PDEs and GMT

The thresholding scheme for mean curvature flow and De Giorgi's ideas

Selim Esedoglu, Tim Laux, Felix Otto,

Max Planck Institute for Mathematics in the Sciences,

Leipzig, Germany

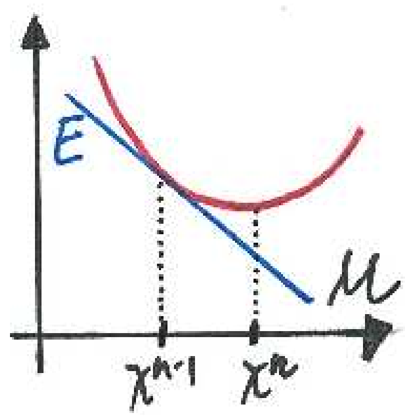
Abstract theme

Flow of hypersurface Σ by mean curvature
$=$ gradient flow of $\mathcal{H}^{d-1}(\Sigma)$ w. r. t. $L^2(\Sigma)$
(functional not semi-convex, induced distance degenerate (Michor&Mumford))

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

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

$=$ De Giorgi's minimizing movements scheme



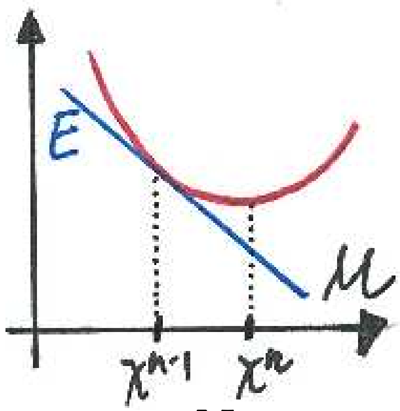
Thresholding scheme $=$ a minimizing movement scheme

Passage to limit in minimizing movements scheme

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

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

= De Giorgi's minimizing movements scheme



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

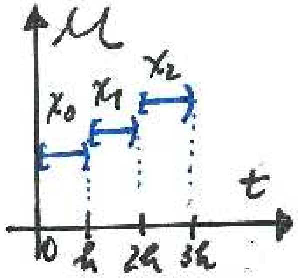
misses dissipation relation $E(\chi(T)) + \int_0^T g_\chi(\frac{d\chi}{dt}, \frac{d\chi}{dt}) dt \leq E(\chi(0))$ by a factor $\frac{1}{2}$. Way out:

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

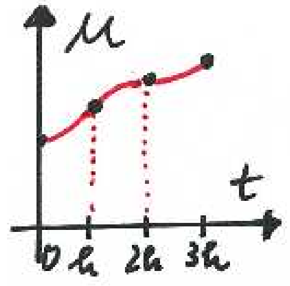
De Giorgi's tools

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

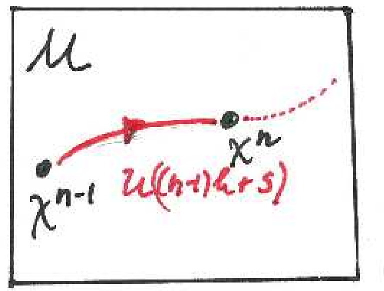
piecewise constant χ^h



"variational" u^h



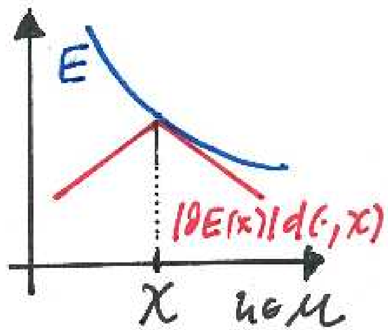
$u^h((n\text{-}1)h+s)$ minimizes $\frac{1}{2s}d^2(u,\chi^{n-1})+E(u)$ among all $u\in\mathcal{M}$



"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:

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

c. f. Sandier-Serfaty '04

... to a convergence result

The thresholding scheme

Merriman & Bence & Osher '92:

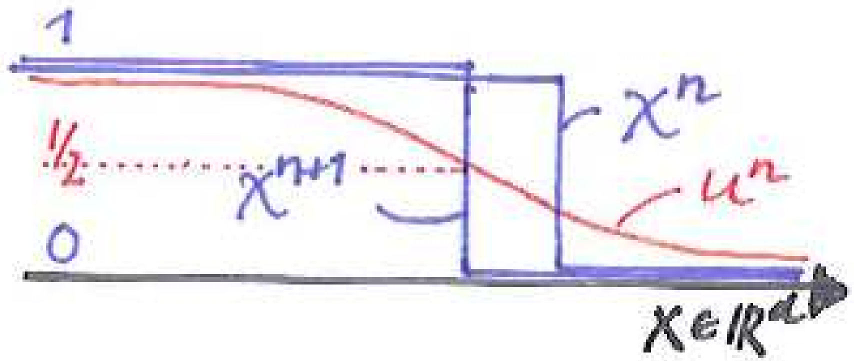
Computational scheme for flow by mean curvature (MCF)

