A scheme for the homogenization of dislocation dynamics

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May 20, 2010

Plan

1. Introduction to dislocations

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2. Mathematical model for particles

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3. Homogenization of the dynamics of dislocation curves

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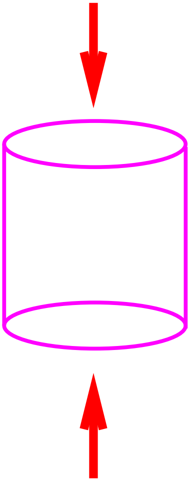
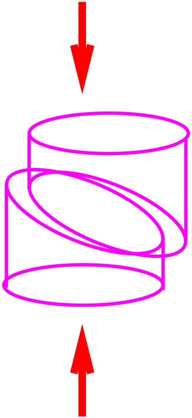
3. Homogenization of the dynamics of dislocation curves
4. A numerical scheme for the cell problem

Introduction to dislocations

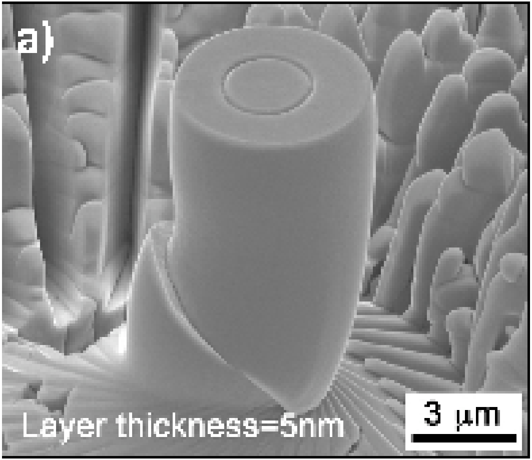
compression of a cylinder



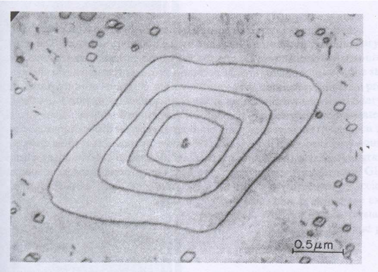
compression of a cylinder



compression of a micro-pillar



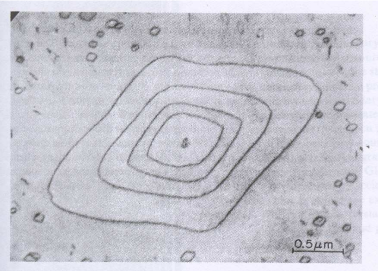
Dislocations in metallic alloys Al-Mg



Definition: a dislocation is a line of crystal defects.

First observation (1956)

Dislocations in metallic alloys Al-Mg



Definition: a dislocation is a line of crystal defects.

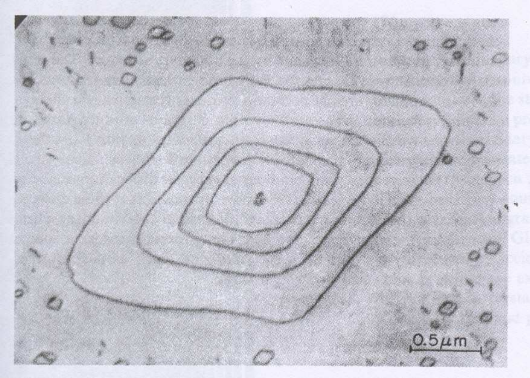
Length $= 10^{-6}m$, Thickness $= 10^{-9}m$

Dynamics of loops

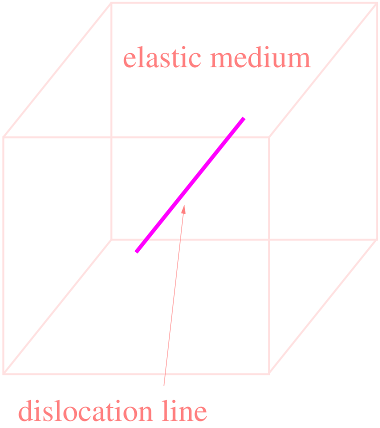
Non local, non monotone dynamics

$$u_t = \left(c_0 \star 1_{\{u \geq 0\}}\right)(x,t)\ |Du| \quad \text{on} \quad \mathbb{R}^N \times (0,T)$$

