Currents and dislocations at the continuum scale

Nicolas Van Goethem

joint work with Riccardo Scala

CMAF-FC-UL-Lisbon

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OUTLINE

- Physical introduction
- Main point: mathematical description of admissible lines and deformations
- Choice of currents: for deformation AND lines

What is a dislocation?

- The 3 scale of matter description
  - Atomic: no precise line location, misfit in atom arrangement
  - Mesoscopic: precise line location, singularity set (of the distortion β), concentration properties:

$$-(\mathrm{curl}\beta)^{\mathrm{T}} = \Lambda = \tau \otimes \mathbf{B}\delta_{\mathcal{L}} : \text{2nd-rank tensor}$$

- Atomic origin

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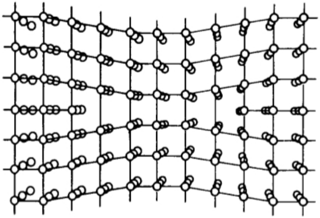
- Atomic origin (multivalued displacement)

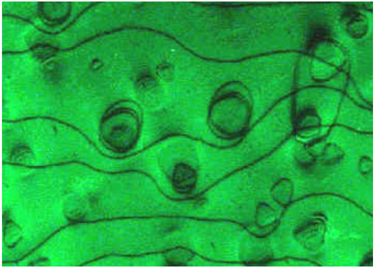
Burgers ·



edge dislocation

Geometry of a dislocation

- Loops
  - overlap
  - intersect
- Endoints on the boundary



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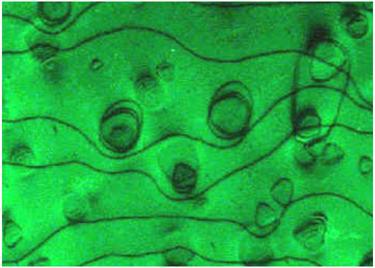
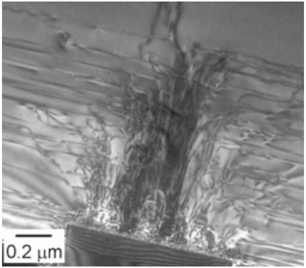


- Clusters
  - mobile geometric necessary dislocations
  - immobile statistically stored
  - forest dislocations



Incompatibility and multivaluedness

- Smooth infinitesimal mesoscopic elasticity. Given $x_0, x, \gamma_{x_0}^x$ (PATH) and $\mathcal{E}$ (STRAIN) $\exists$ $U, W : \mathbb{S}^3 \times \mathbb{M}^3 \to \mathbb{R}$ such that

$$u(x) = U(\mathcal{E}, \mathrm{curl}\ \mathcal{E}; \gamma_{x_0}^x) \quad w(x) = W(\mathrm{curl}\ \mathcal{E}; \gamma_{x_0}^x).$$

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- Displacement u and rotation w well defined $\Leftrightarrow u(x) = U(\mathcal{E}, \mathrm{curl}\ \mathcal{E}; x_0; x) \Leftrightarrow \mathrm{inc}\ \mathcal{E} = \mathrm{curl}(\mathrm{curl}\ \mathcal{E})^T = 0$

$$[u_i](x) = \int_{S_{\gamma_{x_0,x} - \tilde{\gamma}_{x_0,x}}} (y - x) \times \mathrm{inc}\ \mathcal{E} \cdot \mathrm{d}S(y)$$

- INVARIANT of $\mathcal{L}$: MESOSCOPIC Burgers vector:

$$B = [b] = \int_{C_{\mathcal{L}}} [\mathcal{E} + (y - x_0) \times \mathrm{curl}\ \mathcal{E}] \cdot dy$$

Minimization problem

- Nonlinear elasticity: setting of the problem
- Given a family of dislocations $\mathcal{L}$ each with Burgers vector b:
- Dislocation density: $\Lambda = \tau \otimes B\delta_{\mathcal{L}}$
- Deformation variable F, constrained by:

$$\mathrm{curl} F = -\Lambda^{\mathrm{T}} = -B \otimes \tau\delta_{\mathcal{L}} \quad (\star)$$

- Stored energy $\mathcal{W}$, to be minimized under $(\star)$

$$MIN\ \mathcal{W}(F, \Lambda(\mathcal{L}))\ w.r.t.\ F, \mathcal{L}$$

- Class of deformations F (cf. Palombaro and Müller, 2008 and SCALA TALK)
- Class of dislocations $\mathcal{L}$ (THIS TALK)

