Gradient flows: challenges and new directions

The thresholding scheme for mean curvature flow and de Giorgi's ideas for minimizing movements

Selim Esedoglu, Tim Laux, Felix Otto,

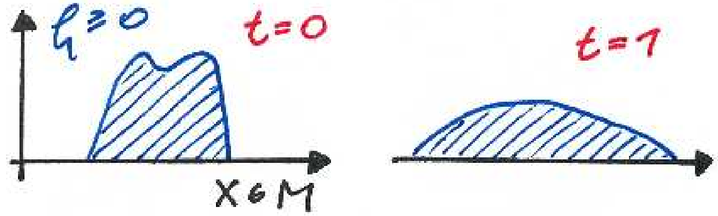
Max Planck Institute for Mathematics in the Sciences,

Leipzig, Germany

Gradient flows and energy landscapes, 3 contributions

I) Porous medium equation

time asymptotics



II) Diffusive phase transition

bounds on coarsening

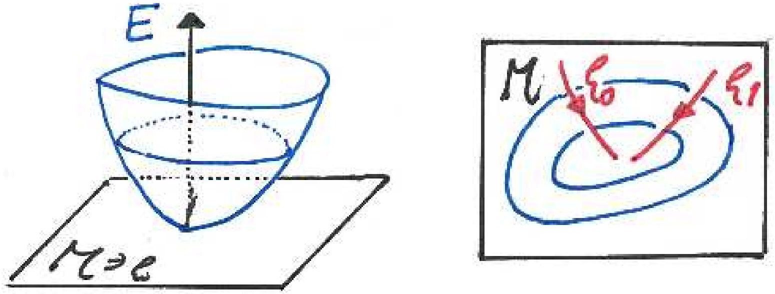
III) Thresholding scheme
for flow
by mean curvature

convergence

Gradient flows and energy landscapes, 3 contributions

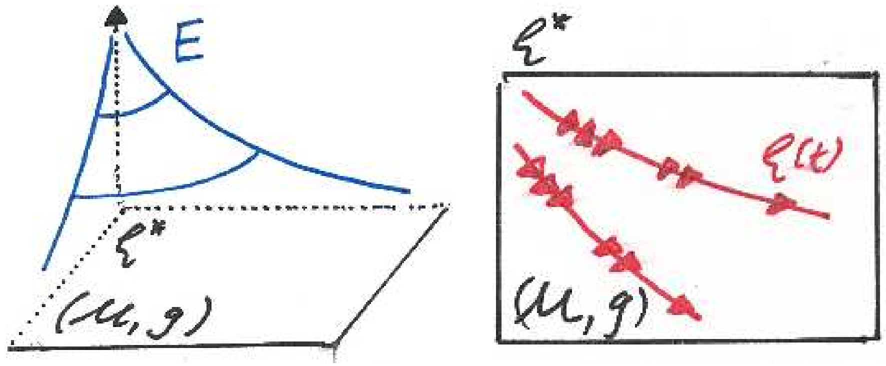
I) Porous medium equation,
contraction in Wasserstein dist.

$$\text{Hess}E \geq 0 \Longrightarrow \frac{d}{dt} d(\rho_0(t), \rho_1(t)) \leq 0$$



II) Diffusive phase transition,
lower bounds on
decrease of surface energy

$$E(\rho) \geq d^{-\alpha}(\rho, \rho^*)$$
$$\Longrightarrow \; E(\rho(t)) \gtrsim t^{-\frac{\alpha}{\alpha+2}}$$



III) Thresholding scheme, convergence to Brakke's inequality

Interpretation as $\quad \rho^n = \text{argmin} \frac{1}{2h} \mathrm{d}^2(\rho, \rho^{n-1}) + E(\rho)$,

Approximate validity of $\quad \frac{d}{dt} E \leq g_\rho(\text{grad} E_{|\rho}, \text{grad} E_{|\rho})$