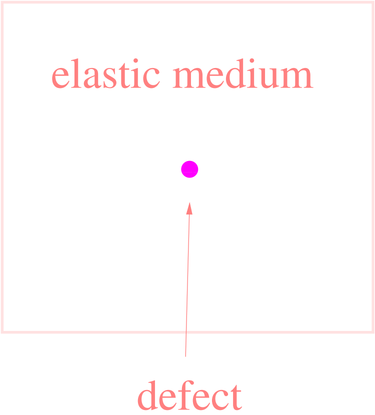
- "Dynamics of sets" (with interior ball)
  [Alvarez, Cardaliaguet, M. (2005)], [Cardaliaguet, Marchi (2006)],
- Level sets
  [Barles, Ley (2006)],
- Notion of weak solutions
  [Barles, Cardaliaguet, Ley, M. (2008)],
  [Barles, Cardaliaguet, Ley, Monteillet (2009)],
- Notion of interior cones
  [Barles, Cardaliaguet, Ley, Monteillet (2009)]


0.5μm

3D continuous model

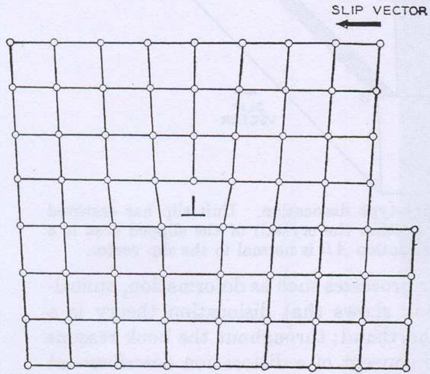


2D continuous model

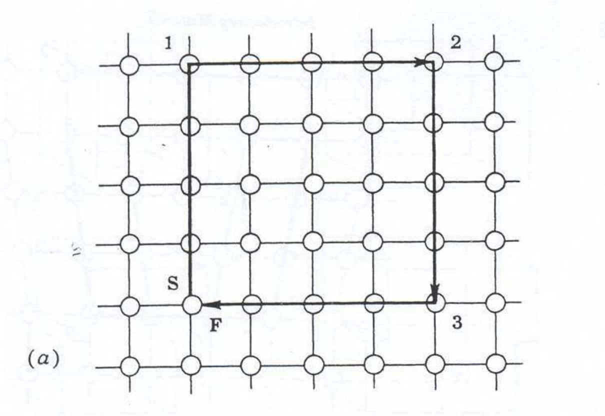


2D atomic model

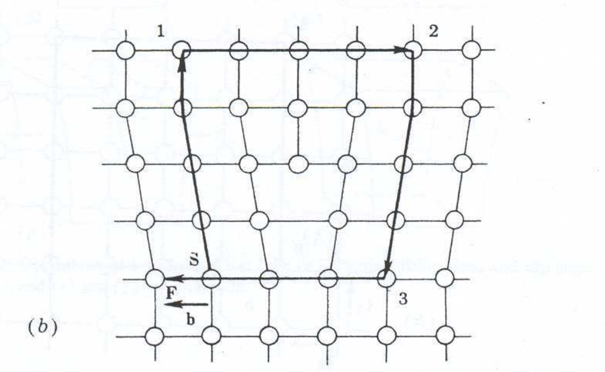
(b)



Perfect crystal



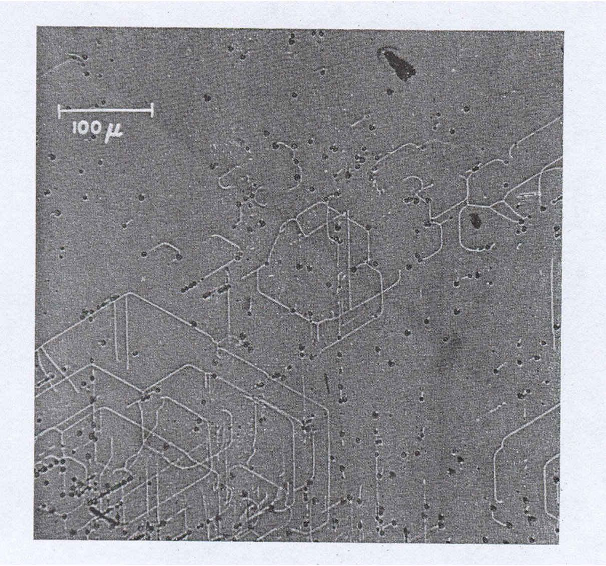
Singular deformation of the crystal



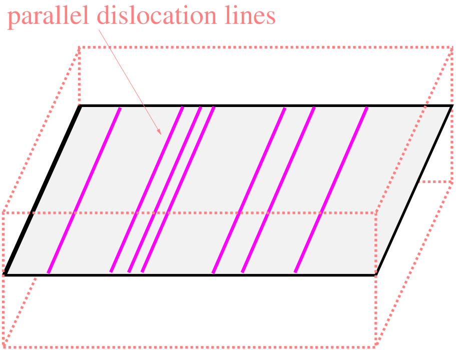
Dynamics of particles

(straight dislocation lines)