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

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

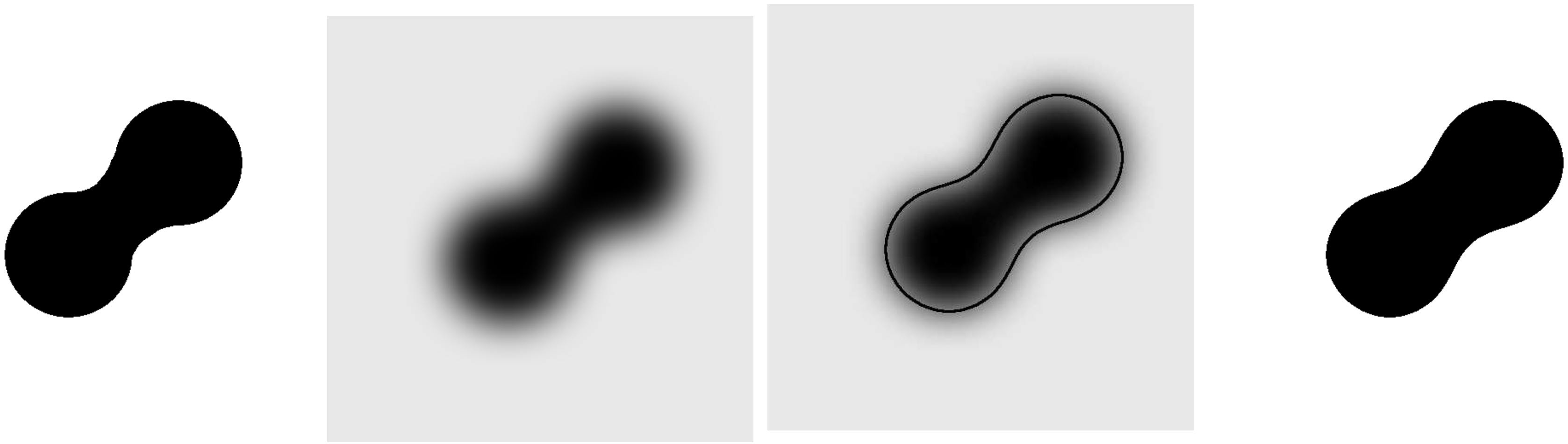
G_h heat kernel at time h

$=$ 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} u^n $\{u^n = \frac{1}{2}\}$ 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:

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

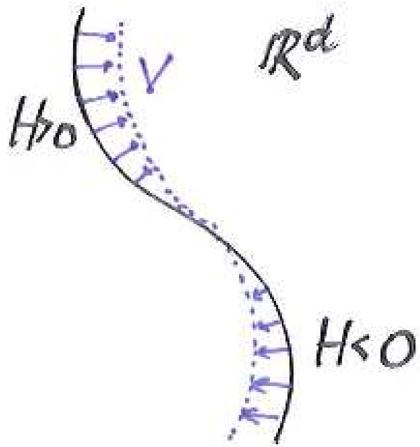
Evans '93,

Barles & Georgelin '95,

Ishii & Pires & Souganidis '99:

convergence to MCF

in sense of viscosity solution (Evans-Spruck)



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 '15,

Strong solutions past singularities for $d = 2$ (networks):

Mantegazza&Novaga&Tortorelli '04, Ilmanen&Neves&Schulze '18

Two issues

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

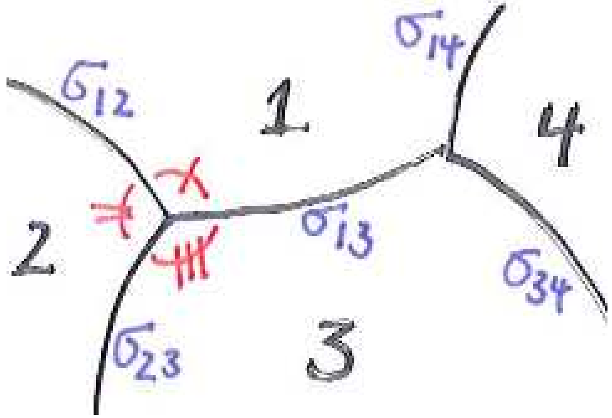
surface tensions σ_{ij}

(Esedoglu & O. '14),

and mobilities (Esedoglu & Salvador '18)

interfacial energy depends

on misorientation of grains



2) (conditional) convergence (Laux & O. '16, '17)

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 $\frac{1}{2h}$distance$^2(\chi, \chi^{n-1})$ + energy(χ)