Structural differences between I, II, III

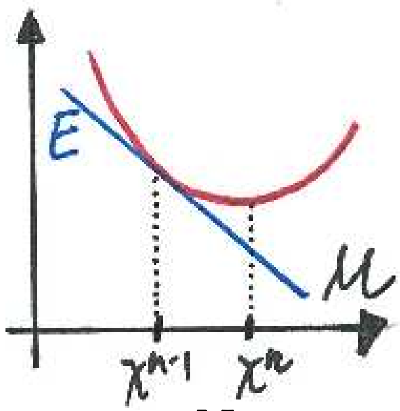
Porous medium equation	Diffusive phase transition	Flow by mean curvature
d explicit	Explicit lower bound on d	d degenerates (Michor&Mumford)
E convex	E non-convex	E non-convex

Abstract theme for III)

Natural time discretization with time step size $h > 0$:

χ^n minimizes $\frac{1}{2h} d^2(\chi, \chi^{n-1}) + E(\chi)$ among all $\chi \in \mathcal{M}$.

= De Giorgi's minimizing movements scheme



Easy a priori estimate $E(\chi^N) + \sum_{n=1}^{N} \frac{1}{2h} d^2(\chi^n, \chi^{n-1}) \le E(\chi^0)$

misses dissipation relation $E(\chi(T)) + \int_0^T g_\chi(\frac{d\chi}{dt}, \frac{d\chi}{dt}) dt \le E(\chi(0))$

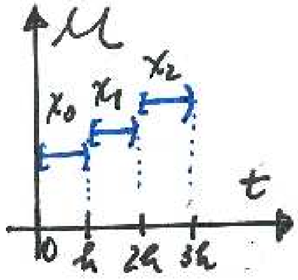
by a factor $\frac{1}{2}$. Way out:

De Giorgi's "variational interpolation", "metric slope".

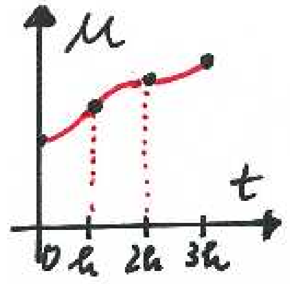
De Giorgi's tools

Two interpolations of $\{\chi^n\}_{n\in\mathbb{N}}$

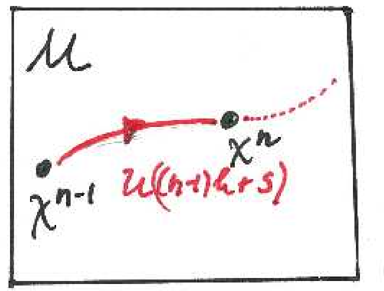
piecewise constant χ^h



"variational" u^h



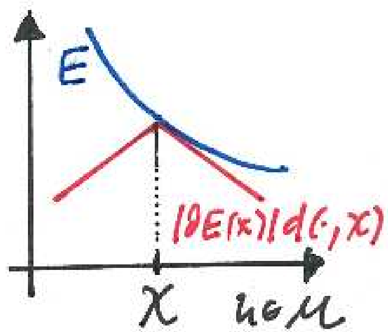
$u^h((n\text{-}1)h+s)$ minimizes $\frac{1}{2s}d^2(u,\chi^{n-1})+E(u)$ among all $u\in\mathcal{M}$



"Metric slope" $|\partial E(\chi)|$

$$:= \limsup_{d(u,\chi)\to 0} \frac{(E(\chi)-E(u))_+}{d(u,\chi)}$$

maximal local downwards slope



De Giorgi's tools provide a path ...

