

Dislocations dynamics and mean curvature motion

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ENPC, CERMICS

New trends in viscosity solutions and nonlinear PDEs

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Plan

- 1 Convergence of dislocations dynamics to mean curvature motion
- 2 Numerical scheme for dislocations dynamics
- 3 Numerical Scheme for the mean curvature motion

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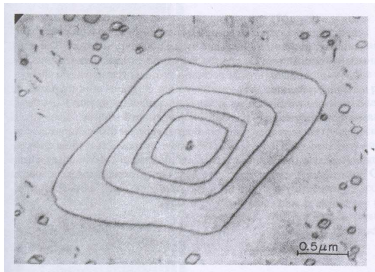
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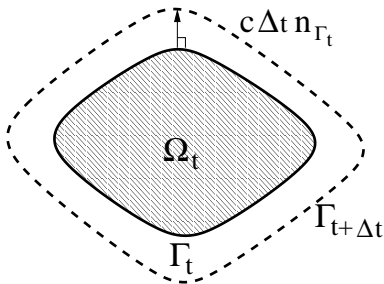
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Observation of dislocations



Definition: a dislocation is a line of crystal defects.

Dynamics of a dislocation



$$\frac{d\Gamma_t}{dt} = c n_{\Gamma_t} \quad \text{with} \quad c = c(\Gamma_t)$$

Slepčev Formulation

- We consider the solutions u^ε of:

$$\begin{cases} u_t^\varepsilon(x, t) = \left((c_0^\varepsilon \star 1_{\{u^\varepsilon(\cdot, t) > u^\varepsilon(x, t)\}}) (x) - \frac{1}{2} \int_{\mathbb{R}^n} c_0^\varepsilon |Du^\varepsilon| \right) \\ u^\varepsilon(\cdot, 0) = u_0(\cdot) \end{cases} \quad (1)$$

where

$$c_0^\varepsilon = \frac{1}{\varepsilon^{n+1} |\ln \varepsilon|} c_0 \left(\frac{x}{\varepsilon} \right)$$

with the particular kernel

$$c_0 \in C^\infty(\mathbb{R}^n), \quad \begin{cases} c_0(x) = \frac{1}{|x|^{n+1}} g \left(\frac{x}{|x|} \right) & \text{if } |x| > 1 \\ c_0(-x) = c_0(x) \geq 0 \end{cases}$$

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Definition of the solutions

Definition (Slepčev)

- u^ε is sub-solution if for Φ test function:

$$\Phi_t \leq \left((c_0^\varepsilon \star 1_{\{u^\varepsilon(\cdot, t_0) \geq u^\varepsilon(x_0, t_0)\}}) (x_0) - \frac{1}{2} \int_{\mathbb{R}^n} c_0^\varepsilon \right) |D\Phi|$$

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Convergence to anisotropic MCM

Theorem (Da Lio, F., Monneau)

Under certain regularity assumptions, when $\varepsilon \rightarrow 0$, u^ε converges locally uniformly on compact sets to u^0 , which is the unique solution of the limit problem:

$$\begin{cases} u_t^0 + F(D^2 u^0, Du^0) = 0 \\ u^0(\cdot, 0) = u_0 \end{cases}$$

with

$$F(M, p) = -\text{trace} \left(MA \left(\frac{p}{|p|} \right) \right)$$

$$A \left(\frac{p}{|p|} \right) = \int_{\theta \in \mathbf{S}^{n-1} \cap \{p^\perp\}} \frac{1}{2} g(\theta) \theta \otimes \theta d\theta$$

Idea of the proof

- Error estimate for regular function s.t. $|D\varphi| > 0$,
- [Barles, Georgelin]: For test function: $|D\varphi| > 0$ or $D\varphi = 0$ and $D^2\varphi = 0$.

Similar Results

- [Garroni, Muller] (Gamma convergence, stationary problem)
- Algorithm of [Merriman, Bence, Osher]
- [Evans], [Barles, Georgelin], [Ishii], [Ishii, Pires, Souganidis], [Bellitini, Novaga], [Chambolle, Novaga]

Error Estimate

We have the following error estimate:

Theorem (F.)

