Crystal dislocation dynamics in higher dimensions

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Joint work with Stefania Patrizi (Texas)

Objectives

We consider the limit as $\varepsilon \to 0^+$ of the solution to the fractional reaction-diffusion equation

$$\begin{cases} \varepsilon \partial_t u^\varepsilon = \frac{1}{\varepsilon |\ln \varepsilon|} \left(\varepsilon \Delta^{1/2} u^\varepsilon - W'(u^\varepsilon) \right) & \text{on } (0,\infty) \times \mathbb{R}^n, \; n \geq 2 \\ u^\varepsilon(0,x) = u_0(x) & \text{on } \mathbb{R}^n. \end{cases}$$

1. Review the Peierls–Nabarro model for straight edge dislocations
   - reduce to one-dimensional, nonlocal PDE
   - evolutionary problem
   - discrete dislocation dynamics
2. Discuss progress on different dislocations
   - cannot reduce to one-dimension
   - evolutionary problem
   - interfaces moving by mean curvature

Straight edge dislocations

A perfect crystal is a simple cubic lattice (infinitely extended).

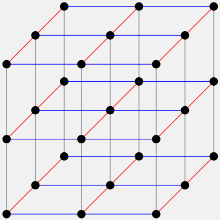

Figure: Cubic lattice

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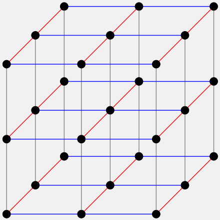

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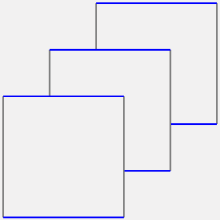

Figure: Stacked planes

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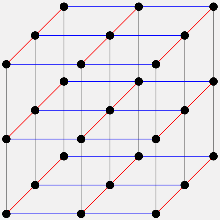

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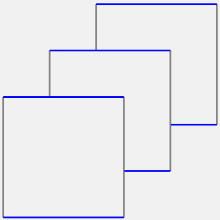

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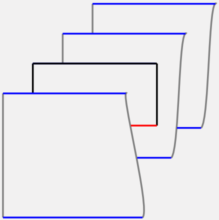
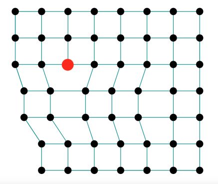


Figure: Dislocation

A straight edge dislocation is caused by the termination of a plane of atoms in the middle of the crystal.

We call the bottom of this ‘plane’ the dislocation line. By symmetry, we associate this line with a single point.

Two dimensional plane



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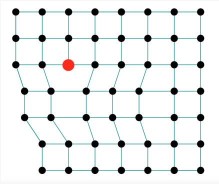

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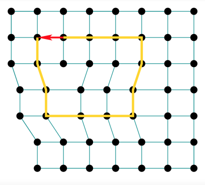

Figure: Burgers vector

In a perfect crystal, if take N steps in each direction, we return to our starting point. For dislocations, we arrive at a different point.

- The arrow joining the starting point to the ending point is called the Burgers vector. It encodes the magnitude and direction of the crystal imperfection.

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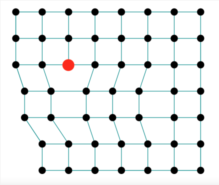

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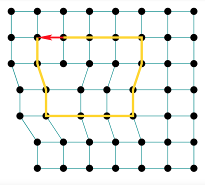

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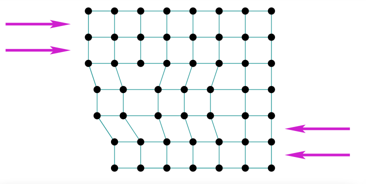

Figure: shearing force

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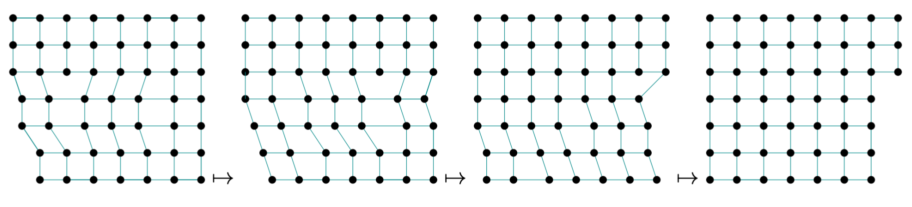
- The arrow joining the starting point to the ending point is called the Burgers vector. It encodes the magnitude and direction of the crystal imperfection.
- The slip line (slip plane) separated the upper and lower half crystals.