Obtain

$$E(\chi^N)+\int_0^{Nh}\frac{1}{2h^2}d^2(\chi^h(t+h),\chi^h(t))dt+\int_0^{Nh}\frac{1}{2}|\partial E(u^h(t))|^2dt$$
$$\leq E(\chi^0)$$

Similar to limit:

$$E(\chi(T))+\int_0^T\frac{1}{2}g_\chi\left(\frac{d\chi}{dt},\frac{d\chi}{dt}\right)dt+\int_0^T\frac{1}{2}g_\chi(\mathrm{grad}E_{|\chi},\mathrm{grad}E_{|\chi})dt$$
$$\leq E(\chi^0)$$

... to a convergence result

The thresholding scheme

Merriman & Bence & Osher '92:

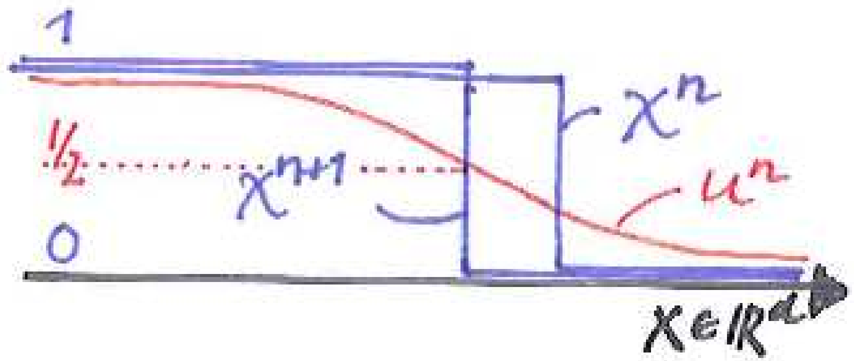
Computational scheme for flow by mean curvature (MCF)

Here just time discretization; time-step size h; $\chi \in \{0, 1\}$

$$\chi^{n-1} \overset{\text{convolution}}{\rightsquigarrow} u^n := G_h * \chi^{n-1} \overset{\text{thresholding}}{\rightsquigarrow} \chi^n := I(u^n \geq \tfrac{1}{2})$$

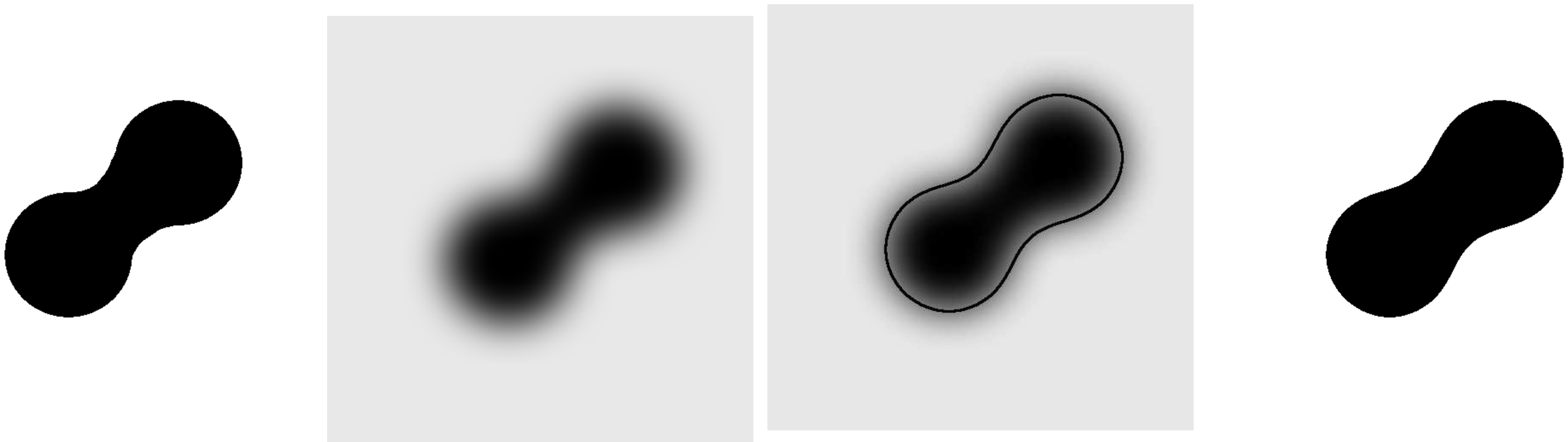
G_h heat kernel at time h

$=$ Gaussian of variance h



Easy to implement

$$\chi^{n-1} \overset{\text{convolution}}{\rightsquigarrow} u^n := G_h * \chi^{n-1} \overset{\text{thresholding}}{\rightsquigarrow} \chi^n := I(u^n \geq \tfrac{1}{2})$$



