A variational model for plasticity via homogenization of straight dislocations

Marcello Ponsiglione
University of Rome *La Sapienza*

Variational model for plasticity

Our aim is to deduce a macroscopic energy of the type

$$\mathcal{F}(\mu, \psi) := \int_\Omega < C\psi : \psi > \; dx + \int_\Omega \varphi\left(\frac{d\mu}{d|\mu|}\right) \, d|\mu|.$$

- μ represents the dislocation density measure;
- ψ is the strain function satisfying Curl $\psi = \mu$;
- C is the elasticity tensor;
- φ is the density of the plastic part of the energy.

The macroscopic energy is deduced as a limit of discrete energy functionals $\mathcal{F}_\varepsilon$.

Description of a screw dislocation line

A deformed crystal C can be described by

- The displacement function $U : C \to \mathbb{R}^3$.
- The strain function $\psi = \nabla U$.

A straight dislocation in the crystal can be described by an infinite line L in the crystal and by a strain ψ such that

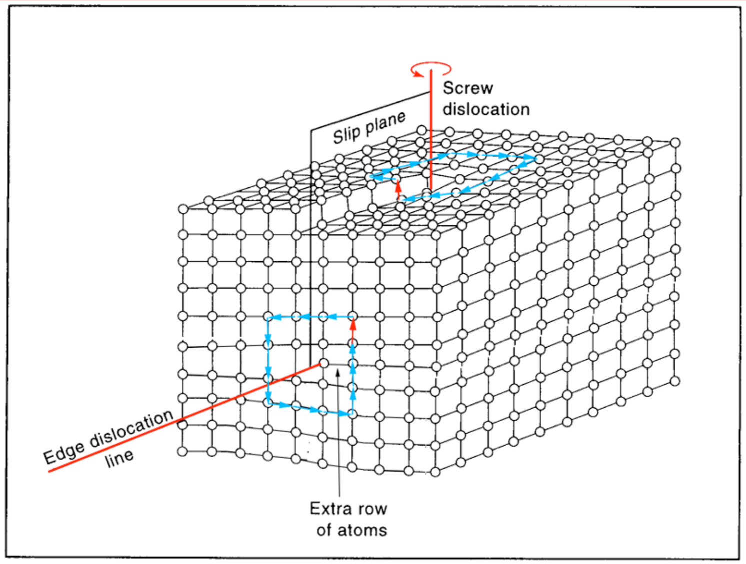
the circulation of ψ around L is a fixed vector $\mathbf{b}$

called *Burgers vector.*

If b is parallel to L, the dislocation is called *screw dislocation*.

Locally in $C \setminus L$, ψ is the gradient of a multi-valued function U.

Screw dislocation



The anti-planar setting

- The reference configuration is an open set $\Omega \subset \mathbb{R}^2$ which represents a horizontal section of an infinite cylindrical crystal.
- Screw dislocations can be represented by a measure on Ω which is a finite sum of *Dirac masses* of the type $\mu := \sum_i z_i |\mathbf{b}| \, \delta_{x_i}$.
- The class of admissible strains associated with a dislocation μ is given by the fields $\psi : \Omega \to \mathbb{R}^2$ whose circulation around the dislocations x_i are equal to $z_i|\mathbf{b}|$ (curl $\psi = \mu$).

The core radius ε and the elastic energy

The admissible strain ψ has a singularity at each dislocation point x_i and it does not have finite energy (ψ is not in $L^2(\Omega;\mathbb{R}^2)$).

To set up a variational formulation it is convenient to introduce an internal scale ε called *core radius*, which is proportional to (the ratio between the size of Ω and) the atomic scale.

We remove balls of radius ε around each point of singularity x_i, and we compute the elastic energy out of this *core region*.

$$E_\varepsilon(\mu,\psi) := \int_{\Omega_\varepsilon(\mu)} |\psi(x)|^2\, dx,$$

where $\Omega_\varepsilon(\mu) := \Omega \setminus \cup_i \overline{B}_\varepsilon(x_i)$.

The logarithmic energy regime

We compute the energy induced by a single dislocation.

$\Omega := B_R$ and $\mu := \delta_0$.

