Strong uniqueness property: if strong solution exists it should coincide with it
- Application to Euler and Navier-Stokes

We will use a different concept of measure-valued solutions

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We design the setup to deal with problems of the form

$$\inf_{u \in W} \int_{\Omega} f(x, u, \nabla u) dx$$

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$$\mathbb{M}(\Omega, \Sigma) = \{(\mu_x)_{x \in \Omega} : \mu_x \geq 0, (1, \mu_x) = 1, x \in \Omega\}$$

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$$I(\mu) = \int_{\Omega} (h_x, \mu_x) dx \quad \text{Is well defined for } \mu \in \mathbb{M}^p(\Omega, \Sigma) \quad h \in C^p(\Omega, \Sigma)$$

The problem: $\inf_{\mu} \int_{\Omega} (h_x, \mu_x) dx$

Theorem 1

Let $h_x \in C^p(\Omega, \Sigma)$ and let $\gamma \in L^1(\Omega)$, and assume that there exists $C > 0$ such that

$$h_x(\sigma) \geq C|\sigma|^p - \gamma(x) \quad \sigma \in \Sigma, x \in \Omega$$

Then the variational problem,

$$\inf_{\mu \in \mathbb{M}^p} \int_{\Omega} (h_x, \mu_x) dx$$

has a solution $\mu \in \mathbb{M}^p(\Omega, \Sigma)$ and

$$\text{supp}(\mu_x) \subseteq \left\{ \bar{\sigma} \in \Sigma : h_x(\bar{\sigma}) = \inf_{\sigma \in \Sigma} h_x(\sigma) \right\}$$

Proof: using duality arguments

Our Framework

For presentation purposes we omit the treatment of concentration!

Instead of modeling with functions in a Sobolev space:

Use parameterized measures $\mu_x(\eta, \xi) \quad x \in \Omega \quad (\eta, \xi) \in \Sigma = \mathbb{R} \times \mathbb{R}^n$

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Recovering function values u $u(x) = (\eta, \mu_x)$ $\nabla u(x) = (\xi, \mu_x)$

$$(h_x, \mu_x) = \int_{\Sigma} h_x(\eta, \xi) d\mu_x(\eta, \xi)$$

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$$(h_x, \mu_x) = \int_{\Sigma} h_x(\eta, \xi) d\mu_x(\eta, \xi)$$

Compatibility condition $(\xi, \mu_x) = \nabla_x(\eta, \mu_x)$ Not the usual Young measures

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Translation: $u \longleftrightarrow \eta \quad \nabla u \longleftrightarrow \xi$

The variational problem: $\inf_{\mu \in \mathcal{K}} \int_{\Omega} \left(\frac{1}{2} |\xi|^2 - f(x)\eta, \mu_x \right) dx$

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Compatibility condition $(\xi, \mu_x) = \nabla_x (\eta, \mu_x)$

Weak formulation of the compatibility condition $\int_{\Omega} (\xi \cdot v(x) + \eta \operatorname{div} v(x), \mu) dx = 0 \quad \forall v \in W$

Summarizing,

$$\inf_{\mu \in \mathcal{K}} \int_{\Omega} \left(\frac{1}{2} |\xi|^2 - f(x)\eta, \mu_x \right) dx$$

$$\mathcal{K} = \left\{ \mu \geq 0 \mid (1, \mu_x) = 1, \quad \int_{\Omega} (\xi \cdot v(x) + \eta \operatorname{div} v(x), \mu_x) dx = 0 \quad \forall v \right\}$$

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Using Duality (Lagrange multipliers)

$$\sup_v \inf_{\mu} \int_{\Omega} \left(\frac{1}{2} |\xi|^2 - f(x)\eta - \xi \cdot v(x) - \eta \operatorname{div} v(x), \mu \right) dx$$

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Giving,

$$(\eta, \xi) \in \operatorname{supp} \mu_x \iff \xi = v(x) \quad - \operatorname{div} v(x) = f(x)$$

Note that

$$v(x) = \int_{\Sigma} (v(x), \mu_x) d\eta d\xi = \int_{\Sigma} (\xi, \mu_x) d\eta d\xi = \nabla u(x)$$