χ^{n-1} $\quad$ u^n $\quad$ $\{u^n = \frac{1}{2}\}$ $\quad$ χ^n

Low complexity: Fast Fourier Transform for convolution

Convergence in the two-phase case

$$\chi^{n-1} \overset{\text{convolution}}{\rightsquigarrow} u^n := G_h * \chi^{n-1} \overset{\text{thresholding}}{\rightsquigarrow} \chi^n := I(u^n \geq \tfrac{1}{2})$$

Thresholding satisfies comparison principle:

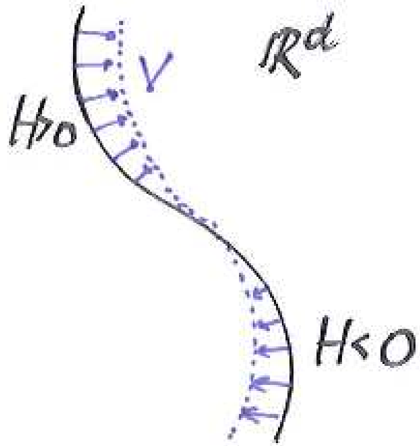
$$\chi^{n-1} \leq \tilde{\chi}^{n-1} \Longrightarrow u^n \leq \tilde{u}^n \Longrightarrow \chi^n \leq \tilde{\chi}^n$$

Evans '93,

Barles & Georgelin '95:

convergence to MCF

in sense of viscosity solution



Straightforward extension to multi-phase version

N phases, eg $\chi = \{\chi_i\}_{i=1,\cdots,N}$ with $\sum_{i=1}^{N} \chi_i = 1$

$\chi^{n-1} \rightsquigarrow u^n, u_i^n := G_h * \chi_i^{n-1} \rightsquigarrow \chi^n, \chi_i^n := I(u_i^n \geq u_j^n \,\forall j)$

Application to grain growth:

eg Elsey & Esedoglu & Smereka '11

Long-time existence of multi-phase MCF:

Kim & Tonegawa via Brakke's notion of MCF '15

Two issues

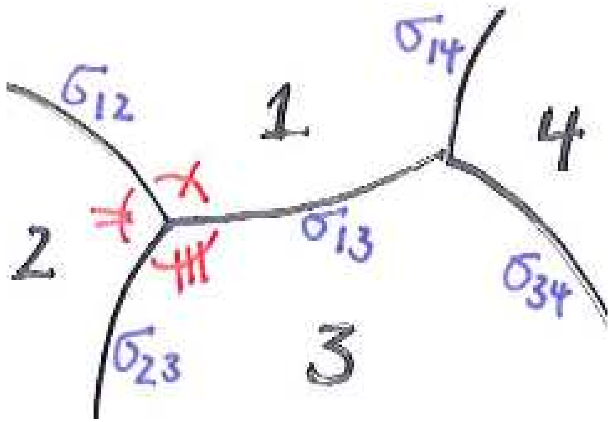
1) Generalization to $\binom{N}{2}$

surface tensions σ_{ij}

(Esedoglu & O. '14)

interfacial energy depends

on misorientation of grains



2) (conditional) convergence (Laux & O. '15, '16)

Both based on **minimizing movement interpretation**

of thresholding (EO'14)

Thresholding as minimizing movement (EO'14)

a) $E_h(\chi) := \sum_{i\neq j} \frac{1}{\sqrt{h}}\int \chi_i\, G_h * \chi_j$

Γ-converges to $c_0 \sum_{i\neq j} \frac{1}{2}\int |\nabla\chi_i| + |\nabla\chi_j| - |\nabla(\chi_i+\chi_j)|$

