Dynamics for a system of screw dislocations

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SISSA, Trieste, Italy

AMS-EMS-SPM Meeting – Porto, Portugal

12 June 2015

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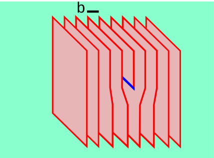

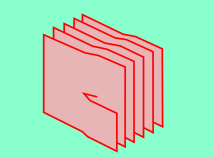

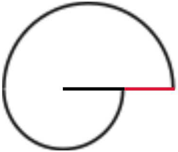

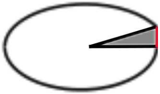

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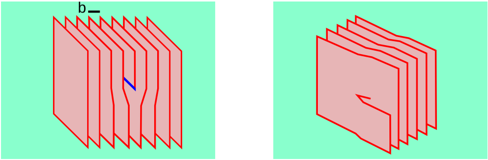

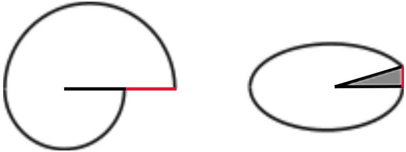

Dislocations modify the physical and chemical properties of a material.

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We do: dynamics for a system of screw dislocations subject to antiplane shear, in the context of linearised elasticity.

Dislocations

Let $\Omega \subset \mathbb{R}^2$ be a Lipschitz domain, let $\mathcal{Z} := \{\mathbf{z}_1, \dots, \mathbf{z}_N\} \subset \Omega$ denote the set of dislocations sites, and let $\mathcal{B} := \{\mathbf{b}_1, \dots, \mathbf{b}_N\}$ be the set of Burgers vectors associated with $\mathcal{Z}$. Let $\mu > 0$ and λ be the Lamé constants of the material and let $\mathbf{L} := \mu\,\mathbf{diag}(1, \lambda^2)$ be the associated elasticity tensor.

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We say that a vector field $\mathbf{h}$ in $\Omega \setminus \mathcal{Z}$ corresponds to a system of dislocations at the points in $\mathcal{Z}$ with Burgers vectors $\mathcal{B}$ if

$$\begin{cases} \mathrm{curl}\, \mathbf{h} = \sum_{i=1}^N \mathbf{b}_i \delta_{\mathbf{z}_i} & \text{in } \Omega, \\ \mathrm{div}\, \mathbf{L}\mathbf{h} = 0 & \text{in } \Omega, \end{cases} \qquad \text{where } \; b_i = \int_{\gamma_i} \mathbf{h} \cdot \mathrm{d}\mathbf{x}; \quad \mathbf{b}_i = b_i \mathbf{e}_3.$$

Here, γ_i is a closed CCW oriented path enclosing only the dislocation $\mathbf{z}_i$.

Energy functional

We consider the elastic energy

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$$J_\varepsilon(\mathbf{h}) = \int_{\Omega_\varepsilon} W(\mathbf{h}(\mathbf{x}))\mathrm{d}\mathbf{x} = c|\log\varepsilon| + U(\mathbf{z}_1, \ldots, \mathbf{z}_N) + o(\varepsilon).$$

The renormalized energy

At a minimum for the energy, the renormalized energy is given by

$$U(\mathbf{z}_1,\dots,\mathbf{z}_N)=U_S(\mathbf{z}_1,\dots,\mathbf{z}_N)+U_I(\mathbf{z}_1,\dots,\mathbf{z}_N)+U_E(\mathbf{z}_1,\dots,\mathbf{z}_N),$$

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with

$$U_S(\mathbf{z}_1,\dots,\mathbf{z}_N)=\sum_{i=1}^N\frac{\mu\lambda b_i^2}{4\pi}\log R+\sum_{i=1}^N\int_{\Omega\setminus C_{R,i}}W(\mathbf{k}_i)\mathrm{d}\mathbf{x},$$

$$U_I(\mathbf{z}_1,\dots,\mathbf{z}_N)=\sum_{i=1}^{N-1}\sum_{j=i+1}^N\int_\Omega\mathbf{k}_j\cdot\mathbf{L}\mathbf{k}_i\mathrm{d}\mathbf{x},$$

$$U_E(\mathbf{z}_1,\dots,\mathbf{z}_N)=\int_\Omega W(\nabla u_0)\mathrm{d}\mathbf{x}+\sum_{i=1}^N\int_{\partial\Omega}u_0\mathbf{L}\mathbf{k}_i\cdot\mathbf{n}\,\mathrm{d}s,$$

where u_0 solves a Neumann problem in Ω.