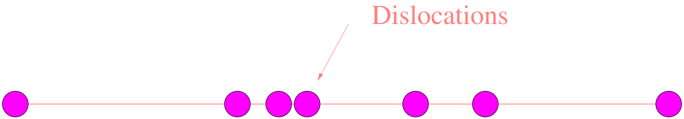
Precipitates = obstacles

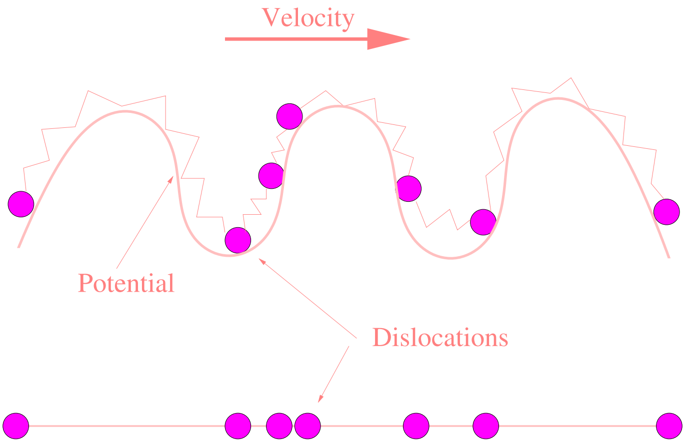


Straight dislocations lines

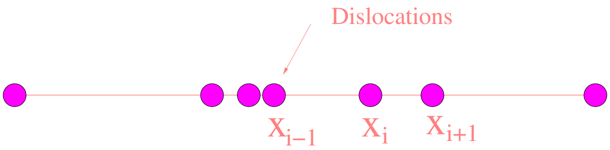


Points



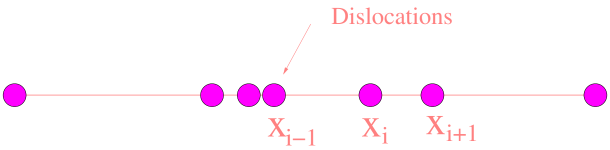

Velocity
Potential
Dislocations

Energy of particles



$$E = \sum_{i<j} V(x_i - x_j) + \sum_i V_0(x_i)$$

Energy of particles

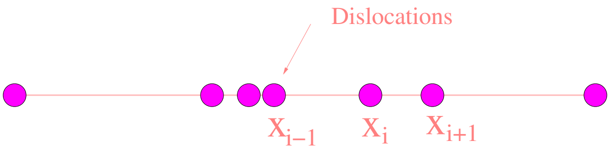


$$E = \sum_{i<j} V(x_i - x_j) + \sum_i V_0(x_i)$$

and

$$V(x) = V(|x|) \quad \text{two-body interactions}$$

Energy of particles



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and

$$V(x) = V(|x|) \quad \text{two-body interactions}$$

$$V_0 \quad \text{periodic:} \quad V_0(x+1) = V_0(x)$$

Overdamped dynamics

$$\text{velocity} \quad = \quad \text{force}$$

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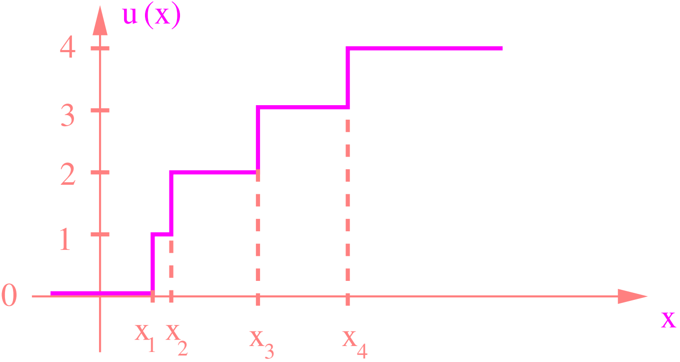
$$\text{velocity} \quad = \quad \text{force}$$