$= c_0 \sum_{i\neq j}$ area of interface between phase i and phase j

$= c_0$ total interfacial energy

b) $-E_h(\chi-\chi') = \sum_i \frac{1}{\sqrt{h}}\int (\chi_i-\chi_i')\, G_h * (\chi_i-\chi_i')$

$= \sum_i \frac{1}{\sqrt{h}}\int |G_{\frac{h}{2}} * (\chi_i-\chi_i')|^2$ is a distance^2 of χ and χ'

c) thresholding means that χ^n minimizes

$2E_h(\chi;\chi^{n-1}) = -E_h(\chi-\chi^{n-1}) + E_h(\chi) + const,$

which is of form $\frac{1}{2h}\text{distance}^2(\chi,\chi^{n-1}) + \text{energy}(\chi)$

Scheme preserves comparison and *gradient flow structure*

Natural generalization to $\{\sigma_{ij}\}$ (EO'14)

a) $E_h(\chi) := \sum_{i,j} \sigma_{ij} \frac{1}{\sqrt{h}} \int \chi_i \, G_h * \chi_j$

Γ-converges to $c_0 \sum_{i,j} \sigma_{ij} \frac{1}{2} \int |\nabla\chi_i| + |\nabla\chi_j| - |\nabla(\chi_i + \chi_j)|$

$= c_0$ total interfacial energy (eg Ambrosio&Braides'90)

provided $\{\sigma_{ij}\}$ satisfies triangle inequality

New element in proof: monotonicity $E_{kh}(\chi) \leq E_h(\chi)$

b) $-E_h(\chi - \chi')$ is a distance^2 of χ and χ'

provided $\{\sigma_{ij}\}$ negative definite on $\delta\chi = (\delta\chi_i)_i$ with $\sum_i \delta\chi_i = 0$.

$\Longleftrightarrow$ ℓ^2-embeddability, ok for Read-Shockley, ok for $N \leq 4$

c) χ^n minimizes $-E_h(\chi - \chi^{n-1}) + E_h(\chi)$ turns into

$\chi^{n-1} \rightsquigarrow u_i^n := \sum_j \sigma_{ij} G_h * \chi_j^{n-1} \rightsquigarrow \chi_i^n := I(u_i^n \leq u_j^n \; \forall j)$

Thresholding scheme of same complexity!

Convergence of multi-phase thresholding

Holds for any number of phases N provided

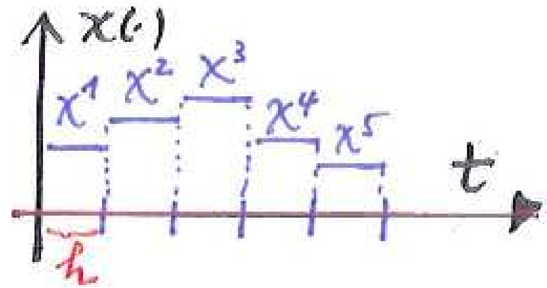
$\{\sigma_{ij}\}_{i,j=1,\cdots,N}$ negative definite & strict triangle inequality

State here for $N = 2$ where $E_h(\chi) = \frac{1}{\sqrt{h}} \int_{[0,1)^d} (1-\chi) G_h * \chi$

χ^0 initial data with $\{E_h(\chi^0)\}_{h\downarrow 0}$ bdd

ie $\int_{[0,1)^d} |\nabla \chi^0| < \infty$,

χ_h piecewise constant interpolation of $\{\chi^n\}_n$



Have 2 *conditional* convergence results:

to BV solution and to Brakke-type solution

Convergence to BV solution (LO'15)