The general problem

$$\inf_{\mu \in \mathcal{K}} \int_{\Omega} (h_x, \mu_x) dx \quad \mathcal{K} = \left\{ \mu \geq 0 \mid (1, \mu_x) = 1, \int_{\Omega} (\xi \cdot v(x) + \eta \operatorname{div} v(x), \mu_x) dx = 0 \quad \forall v \right\}$$

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Formal duality calculation gives,

$$(\eta, \xi) \in \operatorname{supp} \mu_x \iff \nabla_{\xi} h_x(\eta, \xi) = v^*(x) \quad \nabla_{\eta} h_x(\eta, \xi) = \operatorname{div} v^*(x)$$

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Where v^* solves the dual optimization problem

For convex integrand we have a unique solution and the measures can be associated with a function.

$$u(x) \longleftrightarrow \delta_{u(x)}(\eta) \delta_{\nabla u(x)}(\xi)$$

Variational Problems for Special Young Measures

$$\Sigma = \mathbb{R} \times \mathbb{R}^n \quad \sigma = (\eta, \xi) \in \Sigma$$

$$\mathbb{M}(\Omega, \Sigma) = \{(\mu_x)_{x \in \Omega} : \mu_x \geq 0, \quad (1, \mu_x) = 1, \quad x \in \Omega\}$$

$$\mathbb{M}^p(\Omega, \Sigma) = \left\{ \mu \in \mathbb{M}(\Omega, \Sigma) : \int_{\Omega} (|\sigma|^p, \mu_x) dx < \infty \right\}$$

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$$W_0^q(\operatorname{div}; \Omega) = \{v : \Omega \rightarrow \mathbb{R}^n : v \cdot n = 0 \text{ } \partial\Omega, \quad v \in L^q(\Omega) \quad \operatorname{div} v \in L^q(\Omega)\}$$

$$\operatorname{SM}^p(\Omega, \Sigma) = \left\{ \mu \in \mathbb{M}^p(\Omega, \Sigma) : \int_{\Omega} (\xi \cdot v(x) + \eta \operatorname{div} v(x), \mu_x) dx = 0 \quad \forall v \in W_0^q(\operatorname{div}; \Omega) \right\}$$

Study the problem
$$\inf_{\mu \in \operatorname{SM}^p} \int_{\Omega} (h_x, \mu_x) dx$$

Existence? Uniqueness?

The Dual Problem

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$$h_x^*(y, z) = \sup_{\eta, \xi} [y \eta + z \cdot \xi - h_x(\eta, \xi)] \quad \text{The conjugate function.}$$

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$$J(v) = \int_{\Omega} h_x^*(\operatorname{div} v(x), v(x)) dx \quad \mathcal{A} = \{v \in W_0^q(\operatorname{div}; \Omega) : (\operatorname{div}(x), v(x)) \in \operatorname{dom}(h_x^*) \ x \in \Omega\}$$

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Theorem 2:

Let $h \in C^p(\Omega, \Sigma)$, $1 < p < \infty$ and assume that there exists $\gamma \in L^1(\Omega)$ and $C > 0$ such that

$$h_x(\sigma) \geq C|\sigma|^p - \gamma(x)$$

Then the variational problem

$$\sup_{v \in \mathcal{A}} J(v)$$

has a solution $v^* \in W_0^q(\operatorname{div}; \Omega)$.

Theorem 3:

Let $h \in C^p(\Omega, \Sigma)$, $1 < p < \infty$ and assume that there exists a $\gamma \in L^1(\Omega)$ and a $C > 0$ such that

$$h_x(|\sigma|) \geq C|\sigma|^p - \gamma(x)$$

Then the variational problem

$$\inf_{\mu \in \text{SM}^p} I(\mu)$$

has a solution $\mu^* \in \text{SM}^p(\Omega, \Sigma)$ with

$$\text{supp}(\mu_x^*) \subseteq \left\{ (\eta, \xi) \in \Sigma : (\eta, \xi) \in \arg \sup_{\bar{\eta}, \bar{\xi}} [\bar{\xi} \cdot v^*(x) + \bar{\eta} \text{div} v^*(x) - h_x(\bar{\eta}, \bar{\xi})] \right\}$$

where v^* is a solution of the dual problem.