Consider the "function" $u(\theta, r) := \frac{1}{2\pi}\theta$, and let $\psi := \nabla u$.

1) ψ is an admissible strain.
2) $|\psi(\theta, r)| = \frac{1}{2\pi r}$. Therefore

$$E_\varepsilon(\mu, \psi) := \int_{B_R \setminus B_\varepsilon} |\psi(x)|^2 = \int_{B_R \setminus B_\varepsilon} \frac{1}{(2\pi r)^2} =$$

$$\int_\varepsilon^R \frac{1}{2\pi r} = \frac{1}{2\pi}(\log(R) - \log(\varepsilon)) \cong \frac{1}{2\pi}|\log(\varepsilon)|$$

3) ψ minimizes the elastic energy among all the admissible strains (by Jensen inequality).

The phenomenon of concentration of energy

Let $\Omega := B_R$ and $\mu := \delta_0$. Let $\rho_\varepsilon \to 0$ such that

$$\frac{|\log(\rho_\varepsilon)|}{|log(\varepsilon)|} \to 0 \qquad \text{as } \varepsilon \to 0$$

Or equivalently

$$\liminf_{\varepsilon \to 0} \frac{\rho_\varepsilon}{\varepsilon^s} \to \infty \text{ for every fixed } 0 < s < 1.$$

The region B_{ρ_ε} is called hard core region.

Almost all the energy is concentrated in B_{ρ_ε}:

$$\int_{B_{\rho_\varepsilon} \setminus B_\varepsilon} |\psi(x)|^2 = \int_\varepsilon^{\rho_\varepsilon} \frac{1}{2\pi r} =$$

$$\frac{1}{2\pi} |\log(\rho_\varepsilon) - \log(\varepsilon)| \cong \frac{1}{2\pi} |\log(\varepsilon)|.$$

The rescaled elastic energy functionals

Given a dislocation μ, the class of admissible strains $\mathcal{AS}_\varepsilon(\mu)$ associated with μ is given (we consider for simplicity's sake $|\mathbf{b}| = 1$) by

$$\mathcal{AS}_\varepsilon(\mu) := \{\psi \in L^2(\Omega_\varepsilon(\mu); \mathbb{R}^2) : \text{curl } \psi = 0 \text{ in } \Omega_\varepsilon(\mu), \int_{\partial B_\varepsilon(x_i)} \psi(s) \cdot \tau(s)\, ds = \mu(x_i) \text{ for every } x_i \in \text{supp } \mu\}.$$

The (rescaled) elastic energy associated with μ is given by

$$\frac{1}{|\log \varepsilon|} \mathcal{F}_\varepsilon(\mu) := \frac{1}{|\log \varepsilon|} \min_{\psi \in \mathcal{AS}_\varepsilon(\mu)} E_\varepsilon(\psi).$$

Asymptotic behavior of $\mathcal{F}_\varepsilon$ as $\varepsilon \to 0$

Let $\Omega := B_R$. The previous example shows that

$$\frac{1}{|\log \varepsilon|}\mathcal{F}_\varepsilon(z\delta_0) \to \frac{|z|^2}{2\pi}.$$

Cermelli P., Leoni G.: Energy and forces on dislocations. *SIAM J. Math. Anal.* (2005), **37**, no. 4, 1131–1160.

Theorem 1

Let $\mu := \sum_{i=1}^N z_i\delta_{x_i}$. We have

$$\frac{1}{|\log \varepsilon|}\mathcal{F}_\varepsilon(\mu) \to \frac{1}{2\pi}\sum_{i=1}^N |z_i|^2.$$

For ε small $\frac{1}{|\log \varepsilon|}\mathcal{F}_\varepsilon$ counts the dislocations. Therefore the logarithmic rescaling corresponds to a finite number of dislocations.

Γ-convergence of the energy functionals $\mathcal{F}_\varepsilon$.

Let X be the space of measures of the type $\mu := \sum_{i=1}^N z_i \delta_{x_i}$.
The Γ-limit of $\mathcal{F}_\varepsilon$ is the functional $\mathcal{F} : X \to \mathbb{R}$ defined by

$$\mathcal{F}(\mu) := \frac{1}{2\pi} |\mu|(\Omega) \qquad \text{for every } \mu \in X.$$

P.: Elastic energy stored in a crystal induced by screw dislocations, from discrete to continuous. *SIAM J. Math. Anal.* (2007).