Theorem 1. Suppose $\chi_h \to \chi$ in $L^1((0,1)\times[0,1)^d)$ and

$$\int_0^1 E_h(\chi_h(t))dt \to c_0\int_0^1\int_{[0,1)^d}|\nabla\chi|dt.$$

Then there exists $V \in L^2(|\nabla\chi|dt)$ such that

for all $\zeta \in C_0^\infty((0,1)\times[0,1)^d)$

$$\int_0^1\int \partial_t\zeta\chi + \zeta V|\nabla\chi|dt = 0 \text{ (normal velocity } = V)$$

and for all $\xi \in C_0^\infty([0,1]\times[0,1)^d,\mathbb{R}^d)$

$$\int_0^1\int (\nabla\cdot\xi - \nu\cdot D\xi\nu + 2V\nu\cdot\xi)|\nabla\chi|dt = 0 \text{ (mean curv. } = -2V)$$

A *conditional* convergence result

Suppose $\chi_h \to \chi$ in $L^1((0,1) \times [0,1)^d)$ and

$$\int_0^1 E_h(\chi_h(t))dt \to c_0 \int_0^1 \int_{[0,1)^d} |\nabla\chi| dt.$$

Then $\exists\, V \in L^2(|\nabla\chi| dt)$ s. t. $\forall\, \zeta \in C_0^\infty((0,1) \times [0,1)^d)$, $\xi \in C_0^\infty([0,1] \times [0,1)^d, \mathbb{R}^d)$

$$\int_0^1 \int \partial_t\zeta\chi + \zeta V|\nabla\chi| dt = 0$$

$$\int_0^1 \int (\nabla \cdot \xi - \nu \cdot D\xi\nu + 2V\nu \cdot \xi)|\nabla\chi| dt = 0$$

Same assumption and notion of solution as in Luckhaus & Sturzenhecker '95 on

minimizing movement scheme for MCF introduced by Almgren & Taylor & Wang '93,

but more robust proof (no minimal surface regularity theory)

Convergence to Brakke-type solution (LO'16)

Theorem 2. Suppose $\chi_h \to \chi$ in $L^1((0,1)\times[0,1)^d)$ and

$$\int_0^1 E_h(\chi_h(t))dt \to c_0 \int_0^1 \int_{[0,1)^d} |\nabla\chi| dt.$$

Then there exists $H \in L^2(|\nabla\chi| dt)$ such that

for all $\xi \in C^\infty((0,1)\times[0,1)^d, \mathbb{R}^d)$

$$\int_0^1 \int (\nabla\cdot\xi - \nu\cdot D\xi\nu - \nu\cdot\xi H)|\nabla\chi| dt = 0 \text{ (mean curv. } = H)$$

and for all $\zeta \in C^\infty((0,1)\times[0,1)^d, [0,\infty))$

$$\int_0^1 \int (-2\partial_t\zeta + \zeta H^2 + \nu\cdot\nabla\zeta H)|\nabla\chi| dt \leq 0$$

$$(2\text{normal velocity} = -H)$$

Contains correct inequality $2\frac{d}{dt}\int|\nabla\chi| \leq -\int H^2|\nabla\chi|$

"Brakke-type" because
Brakke's inequality is expressed in BV-framework instead of varifold-framework

Proof: localization of minimizing movements principle

Lemma 1. For any nonnegative $\zeta \in C^\infty([0,1)^d)$

$$\chi^n \quad \text{minimizes} \quad \tilde{E}_h(u,\chi^{n-1}) + \frac{1}{2h}\tilde{d}_h^2(u,\chi^{n-1}) \quad \text{among all } u \in X,$$

where

$$\frac{1}{2h}\tilde{d}_h^2(u,u') := \frac{1}{\sqrt{h}}\int \zeta (G_{\frac{h}{2}} * (u-u'))^2,$$

$$\tilde{E}_h(u,\chi) := \frac{1}{\sqrt{h}}\int \zeta (1-u) G_h * u + (u-\chi)[\zeta, G_h *](1-\chi)$$
$$+ (u-\chi)[\zeta, G_{\frac{h}{2}} *] G_{\frac{h}{2}} * (u-\chi).$$

Furthermore, $(X,\tilde{d}_h)$ is a compact metric space provided $\zeta > 0$, and $\tilde{E}_h(\cdot,\chi)$ is continuous.