Force on a dislocation

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Theorem

The gradient of the renormalized energy with respect to $\mathbf{z}_\ell$ *is given in terms of the Eshelby stress* $\mathbf{C} = W(\mathbf{h}_0)\mathbf{I} - \mathbf{h}_0(\mathbf{L}\mathbf{h}_0)^\top$. *In particular,*

$$\nabla_{\mathbf{z}_\ell} U(\mathbf{z}_1, \ldots, \mathbf{z}_N) = -\int_{\partial C_{\ell,R}} \left\{ W(\mathbf{h}_0)\mathbf{I} - \mathbf{h}_0(\mathbf{L}\mathbf{h}_0)^\top \right\} \mathbf{n}\, \mathrm{d}s.$$

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The Peach-Köhler force on the dislocation $\mathbf{z}_\ell$ *has the expression*

$$\mathbf{j}_\ell(\mathbf{z}_\ell) = -\nabla_{\mathbf{z}_\ell} U = b_\ell \mathbf{J}\mathbf{L} \left(\nabla u_0(\mathbf{z}_\ell) + \sum_{i \neq \ell} \mathbf{k}_i(\mathbf{z}_\ell) \right).$$

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We want to be able to explain a picture like this

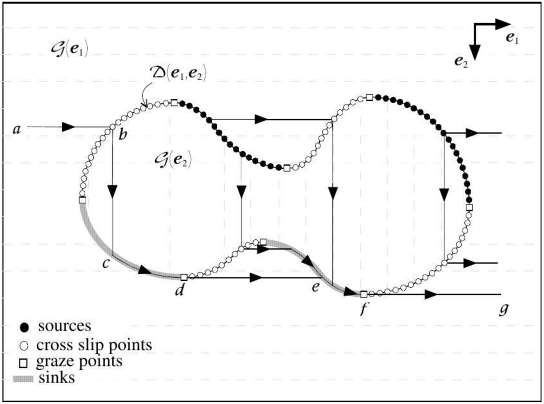

Fig. 1. Generalized gliding motions near a double slip curve $\mathscr{D}(e_1, e_2)$, with e_1 and e_2 the associated glide directions. The curve $abcdefg$ corresponds to a dislocation that glides from a to b, cross slips at b, glides to c, cross slips finely from c to d, glides to e, cross slips finely to f, and then glides to g.

Glide directions and the equation of motion

We assume, for physical reasons, that only a finite number of directions is admissible for motion. Call $\mathcal{G} := \{\mathbf{g}_1, \dots, \mathbf{g}_M\} \subset \mathbb{S}^1$ the set of the *glide directions*.

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$$\dot{\mathbf{z}}_\ell = (\mathbf{j}_\ell \cdot \mathbf{g}_\ell)\mathbf{g}_\ell \,,$$

where $\mathbf{g}_\ell \in \mathcal{G}$ is the direction that maximises the dissipation, *i.e.*,

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Filippov solutions

At those ambiguity points where the right-hand side $(\mathbf{j}_\ell \cdot \mathbf{g}_\ell)\mathbf{g}_\ell$ fails to be single-valued, a weaker notion of solution is needed. The theory developed by Filippov for ODE's takes care of this aspect and allows us to recover the results one can expect from heuristics. Those results are also supported by numerical and experimental evidence.

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The ambiguity set $\mathcal{A}$ is given by solving $\mathbf{j}_\ell \cdot \mathbf{g} = 0$ for $\mathbf{g} = \mathbf{g}_\ell^+ - \mathbf{g}_\ell^-$ $\mathbf{g}_\ell^\pm \in \mathcal{G}$, dissipation-maximizing directions.

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- $\Omega = \mathbb{R}^2$. The set $\mathcal{A}$ is the union of hyperplanes.
- $\Omega \subset \mathbb{R}^2$. The structure of $\mathcal{A}$ is more complicated, due to the presence of the term ∇u_0 in the expression of the force.

Setting for the equations of motion

Set $\mathbf{Z} := (\mathbf{z}_1, \dots, \mathbf{z}_N) \in \Omega^N$ and $\mathcal{G}_\ell(\mathbf{Z}) := \arg\max\{\mathbf{j}_\ell(\mathbf{Z}) \cdot \mathbf{g} : \mathbf{g} \in \mathcal{G}\}$.