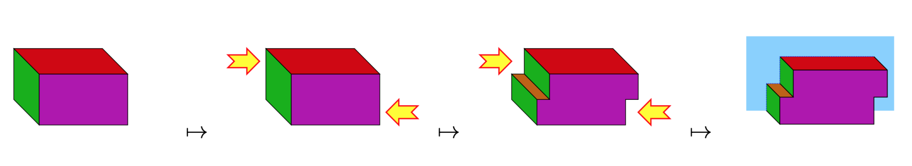
pictures: [S. Dipierro, S. Patrizi, E. Valdinoci (2021)]

Deformation

Evolution in two-dimensions.



Plastic deformation.



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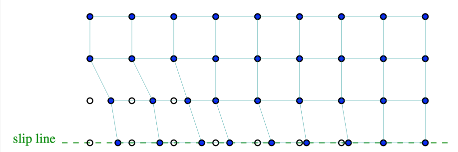
Mismatch between atom locations

The mismatch between atom location and crystal structure:



- $(x, y) \in \mathbb{R} \times [0, \infty)$ denotes a point in the upper half plane.
- $U(x, y) =$ distance between the actual position and its rest position.
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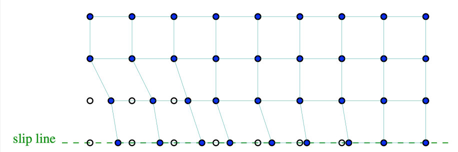

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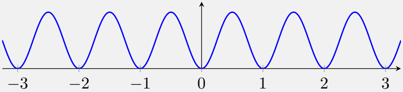
Most of the mismatch occurs along the slip line. To quantify this, let W be a multi-well potential satisfying

$$\begin{cases} W(u) = 0 & u \in \mathbb{Z} \\ W(u) > 0 & u \in \mathbb{R} \setminus \mathbb{Z} \\ W(u+1) = W(u) & u \in \mathbb{R} \\ W''(0) \neq 0. \end{cases}$$



Peierls–Nabarro model

In the Peierls–Nabarro model, the total energy is the energy for bonds between atoms plus the energy for atomic displacement:

$$\mathcal{E} = \mathcal{E}^{\text{elastic}} + \mathcal{E}^{\text{misfit}} = \frac{1}{2} \int_{\mathbb{R}\times\mathbb{R}^+} \left|U(x,y)\right|^2 \, dx\, dy + \int_{\mathbb{R}} W(\phi(x))\, dx.$$

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The equilibrium configuration is obtained my minimizing the energy under the constraint that

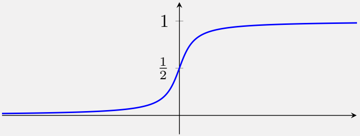
$$\lim_{x\to-\infty}\phi(x) = 0, \quad \lim_{x\to+\infty}\phi(x) = 1, \quad \phi(0) = \frac{1}{2}, \quad \phi' > 0$$

where $x_0 = 0$ is the dislocation point. We call ϕ the phase transition.

In the original Peierls–Nabarro model [see Hirth and Lothe (1991)],

$$W(u) = \frac{1}{4\pi^2}(1 - \cos(2\pi u))$$

$$\phi(x) = \frac{1}{2} + \frac{1}{\pi}\arctan(2x).$$



One-dimensional, nonlocal PDE

Minimizers satisfy the following Euler–Lagrange equation:

$$\begin{cases} \Delta U = U_{xx} + U_{yy} = 0 & \text{in } \mathbb{R} \times \{y > 0\} \\ \partial_y U(x,0) = W'(\phi(x)) & \text{on } \mathbb{R} \times \{y = 0\} \\ U(x,0) = \phi(x) & \text{on } \mathbb{R} \times \{y = 0\}. \end{cases}$$

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By the Caffarelli–Silvestre extension problem for $(-\Delta)^{1/2}$, this is equivalent to the **one**-dimensional, **nonlocal**, **nonlinear** problem

$$\begin{cases} -(-\Delta)^{1/2}\phi(x) = W'(\phi(x)) & \text{in } \mathbb{R} \\ \phi' > 0 \\ \phi(-\infty) = 0, \quad \phi(+\infty) = 1, \quad \phi(0) = \frac{1}{2}. \end{cases}$$