Dynamics

$$\dot{x}_i = -\nabla_{x_i} E + F$$

with

$$F = \text{driving force}$$

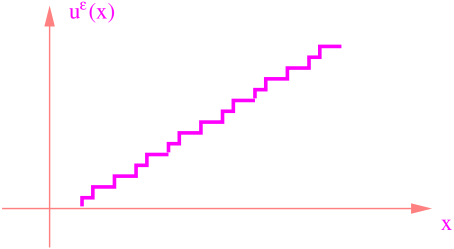


Cumulative distribution

$$u(x,t) = \sum_i H(x - x_i(t))$$

Rescaling

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



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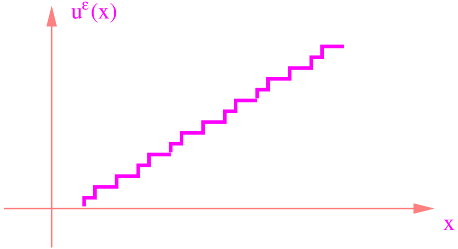
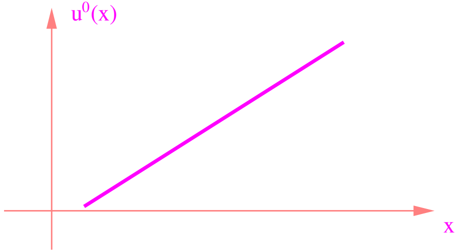


$$u^{\varepsilon} \longrightarrow ?$$

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



$$u^{\varepsilon} \longrightarrow u^{0}$$

Homogenization of dislocation particles

Two-body interactions

$V(x) = -\ln|x|$ for straight dislocations

Long range interactions: $-V'(x) = \dfrac{1}{x}$

Limit $\varepsilon = 0$

Theorem (Forcadel, Imbert, M.)

We have

$$u^\varepsilon(x,t) \longrightarrow u^0(x,t)$$

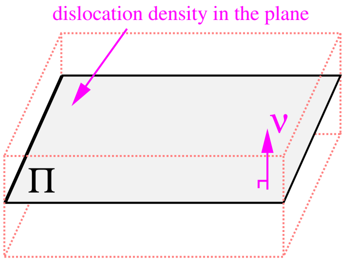
solution of

$$u^0_t = \overline{H}(u^0_x, Lu^0)$$

Here for $w = w(x)$, the operator L is defined by

$$Lw = -(-\Delta)^{\frac{1}{2}} w = \text{pv}\left(\frac{1}{x^2}\right) \star w$$

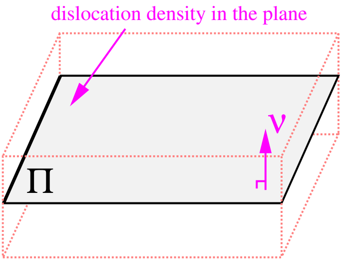
Mechanical interpretation



$$\text{div } \underline{\underline{\sigma}} = 0 \quad \text{with} \quad [U] = bu^0 \quad \text{on} \quad \Pi$$

$\underline{\underline{\sigma}}$: stress, U : displacement, b : Burgers vector

Mechanical interpretation



$$\text{div } \underline{\underline{\sigma}} = 0 \quad \text{with} \quad [U] = bu^0 \quad \text{on} \quad \Pi$$

$\underline{\underline{\sigma}}$: stress, U : displacement, b : Burgers vector

$$Lu^0 = \nu \cdot \underline{\underline{\sigma}} \cdot b$$

Mechanical interpretation

$$\begin{cases} Lu^0 = \sigma & \text{stress} \\ \\ u^0_x = \rho & \text{dislocation density} \end{cases}$$

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1. Orowan law (plastic strain velocity)

$$\dot{e}_p = \sigma\rho$$

Mechanical interpretation

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1. Orowan law (plastic strain velocity)

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2. Norton law with threshold (elasto-visco-plasticity)

$$\dot{e}_p = C \mathsf{sign}(\sigma)((|\sigma| - \sigma_c)^+)^m$$

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2. Norton law with threshold (elasto-visco-plasticity)

$$\dot{e}_p = C \mathsf{sign}(\sigma)((|\sigma| - \sigma_c)^+)^m$$

3. By homogenization we find

$$\dot{e}_p = \overline{H}(\rho, \sigma)$$

Effective Hamiltonian

Theorem (Forcadel, Imbert, M.)