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

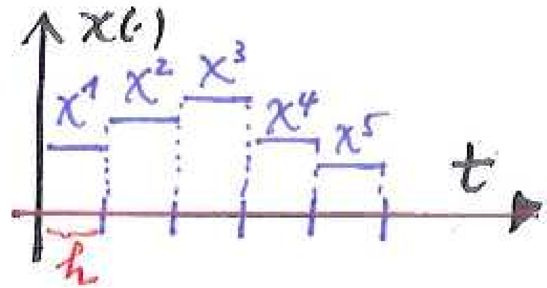
$\{\sigma_{ij}\}_{i,j=1,\cdots,N}$ negative definite & strict triangle inequality

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 3 *conditional* convergence results:

to BV solution, Brakke solution, De Giorgi-type solution

Convergence to BV solution (LO'16 CalcVar)

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

$$\int_0^1 E_h(\chi_h(t))dt \to c_0 \int_0^1 \int |\nabla\chi| dt.$$

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

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

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

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

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

here $\int := \int_{[0,1)^d}$

A *conditional* convergence result

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

$$\int_0^1 E_h(\chi_h(t))dt \to c_0 \int_0^1 \int |\nabla\chi| dt.$$

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'17 arXiv)

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

$$\int_0^1 E_h(\chi_h(t))dt \to c_0 \int_0^1 \int |\nabla\chi| dt.$$

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

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

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

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

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

Convergence to De Giorgi-type solution (LO'18 in preparation)

Theorem 3. Suppose $\chi_h \to \chi$ in $L^1((0,1)\times[0,1)^d)$ and
$\int_0^1 E_h(\chi_h(t))dt \to c_0 \int_0^1 \int |\nabla\chi| dt.$

Then $\exists\ V \in L^2(|\nabla\chi|dt)$ s. t. $\forall\ \zeta \in C_0^\infty((0,1)\times[0,1)^d)$
$\int_0^1 \int \partial_t\zeta\chi + \zeta V|\nabla\chi|dt = 0$ (normal velocity $= V$)

and $\exists\ H \in L^2(|\nabla\chi|dt)$ s. t. $\forall\ \xi \in C^\infty((0,1)\times[0,1)^d, \mathbb{R}^d)$
$\int_0^1 \int (\nabla\cdot\xi - \nu\cdot D\xi\nu - \nu\cdot\xi H)|\nabla\chi|dt = 0$ (mean curv. $= H$)

with the property that for all $T \in (0,1)$

$$2\int|\nabla\chi(T)| + \int_0^T \int \tfrac{1}{2}((2V)^2 + H^2)|\nabla\chi|dt \le 2\int|\nabla\chi^0|.$$

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

Lower semi-continuity in metric term, sketch of proof

Goal: $c_0\int_0^T\int V^2|\nabla\chi| \le \liminf_{h\downarrow 0}\sum_{0<nh<T}\frac{1}{2h}d_h^2(\chi_h^n,\chi_h^{n-1})$

$$= \lim_{h\downarrow 0}\sqrt{h}\int_0^T\int|G_{\frac{h}{2}}*\frac{\chi_h(t+h)-\chi_h(t)}{h}|^2 := \int_0^T\int d\mu.$$

Convergence assumption yields
"convergence of normals down to scale $\sqrt{h}$", i. e.

$$\frac{1}{\sqrt{h}}\left(\chi_h(\cdot+\sqrt{h}\hat{z})-\chi_h\right)_+ \rightharpoonup \left(\hat{z}\cdot\nabla\chi\right)_+$$

Good time scale $\tau := \alpha\sqrt{h}$ with $\alpha\in(0,\infty)$ to be chosen later.

Consider increment $\delta\chi := \chi_h(t+\tau)-\chi_h(t)\in\{-1,0,1\}$;

have $\quad |\delta\chi| = \delta\chi\, G_h*\delta\chi \;+\; \delta\chi(\delta\chi - G_h*\delta\chi)$.

Lower semi-continuity in metric term, sketch of proof

Recall: time scale $\tau := \alpha\sqrt{h}$, increment $\delta\chi := \chi_h(t+\tau) - \chi_h(t)$

splitting $|\delta\chi| = \delta\chi\, G_h{*}\delta\chi + \delta\chi(\delta\chi - G_h{*}\delta\chi)$.

Recall consequence of convergence assumption

$$\frac{1}{\sqrt{h}}\Big(\chi_h(\cdot{+}\sqrt{h}\hat{z}) - \chi_h\Big)_+ \rightharpoonup \Big(\hat{z}\cdot\nabla\chi\Big)_+.$$

Hence if we further split $\delta\chi = \delta\chi_+ - \delta\chi_-$ we have "orthogonality" $\frac{1}{\sqrt{h}}\int \delta\chi_+\, G_h{*}\delta\chi_- \to 0$.