Here $\Delta^{1/2} = -(-\Delta)^{1/2}$ is the fractional operator satisfying the Fourier transform identity $\widehat{(-\Delta)^{1/2}\phi}(\xi) = |\xi|\,\widehat{\phi}(\xi)$ and the pointwise formula

$$(-\Delta)^{1/2}\phi(x) = c_n \,\mathrm{P.V.} \int_{\mathbb{R}^n} \frac{\phi(x) - \phi(y)}{|x-y|^{n+1}}\, dy, \quad n = 1.$$

Evolutionary problem

If we have N straight edge dislocations corresponding to points $x_1, \ldots, x_N$ in the **same** slip plane, then the evolutionary problem is

$$\begin{cases} \partial_t u = \Delta^{1/2} u - W'(u) & \text{in } (0,\infty) \times \mathbb{R} \\ u(0,x) = u_0(x) = \displaystyle\sum_{i=1}^{N} \phi(x - x_i) & \text{on } \mathbb{R}. \end{cases}$$

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To understand how the dislocation points move, we rescale the solution

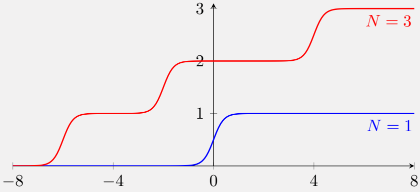
$$u^\varepsilon(t,x) = u\left(\frac{t}{\varepsilon^2}, \frac{x}{\varepsilon}\right).$$

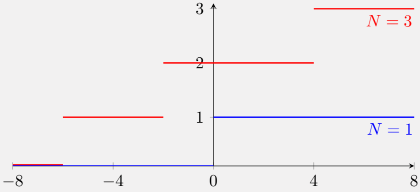
Then, u^ε satisfies the fractional Allen–Cahn equation

$$\begin{cases} \varepsilon \partial_t u^\varepsilon = \frac{1}{\varepsilon}\left(\varepsilon \Delta^{1/2} u^\varepsilon - W'(u^\varepsilon)\right) & \text{in } (0,\infty) \times \mathbb{R} \\ u^\varepsilon(0,x) = \displaystyle\sum_{i=1}^{N} \phi\left(\frac{x - x_i}{\varepsilon}\right) & \text{on } \mathbb{R}. \end{cases}$$

González–Monneau (2010): u^ε converges to the stable minima of W.

Microscopic to mesoscopic scale





At $t = 0$,

$$\lim_{\varepsilon \to 0} u^{\varepsilon}(0, x) = \lim_{\varepsilon \to 0} \sum_{i=1}^{N} \phi\left(\frac{x - x_i}{\varepsilon}\right) = \sum_{i=1}^{N} H\left(x - x_i\right).$$

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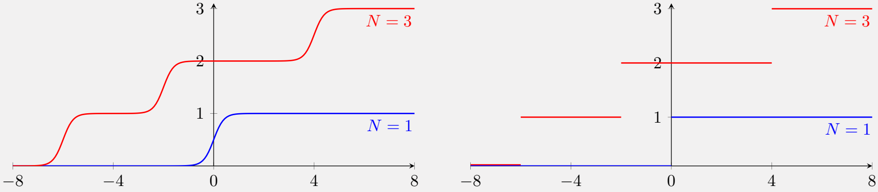

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For $t>0$,

$$\lim_{\varepsilon\to 0} u^{\varepsilon}(t,x) = \sum_{i=1}^{N} H\left(x-y_i(t)\right) \quad \text{where} \quad \begin{cases} \dot{y}_i = \dfrac{c_0}{\pi}\displaystyle\sum_{j\neq i}\frac{1}{y_i-y_j} & \text{t>0} \\ y_i(0) = x_i. \end{cases}$$

Brief literature review

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- Chen (1990): local case $(-\Delta)$ in $\mathbb{R}^n$
- Imbert–Souganidis (preprint): Interface moving by mean curvature

Dislocation dynamics in higher dimensions

We assume that dislocations are contained in the same slip **plane**, but are not necessarily straight edge dislocations.