For $F = 0$, we have

- $\overline{H}(\rho,\sigma) = \sigma|\rho| \quad \textit{if} \quad V_0 \equiv 0$

Effective Hamiltonian

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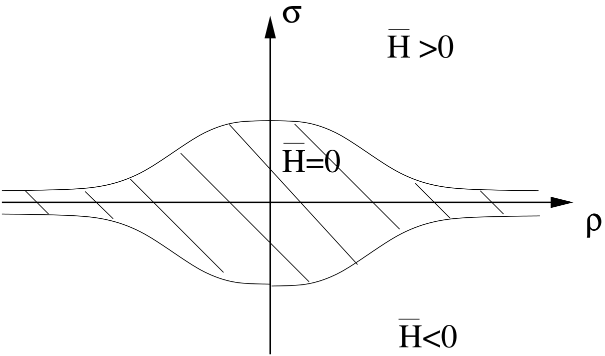
For $F = 0$, we have

- $\overline{H}(\rho, \sigma) = \sigma|\rho| \quad$ *if* $\quad V_0 \equiv 0$

- *Threshold effect* $\quad$ *if* $\quad V_0 \not\equiv 0 \quad$ *with* $\quad \int_0^1 dx\ V_0(x) = 0$ *:*

$$\overline{H}(\rho, \sigma) = 0 \quad \textit{if} \quad (\rho, \sigma) \in B_\delta(0, 0)$$

Effective Hamiltonian



The PDE formulation

Imbedding ODEs in a PDE

$$u(x,t) = \sum_i H(x - x_i(t))$$

solves

$$u_t = |u_x| \left\{ c(x) + \int_{\mathbb{R}} dz \; J(z) E(u(x+z,t) - u(x,t)) \right\}$$

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with

$$\begin{cases} c(x) = V_0'(x) - F \\ J(z) = V''(z) \geq 0 \quad \text{on} \quad \mathbb{R} \setminus \{0\} \\ E = \quad \text{odd integer part} \end{cases}$$

Imbedding ODEs in a PDE

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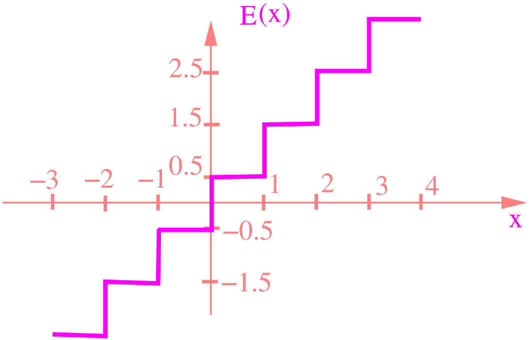
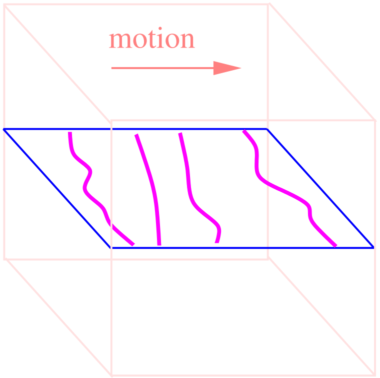
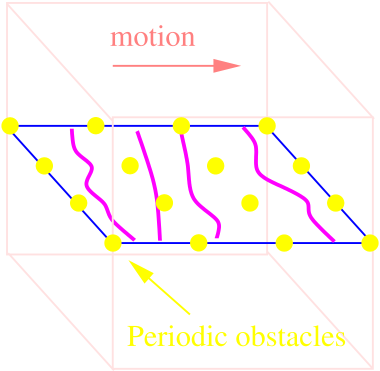


Homogenization of the dynamics of dislocation curves

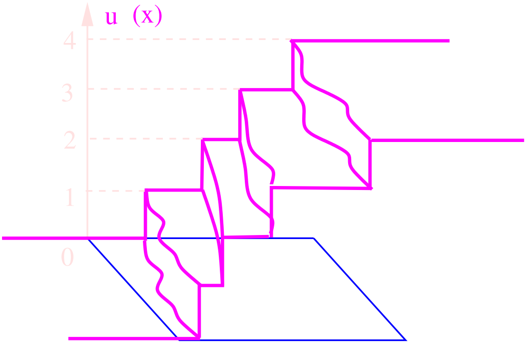


A single plane and a single Burgers vector

Homogenization for curves



Plastic displacement



The microscopic model

$$u_t = |\nabla u| \cdot \left\{ c(x) + \int_{\mathbb{R}^n} dz\ J(z) E(w(x+z) - w(x)) \right\}$$

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with

$$\begin{cases} c(x+k) = c(x) \quad \text{for} \quad k \in \mathbb{Z}^n \\ 0 \leq J(-z) = J(z) = \dfrac{g\left(z/|z|\right)}{|z|^{n+1}} \quad \text{for} \quad |z| \geq R_0 \end{cases}$$

Rescaling

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

Theorem (Forcadel, Imbert, M.)