Theorem 2

The following Γ-convergence result holds.

- i *Γ-limsup equality. For every $\mu \in X$ there exists a sequence $\mu_\varepsilon \rightharpoonup \mu$ such that $\frac{1}{|\log \varepsilon|}\mathcal{F}_\varepsilon(\mu_\varepsilon) \to \mathcal{F}(\mu)$.*
- ii *Γ-liminf inequality. For every $\mu_\varepsilon \rightharpoonup \mu$ we have $\mathcal{F}(\mu) \le \liminf_\varepsilon \frac{1}{|\log \varepsilon|}\mathcal{F}_\varepsilon(\mu_\varepsilon)$.*

Γ-limsup inequality: linear V quadratic

Consider for a while $\mu = 2\delta_x$. We have

$$\frac{1}{|\log \varepsilon|}\mathcal{F}_\varepsilon(\mu) \to \frac{4}{2\pi} = 2\mathcal{F}(\mu).$$

$\mu_\varepsilon \equiv \mu$ IS NOT the recovery sequence.

We have to split multiple dislocations...

Let $v_n \to x$, $w_n \to x$. We have

$$\frac{1}{|\log \varepsilon|}\mathcal{F}_\varepsilon(\delta_{v_n} + \delta_{w_n}) \to \frac{2}{2\pi} = \mathcal{F}(\mu).$$

By a diagonal argument there exists a recovery sequence $\mu_\varepsilon := \delta_{v_{n(\varepsilon)}} + \delta_{w_{n(\varepsilon)}}$ such that

$$\mu_\varepsilon \to \mu, \qquad \frac{1}{|\log \varepsilon|}\mathcal{F}_\varepsilon(\mu_\varepsilon) \to \mathcal{F}(\mu).$$

Convergence of minimizers

Let $A \subset\subset \Omega$. Consider the following problem

$$\min \frac{1}{|\log \varepsilon|} \mathcal{F}_\varepsilon(\mu)$$

among all dislocations μ with $|\mu(A)| = |\mu(\Omega)| = N$.

N could be considered as the *geometrically necessary dislocations.*

It is easy to construct a sequence with finite energy, so that we know that the minimizers μ_ε have finite energy.

We have $\frac{1}{|\log \varepsilon|} \mathcal{F}_\varepsilon(\mu_\varepsilon) \le E$. Can we deduce $\mu_\varepsilon \rightharpoonup \mu$?

This is the so called *equi-coercivity property*.

If this is the case, we deduce $|\mu(A)| = N$, and by the Γ-convergence result we have

$$\frac{1}{|\log \varepsilon|} \mathcal{F}_\varepsilon(\mu_\varepsilon) \to \mathcal{F}(\mu) = \frac{1}{2\pi} |\mu|(A) = \frac{1}{2\pi} N.$$

Unfortunately, the equi-coercivity property does not hold...

Short dipoles

A dipole is a pair of dislocations of the type

$$\mu_\varepsilon := \delta_x - \delta_y.$$

Consider now a sequence of pairs (x_n, y_n) with $|x_n - y_n| \to 0$, and let μ_n be the corresponding dipole. It is easy to see that

$$\frac{1}{|\log \varepsilon|} F_\varepsilon(\mu_\varepsilon) \to 0 \quad \text{as } n \to \infty.$$

We can easily construct a sequence μ_ε such that

$$|\mu_\varepsilon|(\Omega) \to \infty, \qquad \frac{1}{|\log \varepsilon|} F_\varepsilon(\mu_\varepsilon) \to 0 \quad \text{as } \varepsilon \to 0.$$

For ε small, the functional $\frac{1}{|\log \varepsilon|}\mathcal{F}_\varepsilon$ does not count short dipoles

The flat norm

Let us define the *flat norm* as follows.

If $\mu = \delta_x - \delta_y$ is a dipole, then $\|\mu\|_f = |x - y|$.