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The problem of the dynamics consists in solving the system of ordinary differential *inclusions*

$$\begin{cases} \dot{\mathbf{z}}_\ell \in F_\ell(\mathbf{Z}), \\ \mathbf{z}_\ell(0) = \mathbf{z}_{\ell,0}, \end{cases} \qquad F_\ell(\mathbf{Z}) := \{(\mathbf{j}_\ell(\mathbf{Z}) \cdot \mathbf{g})\, \mathbf{g} : \mathbf{g} \in \mathcal{G}_\ell(\mathbf{Z})\},$$

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$$F_\ell(\mathbf{Z}) = \begin{cases} \{\mathbf{0}\} & \text{if } \mathbf{j}_\ell(\mathbf{Z}) = \mathbf{0}, \\ \{(\mathbf{j}_\ell(\mathbf{Z}) \cdot \mathbf{g}_\ell(\mathbf{Z}))\,\mathbf{g}_\ell(\mathbf{Z})\} & \text{if } \mathbf{j}_\ell(\mathbf{Z}) \neq \mathbf{0} \text{ and } \mathcal{G}_\ell(\mathbf{Z}) = \{\mathbf{g}_\ell(\mathbf{Z})\}, \\ \{(\mathbf{j}_\ell(\mathbf{Z}) \cdot \mathbf{g}_\ell^\pm(\mathbf{Z}))\,\mathbf{g}_\ell^\pm(\mathbf{Z})\} & \text{if } \mathbf{j}_\ell(\mathbf{Z}) \neq \mathbf{0} \text{ and } \mathcal{G}_\ell(\mathbf{Z}) = \{\mathbf{g}_\ell^\pm(\mathbf{Z})\}. \end{cases}$$

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for given initial conditions $\mathbf{Z}_0 := (\mathbf{z}_{1,0}, \dots, \mathbf{z}_{N,0})$. Filipov's recipe tells us to look at the system

$$\begin{cases} \dot{\mathbf{Z}} \in \operatorname{co} F(\mathbf{Z}), \\ \mathbf{Z}(0) = \mathbf{Z}_0. \end{cases}$$

The local existence theorem

Set $\mathcal{D}(\boldsymbol{F}) := \Omega^N \setminus \cup_{j<k}\Pi_{jk}$.

Theorem (Local Existence)

Let $\Omega \subset \mathbb{R}^2$ *be a connected open set, let* $\mathbf{Z}_0 \in \mathcal{D}(\boldsymbol{F})$ *be a given initial configuration of dislocations. Then the initial value problem*

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In view of the definition of $\mathcal{D}(\boldsymbol{F})$ and of how T is determined, solutions exists as long as dislocations stay away from $\partial\Omega$ and do not collide.

Uniqueness

Define $\mathcal{A} := \bigcup_{\ell=1}^{N} \mathcal{A}_\ell$, $\mathcal{A}_\ell := \{\mathbf{Z} \in \mathcal{D}(F) : \mathbf{card}(\mathcal{G}_\ell) = 2\}$.

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These conditions ensure we can prove

Theorem (Local Uniqueness – user-friendly version)

If the initial configuration $\mathbf{Z}_0 \in \mathcal{A}_\ell \setminus (\mathcal{S}_\ell \cup \mathcal{E}_{\mathrm{zero}} \cup \mathcal{E}_{\mathrm{src}})$ for some $\ell \in \{1, \dots, N\}$, then (right) uniqueness holds.

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The ambiguity set $\mathcal{A}$ is contained in a countable union of smooth manifolds of dimension $\leqslant 2N - 1$.
Moreover, the set $\mathcal{S}_\ell := \{\mathbf{Z} \in \mathcal{D}(F) : \mathbf{j}_\ell(\mathbf{Z}) \cdot \mathbf{g}_0 = 0, \nabla_{\mathbf{Z}}(\mathbf{j}_\ell(\mathbf{Z}) \cdot \mathbf{g}_0) = 0\}$ has dimension $\leqslant 2N - 2$, for every $\ell \in \{1, \dots, N\}$.