Assume that $u^\varepsilon(\cdot,0) = u_0 \in W^{2,\infty}(\mathbb{R}^n)$.
Then u^ε *converges to* u^0 *solution of*

$$\begin{cases} u^0_t = \overline{H}(\nabla u^0, L(u^0(\cdot,t))) \\ \\ u^0(\cdot,0) = u_0 \end{cases}$$

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$$Lw = -(-\Delta)^{\frac{1}{2}} w \quad \text{if} \quad g \equiv 1$$

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The cell problem for homogenization

Computation of $\overline{H}$

$$\lambda = |\nabla u| \cdot c[u](x)$$

with

$$c[u](x) = c(x) \qquad + \int_{\mathbb{R}^n} dz\ J(z)\left\{E(u(x+z) - u(x)) - p \cdot z\right\}$$

Theorem (Forcadel, Imbert, M.)

There exists a unique $\lambda = \overline{H}(p, 0)$ such that there exists a solution u such that

$$u(x) - p \cdot x \quad \text{is} \quad \mathbb{Z}^n\text{-periodic}$$

Computation of $\overline{H}$

$$\lambda = |\nabla u| \cdot c[u](x)$$

with

$$c[u](x) = c(x) + \sigma + \int_{\mathbb{R}^n} dz\ J(z) \left\{ E(u(x+z) - u(x)) - p \cdot z \right\}$$

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There exists a unique $\lambda = \overline{H}(p, \sigma)$ such that there exists a solution u such that

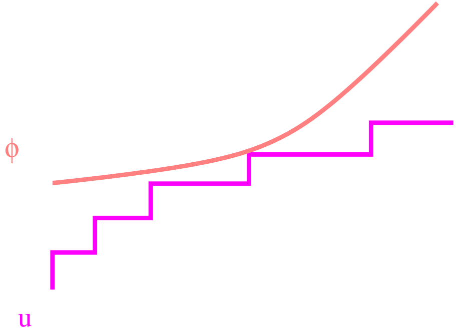
$$u(x) - p \cdot x \quad \text{is} \quad \mathbb{Z}^n\text{-periodic}$$

For $\sigma = 0$, we set

$$c^*[u](x) := c(x) + \int_{\mathbb{R}^n} dz \; J(z) \left\{ E^*(u(x+z) - u(x)) - p \cdot z \right\}$$

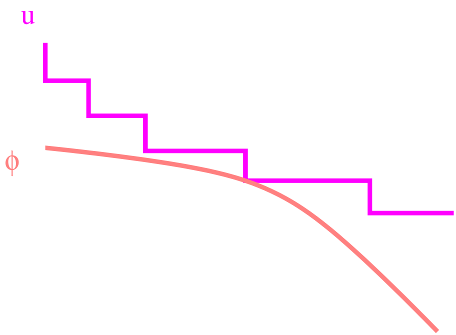
$$c_*[u](x) := c(x) + \int_{\mathbb{R}^n} dz \; J(z) \left\{ E_*(u(x+z) - u(x)) - p \cdot z \right\}$$

Notion of viscosity solution



subsolution:

$$\lambda \leq |\nabla\phi| \cdot c^*[u] \quad \text{at the contact point}$$



supersolution:

$$\lambda \geq |\nabla \phi| \cdot c_*[u] \quad \text{at the contact point}$$

A numerical scheme for the cell problem

Goal: find an approximation of λ by discretization of

$$\lambda = |\nabla u| \cdot c[u]$$

For $\Delta x > 0$ being the inverse of an integer, and for any $I = (I_1, ..., I_n) \in \mathbb{Z}^n$, we define the cube with $x_I = I \cdot \Delta x$

$$Q_I = x_I + [-\Delta x/2, \Delta x/2)^n$$

For $(v_I)_I$, we define the piecewise constant fonction

$$v_\sharp(x) = \sum_{I \in \mathbb{Z}^n} v_I \cdot 1_{\{x \in Q_I\}}$$

Discrete gradients

$$D_i^+ v_I = \frac{v_{I+e_i} - v_I}{\Delta x}, \quad D_i^- v_I = \frac{v_I - v_{I-e_i}}{\Delta x}$$

$$D^\pm v_I = (D_1^\pm v_I, ..., D_n^\pm v_I), \quad Dv_I = (D^+ v_I, D^- v_I)$$

Upwind discretization of the modulus of the gradient

$$G^+(Dv_I) = \sum_{i=1,\ldots,n} \left(\max(0, D_i^+ v_I, -D_i^- v_I)\right)^2$$

$$G^-(Dv_I) = \sum_{i=1,\ldots,n} \left(\max(0, -D_i^+ v_I, D_i^- v_I)\right)^2$$