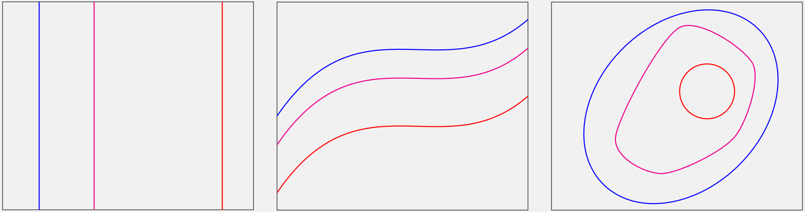

Figure: Slip plane in $\mathbb{R}^2$

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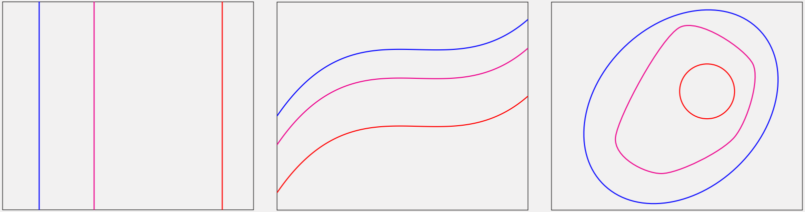

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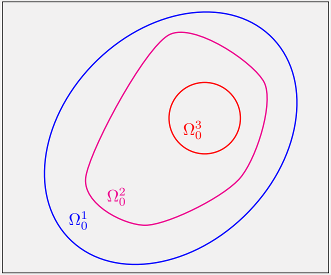
Dislocation dynamics?

Initial configuration

Fix N open (convex) sets $(\Omega_0^i)_{i=1}^N$ in $\mathbb{R}^n$ s.t.

$$\Omega_0^{i+1} \subset\subset \Omega_0^i.$$

We denote the boundary by $\Gamma_0^i = \partial\Omega_0^i$.



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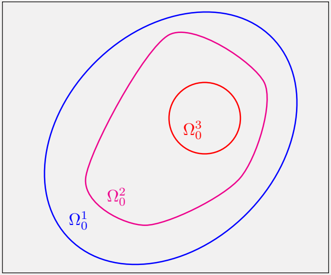

Let $d_i(x)$ denote the signed distance function to Γ_0^i:

$$d_i(x) = \begin{cases} d_i(x, \Gamma_0^i) & \text{if } x \in \Omega_0^i \\ -d_i(x, \Gamma_0^i) & \text{otherwise.} \end{cases}$$

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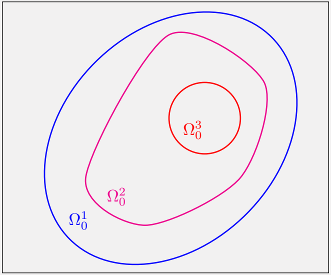

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Recall that for straight-edge dislocations,

$$u(0,x) = u_0(x) = \sum_{i=1}^N \phi\,(x - x_i) = \sum_{i=1}^N \phi(d_i(x)).$$

Fractional reaction-diffusion equation

For $n \geq 2$, we consider viscosity solutions to

$$\begin{cases} \varepsilon \partial_t u^\varepsilon = \dfrac{1}{\varepsilon\,|\ln \varepsilon|}\left(\varepsilon \mathcal{I}_n[u^\varepsilon] - W'(u^\varepsilon)\right) & \text{in } (0,\infty)\times\mathbb{R}^n \\ u^\varepsilon(x,0) = \displaystyle\sum_{i=1}^N \phi\left(\frac{d_i(x)}{\varepsilon}\right) & \text{on } \mathbb{R}^n. \end{cases}$$

where $\mathcal{I}_n = -(-\Delta)^{1/2}$ in $\mathbb{R}^n$ and $\phi : \mathbb{R} \to \mathbb{R}$ is the solution to

$$\begin{cases} c_n \mathcal{I}_1[\phi] = W'(\phi) & \text{in } \mathbb{R} \\ \dot{\phi} > 0 \\ \phi(-\infty) = 0, \quad \phi(+\infty) = 1, \quad \phi(0) = \frac{1}{2}. \end{cases}$$

For a unit vector $e \in \mathbb{S}^{n-1}$, let $\phi_e(x) = \phi(e \cdot x) : \mathbb{R}^n \to \mathbb{R}$. Then,

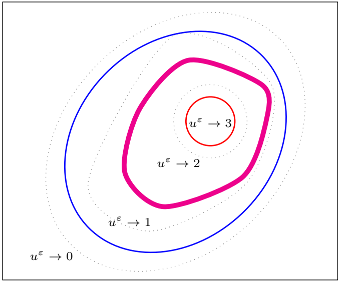
$$\mathcal{I}_n[\phi_e](x) = c_n \mathcal{I}_1[\phi](e \cdot x).$$

Main result

Theorem (Patrizi–V.)