Proof: using duality arguments

Outline of proof

$$L(\mu, \alpha, \beta, v) = \int_{\Omega} (h_x, \mu_x) dv + \int_{\Omega} \alpha(x)[(1, \mu_x) - 1] dx - \int_{\Omega} (\beta_x, \mu_x) dx - \int_{\Omega} (\xi \cdot v(x) + \eta \operatorname{div} v(x), \mu_x) dx$$

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$$g(\alpha, \beta, v) = \inf_{\mu} L(\mu, \alpha, \beta, v)$$

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Linear terms in $L(\mu, \alpha, \beta, v)$ imply

$$\operatorname{dom}(g) = \{(\alpha, \beta, v) : \beta_x(\sigma) = h_x(\sigma) - \alpha(x) - \xi \cdot v(x) - \eta \operatorname{div} v(x) \geq 0 \quad (x, \eta, \xi) \in \Omega \times \Sigma\}$$

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$$(\alpha, \beta, v) \in \operatorname{dom}(g) \Rightarrow$$

$$g(\alpha, \beta, v) = \inf_{\mu} L(\mu, \alpha, \beta, v) = - \int_{\Omega} \alpha(x) dx \leq \inf_{\mu \in \operatorname{SM}^p} L(\mu, \alpha, \beta, v)$$

$$\beta_x(\sigma) \geq 0 \quad \Rightarrow \quad \alpha(x) \geq \sup_{\eta, \xi} [-h_x(\sigma) + \xi \cdot v(x) + \eta \operatorname{div} v(x)] = h_x^*(\operatorname{div} v(x), v(x))$$

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Let $\mathcal{B} = \{(\alpha, v) \in L^1(\Omega) \times \mathcal{A} : \alpha(x) \geq h_x^*(\operatorname{div} v(x), v(x)) \quad x \in \Omega\}$

We have,

$$\sup_{\beta \geq 0, (\alpha, v) \in \mathcal{B}} g(\alpha, \beta, v) = - \inf_{(\alpha, v) \in \mathcal{B}} \int_{\Omega} \alpha(x) dx = - \inf_{v \in \mathcal{A}} \int_{\Omega} h_x^*(\operatorname{div} v(x), v(x)) dx > -\infty$$

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$$g(\alpha, \beta, v) \leq L(\mu, \alpha, \beta, v) \leq \int_{\Omega} (h_x, \mu_x) dx \quad \mu \in \operatorname{SM}^p$$

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$$g(\alpha, \beta, v) \leq L(\mu, \alpha, \beta, v) \leq \int_{\Omega} (h_x, \mu_x) dx \quad \mu \in \operatorname{SM}^p$$

$$\inf_{\mu \in \operatorname{SM}^p} I(\mu) \geq \sup_{\beta \geq 0, \alpha, v} g(\alpha, \beta, v) = - \inf_{v \in \mathcal{A}} \int_{\Omega} h_x^*(\operatorname{div} v(x), v(x)) dx > -\infty$$

Summarizing,

$$\inf_{\mu \in \mathcal{SM}^p} I(\mu) \geq - \int_{\Omega} h_x^*(\operatorname{div} v^*(x), v^*(x)) dx$$

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Taking a minimizing sequence and using weak compactness of measures gives existence.
For the statement about the support of the measure:

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using a selection theorem (Ekeland Temam Ch 8, Thm 1.2) we can find a measurable selection

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using a selection theorem (Ekeland Temam Ch 8, Thm 1.2) we can find a measurable selection

$$(\eta_x, \xi_x) \in \operatorname{arg\,sup}_{(\eta, \xi)} [\xi \cdot v(x) + \eta \operatorname{div} v(x) - h_x(\eta, \xi)]$$

The measure $\mu = \delta_{\eta_x} \delta_{\xi_x}$ attains the lower bound. In addition, if the support does not satisfy the condition mentioned, then it is not optimal.