We assume that

$$v_\sharp(x) - p \cdot x \quad \text{is} \quad \mathbb{Z}^n\text{-periodic}$$

For $x_I = I \cdot \Delta x$, we define

$$R^*[v]_I := \begin{cases} G^+(Dv_I) \cdot c^*[v_\sharp](x_I) & \text{if} \quad c^*[v_\sharp](x_I) \geq 0 \\ G^-(Dv_I) \cdot c^*[v_\sharp](x_I) & \text{if} \quad c^*[v_\sharp](x_I) < 0 \end{cases}$$

Similarly, we define $R_*[v]_I$.

A numerical solution should satisfy

$$R_*[v]_I \leq \lambda_v \leq R^*[v]_I, \quad \text{for every} \quad I \in \mathbb{Z}^n$$

- No uniqueness of λ_v
- The existence of a solution v is unknown

A posteriori error estimate

Theorem (Cacace, Chambolle, M.)

For every discrete function v (periodic + linear), set

$$\overline{\lambda}_v = \sup_{I \in \mathbb{Z}^n} R_*[v]_I, \quad \underline{\lambda}_v = \inf_{I \in \mathbb{Z}^n} R^*[v]_I$$

Then there exists K_v such that

$$\lambda - \overline{\lambda}_v \leq K_v \sqrt{\Delta x}, \quad \underline{\lambda}_v - \lambda \leq K_v \sqrt{\Delta x}$$

- Proof = adaptation of the Crandall-Lions estimate
- $\sqrt{\Delta x}$ replaced by Δx if $n = 1$ (under additional assumptions)

How to find a good candidate v ?

Use the implicit scheme:

$$\begin{cases} R_*[v^{n+1}]_I \leq \dfrac{v_I^{n+1} - v_I^n}{\Delta t} \leq R^*[v^{n+1}]_I \\ \\ v_I^0 = p \cdot x_I \end{cases}$$

Difficulties

- No comparison principle for the solutions
- No uniqueness of the solutions
- Fully implicit scheme $\Longrightarrow$ solvable by an interative procedure

Monotonicity of the discrete time derivative

Theorem (Cacace, Chambolle, M.)

There exists a discrete solution $(v^n)_n$ *of the implicit scheme such that*

$$\overline{\mu}^n = \sup_{I \in \mathbb{Z}^n} \left(\frac{v_I^n - v_I^{n-1}}{\Delta t} \right) \quad \textit{and} \quad \underline{\mu}^n = \inf_{I \in \mathbb{Z}^n} \left(\frac{v_I^n - v_I^{n-1}}{\Delta t} \right)$$

satisfy the following monotonicity property

$$\underline{\mu}^n \le \underline{\mu}^{n+1} \le \overline{\mu}^{n+1} \le \overline{\mu}^n, \quad n \ge 1$$

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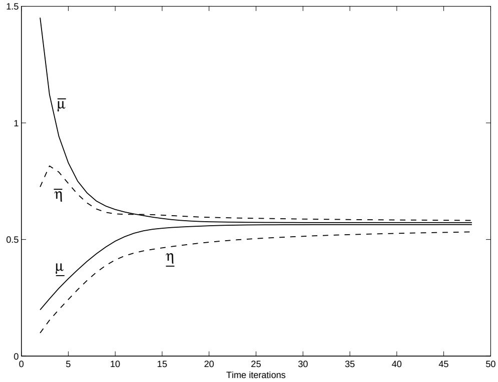
satisfy the following monotonicity property

$$\underline{\mu}^n \le \underline{\mu}^{n+1} \le \overline{\mu}^{n+1} \le \overline{\mu}^n, \quad n \ge 1$$