Allows to replace $\delta\chi(\delta\chi - G_h{*}\delta\chi) \rightsquigarrow$

$$\delta\chi_+(\delta\chi_+ - G_h{*}\delta\chi_+) + \delta\chi_-(\delta\chi_- - G_h{*}\delta\chi_-)$$
$$= \delta\chi_+\, G_h{*}(1\text{-}\delta\chi_+) + \delta\chi_-\, G_h{*}(1\text{-}\delta\chi_-).$$

Lower semi-continuity in metric term, sketch of proof

Recall we still need to control

$$\frac{1}{\tau}\int\Big(\delta\chi_+\, G_h*(1\text{-}\delta\chi_+) + \delta\chi_- G_h*(1\text{-}\delta\chi_-)\Big)$$

where $\delta\chi = \chi_h(t+\tau) - \chi_h(t)$, $\tau = \alpha\sqrt{h}$.

For any normal $\nu_0 \in S^{d-1}$ to be chosen later

$$\int\Big(\delta\chi_+\, G_h*(1\text{-}\delta\chi_+) + \delta\chi_- G_h*(1\text{-}\delta\chi_-)\Big)$$
$$= \int dx \int_{z\cdot\nu_0>0} dz G_h(z)(|\delta\chi_+(x+z)\text{-}\delta\chi_+(x)|+|\delta\chi_-(x+z)\text{-}\delta\chi_-(x)$$

Discrete mixed derivative in time τ and space z;
use 2 pointwise estimates ("time like", "space like"):

$$|\delta\chi_+(x+z)\text{-}\delta\chi_+(x)| + |\delta\chi_-(x+z)\text{-}\delta\chi_-(x)|$$
$$\leq \begin{cases} |\chi_h(t+\tau,x+z)\text{-}\chi_h(t,x+z)| + |\chi_h(t+\tau,x)\text{-}\chi_h(t,x)| \\ |\chi_h(t+\tau,x+z)\text{-}\chi_h(t+\tau,x)| + |\chi_h(t,x+z)\text{-}\chi_h(t,x)| \end{cases}$$

sketch of proof, end

Recall we still need to control

$$\frac{1}{\tau}\int dx \int_{z\cdot\nu_0>0} dz G_h(z)(|\delta\chi_+(x+z)\text{-}\delta\chi_+(x)| + |\delta\chi_-(x+z)\text{-}\delta\chi_-(x)|).$$

Use $|\delta\chi_+(x+z)\text{-}\delta\chi_+(x)| + |\delta\chi_-(x+z)\text{-}\delta\chi_-(x)|$

$$\leq \begin{cases} |\chi_h(t+\tau,x+z)\text{-}\chi_h(t,x+z)| + |\chi_h(t+\tau,x)\text{-}\chi_h(t,x)| & \text{for } z\cdot\nu_0 > \tau V_0 \\ |\chi_h(t+\tau,x+z)\text{-}\chi_h(t+\tau,x)| + |\chi_h(t,x+z)\text{-}\chi_h(t,x)| & \text{for } z\cdot\nu_0 < \tau V_0 \end{cases}$$

with $V_0 \in (0,\infty)$ to be chosen.

Convergence assumption yields $|\partial_t\chi|$

$$\leq \alpha\mu + 2\int_{\hat{z}\cdot\nu_0>\alpha V_0} G_1(\hat{z})d\hat{z}|\partial_t\chi| + \frac{2}{\alpha}\int_{0<\hat{z}\cdot\nu_0<\alpha V_0} G_1(\hat{z})|\hat{z}\cdot\nabla\chi|d\hat{z}.$$

Localize in good point x on boundary and choose

$\nu_0 = \nu(x)$, $V_0 := |V(x)|$, divide by $\alpha \downarrow 0$.

Recover $c_0 V^2 \leq \frac{d\mu}{d|\nabla\chi|}$ with desired $c_0 := \int(\hat{z}_1)_+ G_1(\hat{z})d\hat{z} = \frac{1}{\sqrt{2\pi}}$.

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

Lemma 1. (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

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

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

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

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

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

Limit in slope term: 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 $\frac{1}{2}|\partial E_h(\cdot,\chi)|^2(u) \geq \sup_\xi \left\{\delta E_h(\cdot,\chi)(u,\xi) - \sqrt{h}\int (G_{\frac{h}{2}} * (\xi\cdot\nabla)u)^2\right\}$.

Limit in slope term: Use of the convergence assumption

Lemma 2 (à la Luckhaus-Modica, Reshetnyak).
For any $\{u^h\}_{h\downarrow 0} \subset X$ and $\chi \in \{0,1\}$ with

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

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

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

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

Lemma 3 (Limit in infinitesimal metric / metric tensor).
Under same assumptions

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