Proof: De Giorgi's tools (Ambrosio & Gigli & Savaré '04)

Lemma 2. (X, d) be compact metric space, E continuous, $\chi \in X$.

i) "Variational interpolation". For $t > 0$ let $u(t)$ be a minimizer of

$E(u) + \frac{1}{2t} d^2(u, \chi)$,

which exists by continuity and compactness. Then

$$E(u(t)) + \frac{1}{2t} d^2(u(t), \chi) + \int_0^t \frac{1}{2s^2} d^2(u(s), \chi) ds \le E(\chi).$$

ii) "Metric slope". For $u \in X$ define

$$|\partial E|(u) := \limsup_{v:d(u,v)\downarrow 0} \frac{(E(u)-E(v))_+}{d(u,v)} \in [0, \infty].$$

Then

$$|\partial E|(u(t)) \le \frac{1}{t} d(u(t), \chi).$$

Usage: If $u((n\text{-}1)h+t)$ minimizes $E(u) + \frac{1}{2t} d^2(u, \chi^{n-1})$ then

$$E(\chi^n) + \int_{(n\text{-}1)h}^{nh} \frac{1}{2} |\partial E(\chi^n)|^2 + \frac{1}{2} |\partial E(u(s))|^2 ds \le E(\chi^{n-1}).$$

Proof: Passing to limit in inequality (cf. Sandier&Serfaty '04)

Recall: $E(\chi^n) + \int_{(n-1)h}^{nh} \frac{1}{2}|\partial E(\chi^n)|^2 + \frac{1}{2}|\partial E(u(t))|^2 dt \le E(\chi^{n-1})$.

In localized case: $\tilde{E}_h(\chi^n, \chi^{n-1})$

$$+ \int_{(n-1)h}^{nh} \frac{1}{2}|\partial \tilde{E}_h(\cdot, \chi^{n-1})|^2(\chi^n) + \frac{1}{2}|\partial \tilde{E}_h(\cdot, \chi^{n-1})|^2(\tilde{u}^h(t))dt$$

$$\le \tilde{E}_h(\chi^{n-1}, \chi^{n-1}).$$

Summing yields: $\tilde{E}_h(\chi^h(T), \chi^h(T))$

$$+ \int_0^T \frac{1}{2}|\partial \tilde{E}_h(\cdot, \chi^h(t))|^2(\chi^h(t+h)) + \frac{1}{2}|\partial \tilde{E}_h(\cdot, \chi^h(t))|^2(\tilde{u}^h(t))dt$$

$$+ \int_0^T \frac{1}{h}\Big(\tilde{E}_h(\chi^h(t+h), \chi^h(t)) - \tilde{E}_h(\chi^h(t+h), \chi^h(t+h))\Big)dt \le \tilde{E}_h(\chi^0, \chi^0).$$

Goal: Limit by lower semi-continuity:

$$\int \zeta|\nabla\chi(T)| + \frac{1}{2}\int_0^T \int \zeta H^2|\nabla\chi|dt + \frac{1}{2}\int_0^T \int \nabla\zeta \cdot \nu H|\nabla\chi|dt \le \int \zeta|\nabla\chi^0|.$$

Proof: Metric slope and first variation

Recall $|\partial E(u)| := \limsup_{v:d(u,v)\downarrow 0} \frac{(E(u)-E(v))_+}{d(u,v)}$,

then $\frac{1}{2}|\partial E(u)|^2 \geq \limsup_{v:d(u,v)\downarrow 0}\{(E(u) - E(v))_+ - \frac{1}{2}d^2(u,v)\}$.

First variation $\delta E(u,\xi)$ of function E in configuration $u \in X$
in direction of vector field $\xi \in C^\infty([0,1)^d)^d$:

$\delta E(u,\xi) := \frac{d}{ds}_{|s=0} E(u_s)$ where $\partial_s u_s + \xi \cdot \nabla u_s = 0$ with $u_{|s=0} = u$.