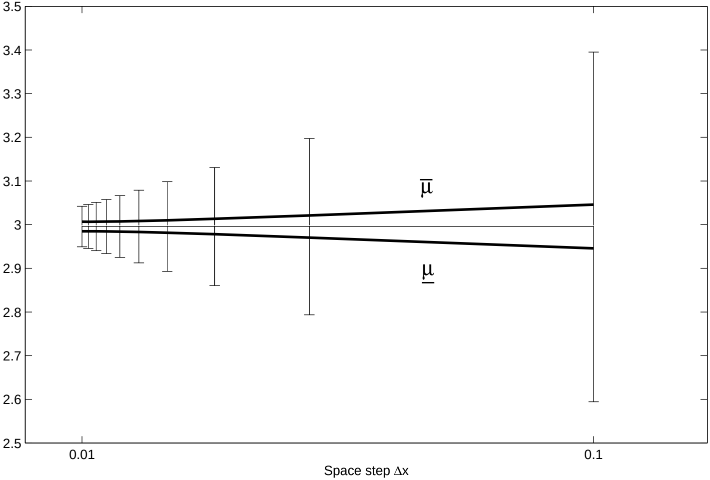
$$\underline{\mu}^n - K_{v^n}\sqrt{\Delta x} \le \lambda \le \overline{\mu}^n + K_{v^n}\sqrt{\Delta x}$$

Convergence in time

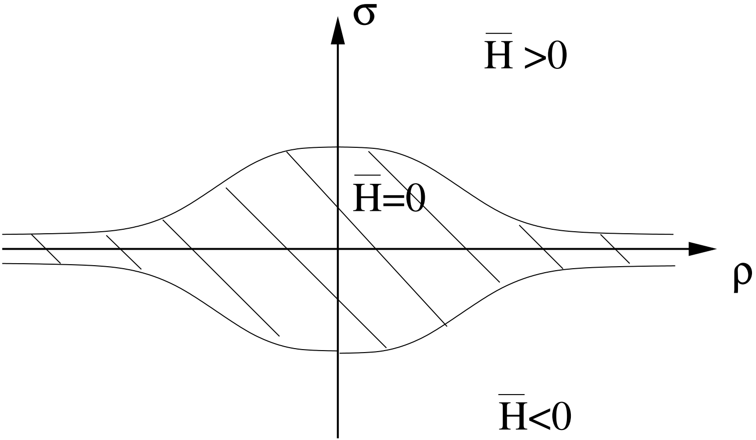


$$\eta^n \sim \frac{v^n}{n\Delta t}$$

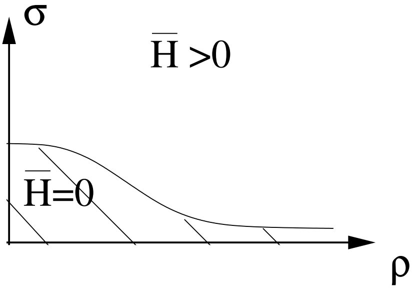
error w.r.t. Δx, (dimension $n = 1$)



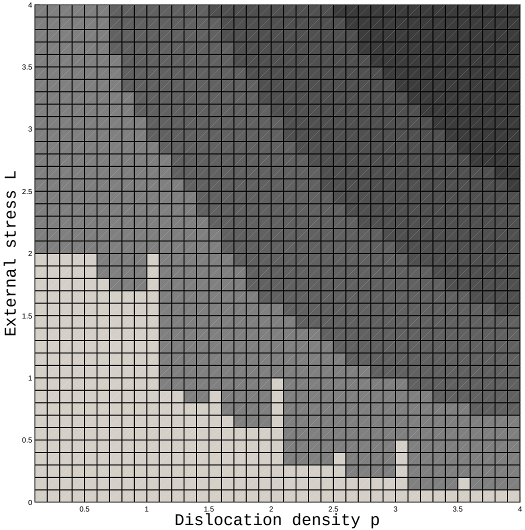
Effective Hamiltonian



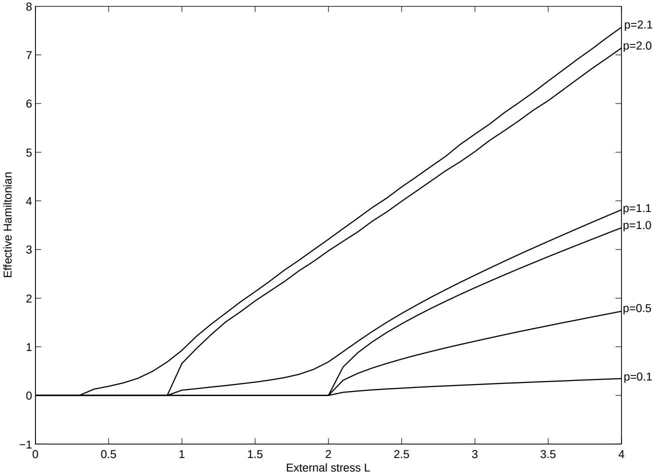
Effective Hamiltonian



Effective Hamiltonian



Effective Hamiltonian $\sigma \mapsto \overline{H}(\sigma, \rho)$



Thank you!