As $\varepsilon \to 0$, the dislocations Γ_t^i move by mean curvature and the solution u^ε satisfies

$$\begin{cases} u^\varepsilon \to 0 & \text{"outside" } \Gamma_t^1 \\ u^\varepsilon \to i & \text{"between" } \Gamma_t^i \text{ and } \Gamma_t^{i+1} \\ u^\varepsilon \to N & \text{"inside" } \Gamma_t^N. \end{cases}$$



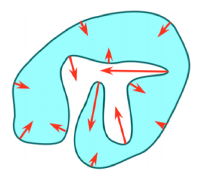
- See Imbert–Souganidis (preprint) for $N = 1$.

Motion by mean curvature

Small times. Let $v = v(x,t)$ be a unit normal vector field to $(\Gamma_t)_{t\geq 0}$.

We say that $(\Gamma_t)_{t\geq 0}$ move by mean curvature if, in a neighborhood of $x \in \Gamma_t$,

$$\begin{cases} \dot{x}(s) = \underbrace{-\operatorname{div}(v)}_{\text{mean curvature}} v, \quad s > t \\ x(t) = x. \end{cases}$$



picture: Math stack exchange

Link

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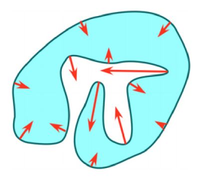

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Large times. Let u be a solution to the mean curvature equation

$$\partial_t u = \mu \operatorname{trace}\left(\left(I - \frac{\nabla u}{|\nabla u|} \otimes \frac{\nabla u}{|\nabla u|}\right) D^2 u\right) \quad \text{in } (0,\infty) \times \mathbb{R}^n,$$

where $\mu = \mu(\phi, n)$. This is a **nonlinear, degenerate, geometric equation.**

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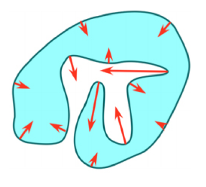

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where $\mu = \mu(\phi, n)$. This is a **nonlinear, degenerate, geometric equation.**

- u is a solution if and only if the zero level sets $(\Gamma_t)_{t \geq 0}$ move by mean curvature. [Evans–Spruck (1991)]
- If $\Phi : \mathbb{R} \to \mathbb{R}$ is smooth, then $\Phi(u)$ is also a solution.

Dislocations move by mean curvature

For each $i = 1, \dots, N$, let $v^i(t,x)$ be the unique solution to

$$\begin{cases} \partial_t v^i = \mu \,\mathrm{trace}\left(\left(I - \frac{\nabla v^i}{|\nabla v^i|} \otimes \frac{\nabla v^i}{|\nabla v^i|}\right) D^2 v^i\right) & \text{in } (0,\infty) \times \mathbb{R}^n \\ v^i(0,x) = v_0^i(x) & \text{on } \mathbb{R}^n. \end{cases}$$

where $\Gamma_0^i = \partial \Omega_0^i$ is the zero level set of the smooth function v_0^i.

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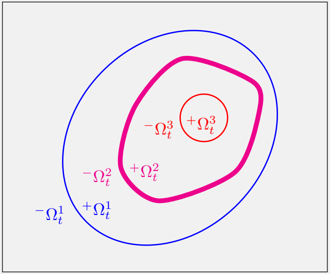
Dislocation dynamics. The level set evolution of $(\Omega_0^i, \Gamma_0^i, (\overline{\Omega_0^i})^c)$ is denoted by the triplet $({}^+\Omega_t^i, \Gamma_t^i, {}^-\Omega_t^i)$ and is given by

- $\Gamma_t^i = \{v^i(t,\cdot) = 0\}$
- ${}^+\Omega_t^i = \{v^i(t,\cdot) > 0\}$
- ${}^-\Omega_t^i = \{v^i(t,\cdot) < 0\}$.