In general, $\|\mu\|_f$ is given by the minimal connection:

$$\|\mu\|_f := \inf\{\mathcal{H}^1(R) : \partial R = \mu\}. \tag{1}$$

Here R is a finite formal sum of oriented segments with integer multiplicity.

Note that by definition if $\mu_n := \delta_{x_n} - \delta_{y_n}$ with $|x_n - y_n| \to 0$,

$$\|\mu_n\|_f = |x_n - y_n| \to 0.$$

The flat norm, as well as the elastic energy, does not see short dipoles.

The Γ-convergence result

Theorem 3

The following Γ-convergence result holds.

i) *Equi-coercivity. Let* $\varepsilon \longrightarrow 0$, *and let* $\{\mu_\varepsilon\}$ *be a sequence such that* $\frac{1}{|\log\varepsilon|}\mathcal{F}_\varepsilon(\mu_\varepsilon) \le E$.

Then (up to a subsequence) $\mu_\varepsilon \stackrel{f}{\longrightarrow} \mu$ *for some* $\mu \in X$.

ii) *Γ-convergence. The functionals* $\frac{1}{|\log\varepsilon|}\mathcal{F}_\varepsilon$ *Γ-converge to* $\mathcal{F}$ *as* $\varepsilon \longrightarrow 0$ *with respect to the flat norm, i.e., the following inequalities hold.*

Γ-liminf inequality: $\mathcal{F}(\mu) \le \frac{1}{|\log\varepsilon|}\liminf \mathcal{F}_\varepsilon(\mu_\varepsilon)$ *for every* $\mu \in X$, $\mu_\varepsilon \stackrel{f}{\longrightarrow} \mu$ *in* X.

Γ-limsup inequality: given $\mu \in X$, *there exists* $\{\mu_\varepsilon\} \subset X$ *with* $\mu_\varepsilon \stackrel{f}{\longrightarrow} \mu$ *such that* $\limsup \frac{1}{|\log\varepsilon|}\mathcal{F}_\varepsilon(\mu_\varepsilon) \le \mathcal{F}(\mu)$.

Convergence of minimizers

Let $A \subset\subset \Omega$. Consider the following problem

$$\min \frac{1}{|\log \varepsilon|} \mathcal{F}_\varepsilon(\mu)$$

among all dislocations μ with $|\mu(A)| = |\mu(\Omega)| = N$.

The minimizers μ_ε have finite energy, so that by the equi-coercivity property we have

$$\mu_\varepsilon \xrightarrow{f} \mu \qquad \text{for some } \mu \in X.$$

By the Γ-convergence result we have

$$\frac{1}{|\log \varepsilon|} \mathcal{F}_\varepsilon(\mu_\varepsilon) \to \mathcal{F}(\mu) = \frac{1}{2\pi} N.$$

Moreover, since $\|\mu_\varepsilon\|_f$ is uniformly bounded, we deduce that μ_ε has a finite number of clusters with non-zero effective multiplicity.

A comment about the use of linear elasticity in our model

Let $C > 0$. The Γ-convergence result holds even if in the definition of Ω_ε we remove balls of radius $C\varepsilon$ instead of ε.

This fact gives a partial justification of the use of linearized elasticity in $\Omega_{C\varepsilon}(\mu)$. In fact, the recovering sequence ψ_ε satisfies

$$\|\psi_\varepsilon\|_{L^\infty(\Omega_{C\varepsilon}(\mu_\varepsilon);\mathbb{R}^2)} \leq \frac{1}{2\pi C\varepsilon} + O(n),$$

Since the admissible strains should be rescaled by ε (like the Burgers vector), we deduce that $|\psi_\varepsilon|$ can be chosen arbitrarily small, choosing C big enough.

The discrete model

We consider the illustrative case of a *square lattice* of size ε with *nearest-neighbor interactions*, following along the lines of the more general theory introduced in

Ariza M. P., Ortiz M.: Discrete crystal elasticity and discrete dislocations in crystals. *Arch. Rat. Mech. Anal.* **178** (2006), 149-226.

The discrete model seems very natural, and provides a theoretical justification of the continuum model.

A line tension model

The asymptotic elastic energy as $\varepsilon \longrightarrow 0$ is essentially given by the number of dislocations present in the crystal.