Under certain regularity assumptions, we have the following error estimate between u^ε and u^0 , for $T \leq 1$:

$$|u^\varepsilon - u^0| \leq C \left(\frac{T}{\sqrt{|\ln \varepsilon|}} \right)^{\frac{1}{3}}.$$

Proof: Use the argument of [Barles, Georgelin] in a quantitative way.

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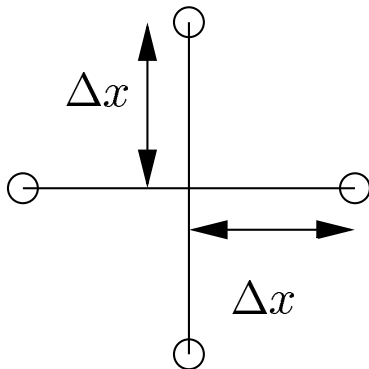
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Discretization



Monotone scheme

$$c_0^\varepsilon = \frac{1}{\varepsilon^{n+1} |\ln \varepsilon|} c_0 \left(\frac{x}{\varepsilon} \right)$$

- Equation: $u_t(x, t) = \left(c[u](x, t) - \frac{1}{2} \int_{\mathbb{R}^n} c_0 \right) |Du|$

- Scheme: $\frac{v_I^{n+1} - v_I^n}{\Delta t} = \left(c_I^{n+1}[v] - \frac{1}{2} \int_{\mathbb{R}^n} c_0 \right) |Dv|_I^{n+1}$

- Non-local velocity: $c[u](x, t) = (c_0 \star 1_{\{u(\cdot, t) > u(x, t)\}})(x)$

- Non-local velocity: $c_I^{n+1}[v] = \sum_{J \in \mathbb{Z}^N} \tilde{c}_{I-J}^0 1_{\{v_J^{n+1} \geq v_I^{n+1}\}}(\Delta x)^N$

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Property of the scheme

Property of the scheme:

- Implicit, but practically computable \Rightarrow no CFL condition
- Discrete Slepcev formulation
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Discrete-continuous error estimate

Theorem (F.)

Under certain regularity assumptions, we have the following error estimate between the continuous solution u of the dislocations dynamics equation (with c_0) and its numerical approximation v :

$$\sup_{\mathbb{R}^N \times (0, T)} |u - v| \leq K\sqrt{T} (\Delta x + \Delta t)^{1/2}$$

provided $|\Delta X| + \Delta t \leq \frac{1}{K^2}$.

Rescaling

$$u^\varepsilon(x, t) = \varepsilon u\left(\frac{x}{\varepsilon}, \frac{t}{\varepsilon^2 |\ln \varepsilon|}\right)$$

$$\begin{aligned} |u^\varepsilon - v^\varepsilon| &\leq K \frac{\sqrt{T}}{\sqrt{|\ln \varepsilon|}} \sqrt{\Delta x + \frac{\Delta t}{\varepsilon |\ln \varepsilon|}} \\ &\leq K \frac{\sqrt{T}}{\sqrt{\varepsilon |\ln \varepsilon|}} \sqrt{\Delta x + \Delta t} \end{aligned}$$

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Numerical scheme for mean curvature motion

- Using the previous result, we get, for $T \leq 1$:

$$\begin{aligned}
 |u^0 - v^\varepsilon| &\leq |u^0 - u^\varepsilon| + |u^\varepsilon - v^\varepsilon| \\
 &\leq C \left(\frac{T}{\sqrt{|\ln \varepsilon|}} \right)^{\frac{1}{3}} + \frac{K}{\sqrt{\varepsilon} |\ln \varepsilon|} \sqrt{T} \sqrt{\Delta x + \Delta t} \\
 &\leq C \left(\frac{T}{\sqrt{|\ln \varepsilon|}} \right)^{\frac{1}{3}}
 \end{aligned}$$

for $\varepsilon \sim \Delta x$ and $\Delta t \leq \Delta x$.