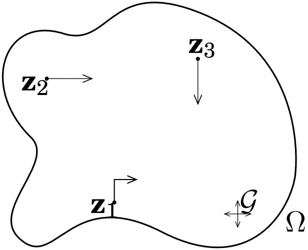
These conditions ensure we can prove

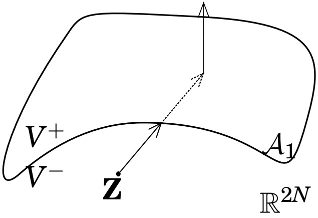
Theorem (Local Uniqueness – user-friendly version)

If the initial configuration $\mathbf{Z}_0 \in \mathcal{A}_\ell \setminus (\mathcal{S}_\ell \cup \mathcal{E}_{\mathrm{zero}} \cup \mathcal{E}_{\mathrm{src}})$ for some $\ell \in \{1, \dots, N\}$, then (right) uniqueness holds.

Uniqueness holds until either a collision occurs, or a dislocation hits the boundary, or a source is reached, or the ambiguity set is no longer smooth.

Cross-Slip and Fine Cross-Slip





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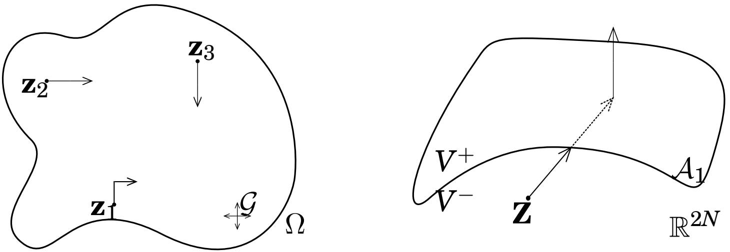

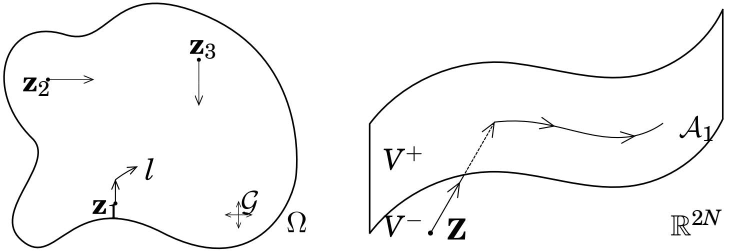

Motion - I: one dislocation in the half-plane

Let us consider a single dislocation $\mathbf{z} = (0, z_2)$ with Burgers modulus b, and let $\Omega = \mathbb{R}^2_+$ be the upper half-plane. Let also $\mathbf{L} = \mathbf{I}$.

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$$\begin{pmatrix} \dot{z}_1 \\ \dot{z}_2 \end{pmatrix} = -\frac{b^2}{4\pi}\begin{pmatrix} 0 \\ z_2 \end{pmatrix}, \qquad \mathbf{z}(0) = \begin{pmatrix} 0 \\ d_0 \end{pmatrix}.$$

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This can be solved and we get

$$z_1(t) = 0,\ \forall t; \quad z_2(t) = \sqrt{d_0^2 - \frac{b^2}{2\pi}t},\ t \in [0, T], \qquad T = \frac{2\pi}{b^2}d_0^2.$$

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$$\dot{r} = \frac{b^2}{2\pi}\frac{r}{1-r^2}, \qquad r(0) = r_0\,,$$

we know the dislocation will hit the boundary of the disk in finite time at

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If not, more complicated expression; problem still solvable.

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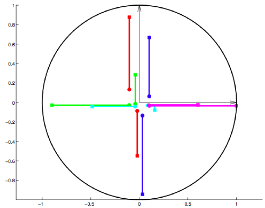
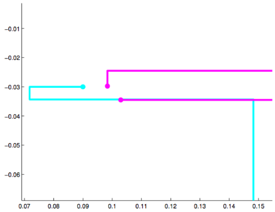
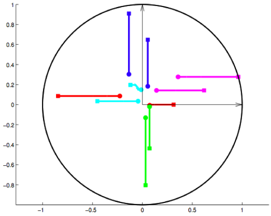
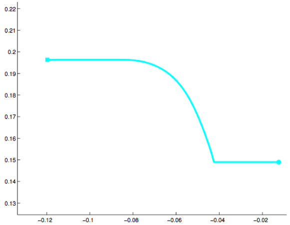
Yet, the expression of the force above allows us to say that the ambiguity set is smooth away from collisions, and this is good for the dynamics.

Motion - IV: some simulations









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Thank you very much for your attention!