Admissible deformations

- Deformation variable F, defect variable Λ
- constrained by $\mathrm{curl} F = -\Lambda_{\mathcal{L}}^{\mathrm{T}}$
- $B = \int_{C_{\mathcal{L}}(r)} F d\mathcal{H}^1$

$$\Rightarrow F \sim \frac{1}{r} \quad \text{close to } \mathcal{L}$$

- $\Rightarrow \frac{1}{2}\mathbb{A}\mathcal{E}\cdot\mathcal{E}$ unbounded $\Rightarrow F \notin L^2$...but linear assumption OK away from $\mathcal{L}$...
- Thus: $F \in L^p, 1 < p < 2$ (cavitation: $1 < p < 3/2$)
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  - (ii) no extreme deformations: $W(F) \to \infty$ as $\det F \to 0$

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- Energy (model choice: nonlinear everywhere+constraint)

$$\hat{\mathcal{W}}(F) = \mathcal{W}(F, \Lambda) = \mathcal{W}(F, \mathrm{curl} F)$$

Energy

- Energy form

$$\hat{\mathcal{W}}(F) = \mathcal{W}(F,\Lambda) = \int_\Omega W_{\mathrm{e}}(F)dx + \mathcal{W}_{\mathrm{defect}}(\Lambda)$$

- assumptions on W_{e}:
  - Polyconvexity, i.e., convexity in the minors (in particular $\det F$)
  - Bound from below (growth): coercivity in L^p
  - example: Ogden material

$$W(F) = \begin{cases} a \parallel F \parallel^p + b \parallel \mathrm{cof} F \parallel^q + c \mid \det F \mid^r - d \log(\det F) + e, \\ +\infty, \text{ if } F \notin \mathbb{M}^3_+ \end{cases}$$

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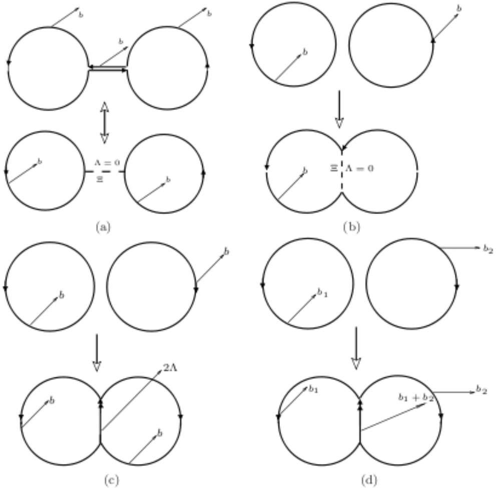
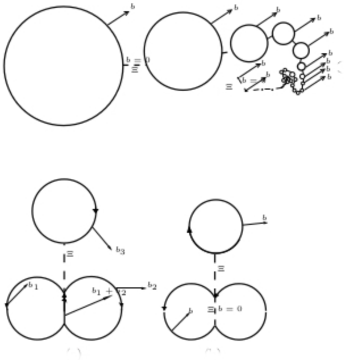
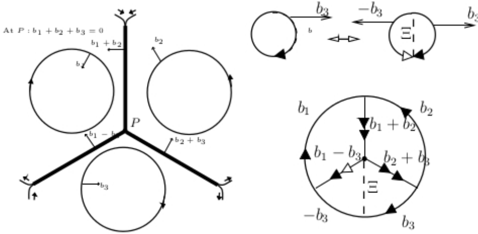
- assumptions for $\mathcal{W}_{\mathrm{defect}}$ (cf. Conti and Garroni, 2014):
  - $\mathcal{W}_{\mathrm{defect}}(\Lambda_{\mathcal{L}}) := \int_L \psi(\theta b, \tau) d\mathcal{H}^1$
  - with coercivity and lsc (by relaxation)

MESOSCOPIC SCALE: Physical properties of the line (1)



MESOSCOPIC SCALE: Physical properties of the line (2)





(a) (b)

Main model object: Currents (intro 1)

- $\mathcal{D}^M(\Omega) = \mathcal{D}(\Omega; \Lambda^M \mathbb{R}^n)$: C^∞-differential forms with degree M with compact support in Ω.
- $\mathcal{D}_M(\Omega) := \mathcal{D}'(\Omega; \Lambda^M \mathbb{R}^n)$: *$M$-dimensional currents on Ω*
- weak convergence:

$$\langle T_k, \omega \rangle \to \langle T, \omega \rangle$$

  for every $\omega \in \mathcal{D}^M(\Omega)$.