Our result says

$$\begin{cases} u^\varepsilon \to 0 & \text{in } {}^-\Omega_t^1 \\ u^\varepsilon \to i & \text{in } {}^+\Omega_t^i \cap {}^-\Omega_t^{i+1} \\ u^\varepsilon \to N & \text{in } {}^+\Omega_t^N. \end{cases}$$

The ansatz

Assume that $u^\varepsilon(t,x)$ be the **smooth** solution to

$$\begin{cases} \varepsilon \partial_t u^\varepsilon = \dfrac{1}{\varepsilon\,|\ln \varepsilon|}\left(\varepsilon \mathcal{I}_n[u^\varepsilon] - W'(u^\varepsilon)\right) & \text{in } (0,\infty)\times\mathbb{R}^n \\ u^\varepsilon(x,0) = \displaystyle\sum_{i=1}^{N} \phi\left(\frac{d_i(x)}{\varepsilon}\right) & \text{on } \mathbb{R}^n. \end{cases}$$

Consider the formal ansatz given by

$$u^\varepsilon(t,x) \simeq \sum_{i=1}^{N} \phi\left(\frac{d_i(t,x)}{\varepsilon}\right)$$

where $d_i(t,x)$ is the signed distance function to Γ_t^i:

$$d_i(t,x) = \begin{cases} d(t,\Gamma_t^i) & \text{if } x \in {}^{+}\Omega_t^i \\ 0 & \text{if } x \in \Gamma_t^i \\ -d(t,\Gamma_t^i) & \text{if } x \in {}^{-}\Omega_t^i. \end{cases}$$

Assume that d_i is smooth and the curves Γ_t^i and Γ_t^{i+1} are separated.

Heuristics: formal computation for ansatz

$$\varepsilon\partial_t u^\varepsilon \simeq \varepsilon\partial_t \left(\sum_{i=1}^{N} \phi\left(\frac{d_i}{\varepsilon}\right) \right)$$

$$\varepsilon\mathcal{I}_n[u^\varepsilon] - W'(u^\varepsilon) \simeq \sum_{i=1}^{N} \varepsilon\mathcal{I}_n\left[\phi\left(\frac{d_i(t,\cdot)}{\varepsilon}\right)\right](x) - W'\left(\sum_{i=1}^{N}\phi\left(\frac{d_i}{\varepsilon}\right)\right)$$

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\varepsilon \mathcal{I}_n[u^\varepsilon] - W'(u^\varepsilon) &\simeq \sum_{i=1}^{N} \varepsilon \mathcal{I}_n\left[\phi\left(\frac{d_i(t,\cdot)}{\varepsilon}\right)\right](x) - W'\left(\sum_{i=1}^{N} \phi\left(\frac{d_i}{\varepsilon}\right)\right) \\
&= \sum_{i=1}^{N} \left(\varepsilon \mathcal{I}_n\left[\phi\left(\frac{d_i(t,\cdot)}{\varepsilon}\right)\right](x) - c_n \mathcal{I}_1[\phi]\left(\frac{d_i(t,x)}{\varepsilon}\right) \right) \\
&\quad + \sum_{i=1}^{N} c_n \mathcal{I}_1[\phi]\left(\frac{d_i}{\varepsilon}\right) - W'\left(\sum_{i=1}^{N} \phi\left(\frac{d_i}{\varepsilon}\right)\right)
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&= \sum_{i=1}^N a_\varepsilon^i + \sum_{i=1}^N W'\left(\phi\left(\frac{d_i}{\varepsilon}\right)\right) - W'\left(\sum_{i=1}^N \phi\left(\frac{d_i}{\varepsilon}\right)\right).
\end{aligned}$$

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$$\int_{\mathbb{R}} \left(\varepsilon \partial_t u^\varepsilon - \frac{1}{\varepsilon\,|\ln \varepsilon|} \left(\varepsilon \mathcal{I}_n[u^\varepsilon] - W'(u^\varepsilon) \right) \right) \dot{\phi}(\xi)\, d\xi = 0.$$

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&\simeq C \varepsilon^2 + \partial_t d_{i_0}(t,x) \int_{\mathbb{R}} (\dot{\phi})^2\, d\xi \simeq c_0^{-1} \partial_t d_{i_0}(t,x)
\end{aligned}$$

where we use that $\dot{\phi}$ satisfies $\dot{\phi}(z) \simeq \frac{C}{|z|^2}$ when $|z| >> 1$.