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Oscillating coefficients

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$$h_x = h_x(\eta, \xi, \Lambda) = \frac{1}{2}(\Lambda \xi, \xi) - f(x)\eta \quad dg(x, \Lambda) = \int_{\Sigma} d\mu_x(\eta, \xi, \Lambda)$$

Assumption about the oscillations in C

$$\int_{\mathbb{S}^n} \Lambda^{-1} dg(x, \Lambda) \geq \alpha I \quad \alpha > 0$$
$$\int_{\mathbb{S}^n} \|\Lambda\| dg(x, \Lambda) < \infty$$

$$h_x^*(w, z, \Lambda) = \frac{1}{2}(z, \Lambda^{-1} z) \quad \operatorname{dom}(h_x^*) = \{(w, z, \Lambda) : w = -f(x)\}$$

The dual problem is

$$\inf_v \frac{1}{2} \int_{\Omega} (v(x), A^{-1}v(x)) dx \quad \text{subject to} \quad -\operatorname{div} v(x) = f \quad v \cdot n = 0 \quad \partial\Omega$$

where $A^{-1} = \int_{S^n} \Lambda^{-1} dg(x, \Lambda)$

Which gives the known result,

$$-\operatorname{div} (A\nabla\lambda) = f \quad x \in \Omega \quad \nabla\lambda \cdot n = 0 \quad x \in \partial\Omega$$

$$(\cdot, \xi, \Lambda) \in \operatorname{supp}(\mu_x) \longrightarrow \xi = \Lambda^{-1}\nabla\lambda^*(x) \quad x \in \Omega$$

This gives in addition to the effective equation for the weak limit, also the characterization of the oscillations, and allow calculation of all moments.

Variational Evolution Equations

The evolution of the parameterized measure

$$\frac{\partial \mu_x}{\partial t} + \operatorname{div}_\sigma (V \mu_x) = 0 \quad V = (V^\eta, V^\xi)$$

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A potential formulation of a gradient flow,

$$\min_{V \in \mathcal{V}} \int_{\Omega} \left(\frac{1}{2} |V|^2, \mu_x \right) dx + \int_{\Omega} (V \cdot D_\sigma h_x, \mu_x(t)) dx$$

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This formulation does NOT reduce back to Sobolev space solution if it exists.

Motivated by minimizing movements,

$$\min_u \frac{1}{2\tau} \|u - u^n\|^2 + \int_{\Omega} h(x, \nabla u) dx$$

to derive the gradient flow for that case, and noticing that the L2 norm above is the Wasserstein distance but only in the η variable, we arrive at the following gradient flow formulation

$$\min_{V \in \mathcal{V}} \int_{\Omega} \left(\frac{1}{2} |V^\eta|^2, \mu_x \right) dx + \int_{\Omega} (V \cdot D_\sigma h_x, \mu_x(t)) dx$$

Equations in Weak Form??

Review the minimization problem, and the associated equation in weak form,

Start with $\inf_{\mu \in \text{SMP}^p} \int_{\Omega} (h_x, \mu_x) dx$

And consider perturbations that preserve the total mass and the compatibility condition we arrive at,

$$\int_{\Omega} (V \cdot Dh_x, \mu_x) dx = 0 \quad \text{For } v: \int_{\Omega} (V \cdot Bv(x), \mu_x) dx = 0 \quad v(x) \in W^q(\text{div}; \Omega)$$

$$Bv(x) = \begin{bmatrix} \text{div } v(x) \\ v(x) \end{bmatrix}$$

There exists $\lambda(x)$ such that $(Dh_x - B\lambda(x))\mu_x = 0$ $Dh_x = \begin{bmatrix} D_{\eta} h_x(\eta, \xi) \\ D_{\xi} h_x(\eta, \xi) \end{bmatrix}$

The problem: Find a special Young measure μ satisfying

$$\int_{\Omega} (V_x \cdot H_x, \mu_x) dx = 0 \quad \text{For } v: \int_{\Omega} (V_x \cdot Bv(x), \nu_x) dx = 0 \quad v(x) \in W_0^q(\text{div}; \Omega), \nu \in \text{SM}^p$$

Needs a Lax-Milgram type of theorem in Banach spaces

This implies ?

$$\text{There exists } \lambda(x) \text{ such that } (H_x - B\lambda(x))\mu_x = 0$$

The last statement says that the support of μ_x is where $H_x(\eta, \xi) = B\lambda(x)$

Is this enough to determine the solution?

Thank you!