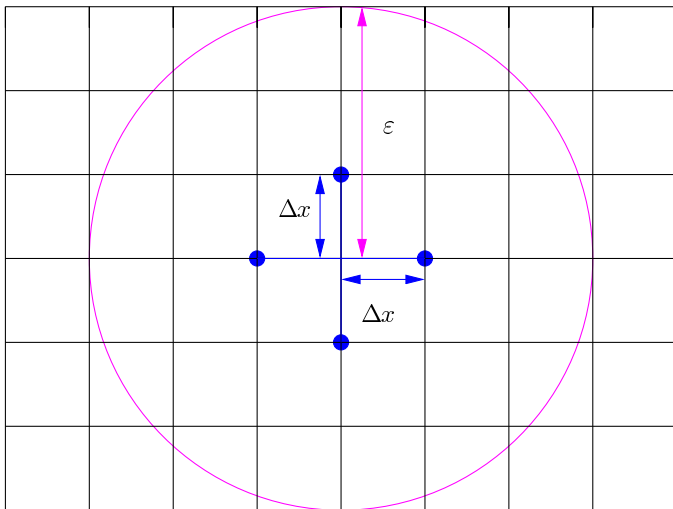
Numerical scheme for mean curvature motion

Theorem (NF)

Let $T \leq 1$. Under certain regularity assumptions, we have the following error estimate between the continuous solution u^0 of the mean curvature motion and its numerical approximation v^ε :

$$\sup_{\mathbb{R}^N \times (0, T)} |u^0 - v^\varepsilon| \leq C \left(\frac{T}{\sqrt{|\ln(\varepsilon)|}} \right)^{\frac{1}{3}} \quad \text{where } \varepsilon \sim \Delta x, \Delta t \leq \Delta x$$

Discretization



References

- [Crandall, Lions], [Oberman]
- Algorithm of [Merriman, Bence, Osher]
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Monotone scheme

- Scheme:

$$v_I^0 = \tilde{u}_0(x_I),$$

$$v_I^{n+1} = v_I^n + \Delta t c^\Delta[v](x_I, t_{n+1}) E^{\text{sign}(c^\Delta[v](x_I, t_{n+1}))} (D^+ v_I^{n+1}, D^- v_I^{n+1}) \quad (2)$$

- Non-local velocity:

$$c^\Delta[v](x_I, t_{n+1}) = \sum_{J \in \mathbb{Z}^N} \bar{c}_0(x_{I-J}) 1_{\{v_J^{n+1} \geq v_I^{n+1}\}} \Delta x_1 \dots \Delta x_N \quad (3)$$

$$- \frac{1}{2} \sum_{J \in \mathbb{Z}^N} \bar{c}_0(x_J) \Delta x_1 \dots \Delta x_N$$

- Kernel:

$$\bar{c}_0(x_I) = \frac{1}{|Q_I|} \int_{Q_I} c_0(x) dx \quad (4)$$

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Monotone scheme

where Q_I is the square cell

$$Q_I = [x_{i_1} - \Delta x_1/2, x_{i_1} + \Delta x_1/2] \times \dots \times [x_{i_N} - \Delta x_N/2, x_{i_N} + \Delta x_N/2]$$

- E^\pm ; approximation of the Euclidean norm ([Osher-Sethian]):

$$E^+ = \left\{ \sum_i \max(D_{x_i}^+ v_I^n, 0)^2 + \sum_i \min(D_{x_i}^- v_I^n, 0)^2 \right\}^2$$

$$E^- = \left\{ \sum_i \min(D_{x_i}^+ v_I^n, 0)^2 + \sum_i \max(D_{x_i}^- v_I^n, 0)^2 \right\}^2$$

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Definition of the solutions

Definition (Numerical sub, super and solution of the scheme)

We say that v is a discrete sub-solution (resp super-solution) of the scheme (2) if for all $I \in \mathbb{Z}^N$, $n \in \mathbb{N}$, we have

$$v_I^{n+1} \leq v_I^n + \Delta t c^\Delta[v](x_I, t_{n+1}) E^{\text{Sign}(c^\Delta[v](x_I, t_{n+1}))} (D^+ v_I^{n+1}, D^- v_I^{n+1})$$

(resp.

$$v_I^{n+1} \geq v_I^n + \Delta t \tilde{c}^\Delta[v](x_I, t_{n+1}) E^{\text{Sign}(\tilde{c}^\Delta[v](x_I, t_{n+1}))} (D^+ v_I^{n+1}, D^- v_I^{n+1}))$$

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