The energy per unit volume is proportional to the length of the dislocation lines, so that our result provides in the limit as $\varepsilon \longrightarrow 0$ a line tension model.

Garroni A., Müller S.: Γ-limit of a phase-field model of dislocations. *SIAM J. Math. Anal.* **36** (2005), no. 6, 1943–1964.
Garroni A., Müller S.: A variational model for dislocations in the line tension limit. *Arch. Rat. Mech. Anal.* **181** (2006), no. 3, 535–578.

Case of planar elasticity

- The reference configuration is an open set $\Omega \subset \mathbb{R}^2$ which represents an horizontal section of the cylindrical crystal.
- The Burgers vectors are a finite set $S \subset \mathbb{R}^2$

$$S := \{b_1, \ldots, b_s\}.$$

- The dislocations are represented by a measure on Ω, which is a finite sum of *Dirac masses*, $\mu := \sum_i z_i b_i \, \delta_{x_i}$.
- The class of admissible strains corresponding to μ is given by the functions $\psi : \Omega_\varepsilon \to M^{2\times 2}$ whose circulation around each x_i is equal to $z_i b_i$.
- The elastic energy corresponding to a pair $(\mu_\varepsilon, \psi_\varepsilon)$ is given by

$$\mathcal{F}_\varepsilon(\mu_\varepsilon, \psi_\varepsilon) = \int_{\Omega_\varepsilon} W(\psi_\varepsilon) dx = \int_{\Omega_\varepsilon} C\psi : \psi \, dx$$

The self energy

The self energy corresponding to a dislocation measure $\mu_\varepsilon := \sum z_i \delta_{x_i} b_i$ is equal to the sum of the energies corresponding to $z_i \delta_{x_i} b_i$

$$E_\varepsilon^{self}(\mu_\varepsilon) := \sum_i \mathcal{F}_\varepsilon(z_i \delta_{x_i} b_i).$$

In view of the concentration phenomenon of the energy we have

$$E_\varepsilon^{self}(z\delta_x b) \cong \min_\psi \int_{B_{\rho_\varepsilon(x)}} W(\psi) \cong |\log \varepsilon| |z|^2 f(b)$$

where $\frac{|\log(\rho_\varepsilon)|}{|log(\varepsilon)|} \longrightarrow 0 \qquad$ as $\varepsilon \longrightarrow 0$

$$E_\varepsilon^{self}(\mu_\varepsilon) \cong \sum_i \min_\psi \int_{B_{\rho_\varepsilon}(x_i)} W(\psi) \cong |\log \varepsilon| \sum_i z_i^2 f(b_i)$$

The self energy is the energy stored in the hard core region.

In collaboration with A. Garroni and G. Leoni.

We study the Γ-convergence of elastic functionals as the number of dislocations

$$N_\varepsilon \to \infty \qquad \text{per } \varepsilon \to 0.$$

More precisely we rescale the elastic energy functionals considering

$$\frac{1}{N_\varepsilon |\log \varepsilon|} \mathcal{F}_\varepsilon.$$

In this case, in contrast with the case $N_\varepsilon \equiv N$, we also have to take into account the interaction energy.

$$E_\varepsilon^{inter}(\mu_\varepsilon, \psi_\varepsilon) := \int_{\Omega \setminus \text{Hard Core of } \mu_\varepsilon} W(\psi_\varepsilon)\, dx.$$

$E_\varepsilon^{self} \cong N_\varepsilon |\log \varepsilon|$.

$E_\varepsilon^{inter} \cong$ ......?

Asymptotic behavior of E_ε^{inter} (Heuristically...)

Assume that N_ε dislocations are uniformly distributed in $B_1(0)$. Then

A ball of radius r contains almost $\pi r^2 N_\varepsilon$ dislocations.