Heuristics: formal computation for ansatz

The term $\frac{1}{\varepsilon|\ln\varepsilon|}\left(\varepsilon\mathcal{I}_n[u^\varepsilon] - W'(u^\varepsilon)\right)$ gives three pieces.

1. $\rightsquigarrow \quad \sum_{i=1}^{N} \frac{1}{\varepsilon\,|\ln\varepsilon|}\int_{\mathbb{R}} W'\left(\phi\left(\frac{d_i}{\varepsilon}\right)\right)\dot{\phi}(\xi)\,d\xi$
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Since u^ε is a solution,

$$\begin{aligned} 0 &= \int_{\mathbb{R}}\left(\varepsilon\partial_t u^\varepsilon - \frac{1}{\varepsilon\,|\ln\varepsilon|}\left(\varepsilon\mathcal{I}_n[u^\varepsilon] - W'(u^\varepsilon)\right)\right)\dot\phi(\xi)\,d\xi \\ &\simeq c_0^{-1}\left(\partial_t d_{i_0} - \mathrm{trace}\left(\left(I - \frac{\nabla d_{i_0}}{|\nabla d_{i_0}|}\otimes\frac{\nabla d_{i_0}}{|\nabla d_{i_0}|}\right)D^2 d_{i_0}\right)\right). \end{aligned}$$

□

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$$E^i = \mathrm{Int}\left\{(t,x)\in(0,\infty)\times\mathbb{R}^n : \limsup_{\varepsilon\to 0}{}_* \frac{u^\varepsilon - (i-1)}{\varepsilon\,|\ln\varepsilon|} \leq 0\right\}.$$

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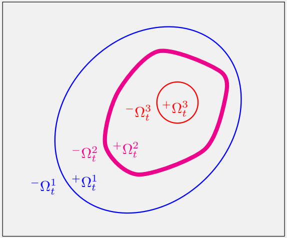
2. Show that

$$^+\Omega_t^i \subset D_t^i \subset {}^+\Omega_t^i \cup \Gamma_t^i$$
$$^-\Omega_t^i \subset E_t^i \subset {}^-\Omega_t^i \cup \Gamma_t^i.$$



Consequently,

$$\begin{cases}\liminf_{\varepsilon\to0}{}_* u^\varepsilon \geq i & \text{in } {}^+\Omega_t^i \subset D_t^i\\ \limsup_{\varepsilon\to0}{}^* u^\varepsilon \leq i & \text{in } {}^-\Omega_t^{i+1} \subset E_t^{i+1}.\end{cases}$$

Explicit barriers

A key step in the abstract method is the construction of barriers (strict subsolutions).

Lemma (Patrizi-V.)

Let $\sigma = W''(0)\tilde{\sigma}$ be a small fixed constant. For sufficiently small $\varepsilon > 0$, the function $v^{\varepsilon}(t, x)$ given by

$$v^{\varepsilon}(t,x) = \sum_{i=1}^{N} \phi\left(\frac{d_i(t,x) - \tilde{\sigma}}{\varepsilon}\right) + \textit{lower order correctors}$$

is a strict subsolution to

$$\varepsilon \partial_t v^{\varepsilon} - \frac{1}{\varepsilon\left|\ln \varepsilon\right|}\left(\varepsilon \mathcal{I}_n[v^{\varepsilon}] - W'(v^{\varepsilon})\right) < -\frac{\sigma}{2}$$

and satisfies

$$v^{\varepsilon}(t,x) - \sum_{i=1}^{N} \mathbb{1}_{\{d_i(t,x) \geq \tilde{\sigma}/2\}} \simeq \varepsilon\left|\ln \varepsilon\right|.$$

Future work

This project is only a small step towards our greater goal.

1. Dislocations given by the graph of a function
2. $N = N_\varepsilon \to \infty$ (microscopic to macroscopic scale)
3. Collisions
4. Δ^s for $0 < s < 1/2$ (fractional mean curvature)
5. etc...

Thank you for your attention!