Have $\frac{1}{2}|\partial \tilde{E}_h(\cdot,\chi)|^2(u) \geq \sup_\xi \left\{\delta \tilde{E}_h(\cdot,\chi)(u,\xi) - \sqrt{h}\int \zeta(G_{\frac{h}{2}} * (\xi\cdot\nabla)u)^2\right\}$.

Lemma 3 (Localization and first variation commute).
For any $u, \chi \in X$ and $\xi \in C^\infty([0,1)^d)^d$

$$|\delta \tilde{E}_h(\cdot,\chi)(u,\xi) - \delta E_h(u,\zeta\xi)| \lesssim_{\zeta,\xi} h^{\frac{1}{4}} \frac{d_h(u,\chi)}{h}.$$

$\frac{d_h(u,\chi)}{h}$ is controlled by standard a priori estimate

Proof: Recovering the transport term

From $\int_0^T \frac{1}{h}\Big(\tilde{E}_h(\chi^h(t+h),\chi^h(t)) - \tilde{E}_h(\chi^h(t+h),\chi^h(t+h))\Big)dt$

to $\frac{1}{2}\int_0^T \int \nabla\zeta \cdot \nu H |\nabla\chi| dt$.

Lemma 4. For any $u, \chi \in X$

$$\left|\frac{1}{h}\Big(\tilde{E}_h(u,\chi) - \tilde{E}_h(u,u)\Big) + \frac{1}{2}\delta\frac{1}{2h}d_h^2(\cdot,\chi)(u,\nabla\zeta)\right| \lesssim_{\zeta,\xi} h^{\frac{1}{4}}\frac{d_h(u,\chi)}{h} + h\frac{d_h^2(u,\chi)}{h^2} + h^{\frac{1}{2}}(E_h(u)+E_h(\chi))^{\frac{1}{2}}.$$

Then Euler-Lagrange equation for (un-localized) minimizing movements:

χ^n minimizes $\frac{1}{2h}d_h^2(u,\chi^{n-1}) + E_h(u)$ in form of

$\delta\frac{1}{2h}d_h^2(\cdot,\chi^{n-1})(\chi^n,\xi) = -\delta E_h(\chi^n,\xi)$ for any $\xi \in C^\infty([0,1)^d)^d$.

Proof: Use of the convergence assumption

Lemma 5 (à la Luckhaus-Modica, Reshetnyak).
For any $\{u^h\}_{h\downarrow 0} \subset X$ and $\chi \in \{0,1\}$ with

$$u^h \overset{L^1}{\to} \chi, \quad E_h(u^h) \to E_0(\chi)$$

we have for all $\zeta \in C^\infty([0,1)^d), \xi \in C^\infty([0,1)^d)^d$

$$\tilde{E}_h(u^h, u^h) = \frac{1}{\sqrt{h}} \int \zeta (1 - u^h) G_h * u^h \to c_0 \int \zeta |\nabla \chi|,$$

$$\delta E_h(u^h, \xi) \to \delta E_0(\chi, \xi) = c_0 \int (\nabla \cdot \xi - \nu \cdot D\xi\nu) |\nabla \chi|.$$

Recall $\frac{1}{2}|\partial \tilde{E}_h(\cdot, \chi)|^2(u) \geq \sup_\xi \left\{ \delta \tilde{E}_h(\cdot, \chi)(u, \xi) - \sqrt{h} \int \zeta (G_{\frac{h}{2}} * (\xi \cdot \nabla) u)^2 \right\}$

Lemma 6 (Limit in infinitesimal metric / metric tensor).
Under same assumptions

$$\sqrt{h} \int \zeta (G_{\frac{h}{2}} * (\xi \cdot \nabla) u^h)^2 \to c_0 \int \zeta (\xi \cdot \nu)^2 |\nabla \chi|.$$