Therefore the average $|\overline{\psi}_\tau(r)|$ of the tangential component of the strain on $\partial B_r(0)$ is of the order

$$|\overline{\psi}_\tau(r)| \cong \pi r^2 N_\varepsilon / 2\pi r = N_\varepsilon r/2.$$

$$E_\varepsilon^{inter}(\mu,\psi) \cong \int_0^1 dr \int_0^{2\pi r} |\overline{\psi}_\tau(r,\theta)|^2 \, d\theta \cong$$

$$\int_0^1 dr \int_0^{2\pi r} N_\varepsilon^2 r^2/4 = CN_\varepsilon^2.$$

Energy regimes: $N_\varepsilon|\log\varepsilon|$ V N_ε^2

Fix $\varepsilon \to N_\varepsilon$. The behavior of N_ε as $\varepsilon \to 0$ determines three different energy regimes:

1. Well separated dislocations ($N_\varepsilon << |\log(\varepsilon)|$): In this regime we have that the self energy is of order $N_\varepsilon|\log\varepsilon|$, and it is predominant with respect to the interaction energy.
2. Critical regime ($N_\varepsilon \approx |\log(\varepsilon)|$): The self energy and the interaction energy have the same magnitude $N_\varepsilon|\log\varepsilon|$.
3. Super-critical regime ($N_\varepsilon >> |\log(\varepsilon)|$): The interaction energy is of order $|N_\varepsilon|^2$ and it is predominant with respect to the self energy.

The class of admissible dislocations

Let us fix the sequence of hard core radii ρ_ε satisfying

i) $\liminf_{\varepsilon\to 0} \frac{\rho_\varepsilon}{\varepsilon^s} \to \infty$ for every $0 < s < 1$;

ii) $|N_\varepsilon|\rho_\varepsilon^2 \to 0$ for $\varepsilon \to 0$.

Assumption: The distance between the dislocations is at least $2\rho_\varepsilon$.

$$X_\varepsilon := \{\mu \in \mathcal{M}(\Omega) : \mu = \sum_{i=1}^{M} \delta_{x_i} b_i,\ M \in \mathbb{N},\ B_\varepsilon(x_i) \in \Omega,$$
$$|x_j - x_k| \geq 2\rho_\varepsilon \text{ for every } j \neq k,\ b_i \in \mathbb{S}\}. \quad (2)$$

Here $S := \{b_1, \dots, b_s\}$ is the set of Burgers vectors and $\mathbb{S}$ is the span generated by S in $\mathbb{Z}$.

Γ-convergence in the critical case

Theorem 4

i) *Compactness.* *Let* $\{(\mu_\varepsilon, \psi_\varepsilon)\}$ *be a sequence in* $\mathcal{M}(\Omega) \times L^2(\Omega; M^{2\times 2})$ *with* $\frac{1}{|\log\varepsilon|^2}\mathcal{F}_\varepsilon(\mu_\varepsilon, \psi_\varepsilon) \le C$*. Up to subsequences we have*

$$\frac{1}{|\log\varepsilon|}\mu_\varepsilon \overset{*}{\rightharpoonup} \mu \qquad \text{with } \mu \in \mathcal{M}; \tag{3}$$

$$\frac{1}{|\log\varepsilon|}\psi_\varepsilon \rightharpoonup \psi \qquad \text{with } \psi \in L^2(\Omega; M^{2\times 2}) \tag{4}$$

Moreover $\mu \in H^{-1}(\Omega)$, *Curl* $\psi = \mu$.

ii) *Γ-convergence.* *The functionals* $\frac{1}{|\log\varepsilon|^2}\mathcal{F}_\varepsilon$ *Γ-converge to*

$$\mathcal{F}(\mu, \psi) := \int_\Omega < C\psi : \psi > \, dx + \int_\Omega \varphi\left(\frac{d\mu}{d|\mu|}\right) d|\mu|.$$

Definition of the density of the plastic energy

Let $S := \{b_1, \dots, b_s\}$ be the set of Burgers vectors and $\mathbb{S}$ be its span on $\mathbb{Z}$.

The density of the plastic energy $\varphi : \mathbb{R}^2 \to \mathbb{R}$ is defined through the following relaxation procedure

$$\varphi(b) := \min\{\sum_{k=1}^{N} \lambda_k f(\xi_k), \sum_{k=1}^{N} \lambda_k \xi_k = b, \xi_k \in \mathbb{S}\}. \tag{5}$$

Remark: φ is positively 1-homogeneous

Dislocation walls