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  for every $\omega \in \mathcal{D}^M(\Omega)$.
- $[S] \in \mathcal{D}_M(\mathbb{R}^n)$ will denote the currents obtained by integration on S:

$$[S](\omega) = \int_S \langle \omega, \vec{S} \rangle d\mathcal{H}^M \quad \text{for } \omega \in \mathcal{D}^M(\Omega) \tag{1}$$

Main model object: Currents (intro 2)

- Boundary of a current $\mathcal{D}_M(\Omega)$ is a current $\partial T \in \mathcal{D}_{M-1}(\Omega)$ defined by

$$\partial T(\omega) := T(d\omega) \quad \text{for } \omega \in \mathcal{D}^{M-1}(\Omega)$$

  - $\omega = f_i dx_i \Rightarrow d\omega = \frac{\partial f_j}{\partial x_i} dx_i \wedge dx_j$

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- Mass of a current $T \in \mathcal{D}_M(\Omega)$:

$$|T| := \sup_{\omega \in \mathcal{D}^M(\Omega), |\omega| \leq 1} T(\omega)$$

- Other important quantity:

$$N(T) := |T| + |\partial T|$$

Currents (3): integer-multiplicity currents

- Short notation: $T = \{S, \tau, \theta\}$
- Let $\tau(x) \in T_x S$ is a simple unit M-vector for $\mathcal{H}^M$-a.e. $x \in S$, $\theta : S \to \mathbb{Z}$ be $\mathcal{H}^M$-integrable,
- Integer-multiplicity M-current:

$$T(\omega) = \int_S \langle \omega(x), \tau(x) \rangle \theta(x) d\mathcal{H}^M(x) \qquad \text{for } \omega \in \mathcal{D}^M(\Omega)$$

- Compactness for i.m. currents

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Theorem (Federer 1)

Let $\{T_i\} \subset \mathcal{D}_M(\Omega)$ be a sequence of integer multiplicity currents such that

$$N_U(T_i) < C \qquad \textit{for all } i \textit{ and } U \subset\subset \Omega,$$

with $C > 0$. Then there exist an integer multiplicity current $T \in \mathcal{D}_M(\Omega)$ and a subsequence $\{T_{k(i)}\}_i$ such that $T_{k(i)} \rightharpoonup T$ weakly in Ω as $i \to \infty$.

Currents (4): indecomposability

- An integer-multiplicity current $T \in \mathcal{D}_M(\mathbb{R}^n)$ is said *indecomposable* if there exists no integral current R such that $R \neq 0 \neq T - R$ and

$$N(T) = N(R) + N(T - R)$$

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- Theorem (Federer 2)
  - *For every integer-multiplicity current T there exists a sequence of indecomposable integral currents T_i such that*
    $T = \sum_i T_i$ *and* $N(T) = \sum_i N(T_i)$.
  - *Suppose T is an indecomposable integer-multiplicity 1-current on $\mathbb{R}^n$. Then there exists a Lipschitz function* $: \mathbb{R} \to \mathbb{R}^n$ *with* $\mathrm{Lip}(f) \leq 1$ *s.t.*

$$f \llcorner [0, |T|] \text{ is injective and } T = f_\sharp[0, |T|].$$

Moreover $\partial T = 0$ *if and only if* $f(0) = f(|T|)$*.*

Currents (5): Cartesian maps

- Let $u \in W^{1,p}(\Omega, \mathbb{R}^n)$. Graph of u: $\mathcal{G}_u \subset \Omega \times \mathbb{R}^n$ as

$$\mathcal{G}_u := \{(x, u(x)) : x \in R_u \cap \Omega\}.$$

- Graph of u is a rectifiable
- Define: $\mathcal{A}^p(\Omega, \mathbb{R}^n) := \{u \in W^{1,p}(\Omega, \mathbb{R}^3) : M^{\beta}_{\bar{\alpha}}(Du) \in L^p(\Omega); \forall \alpha, \beta$ with $|\alpha| + |\beta| = 3\}$

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- Define: $G_u(\omega) = \int_\Omega \langle \omega, \vec{G}_u \rangle d\mathcal{H}^n \llcorner \mathcal{G}_u$
- $\mathrm{Cart}^p(\Omega, \mathbb{R}^n) := \{u \in \mathcal{A}^p(\Omega; \mathbb{R}^n) : \partial G_u \llcorner (\Omega \times \mathbb{R}^n) = 0\}$

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- Theorem (Compactness)

  Let $u_k \in \mathrm{Cart}^p(\Omega, \mathbb{R}^n)$ such that $u_k \rightharpoonup u$ weakly in $L^p(\Omega, \mathbb{R}^n)$, $M_{\bar{\alpha}}^{\beta}(Du_k) \rightharpoonup v_{\bar{\alpha}}^{\beta}$ weakly in $L^p(\Omega)$, for all α, β with $|\alpha| + |\beta| = n$, then $u \in \mathrm{Cart}^p(\Omega, \mathbb{R}^n)$ and $v_{\bar{\alpha}}^{\beta} = M_{\bar{\alpha}}^{\beta}(Du)$

Dislocations as currents (1)

- $\mathcal{L} = \sum_{i \in \mathcal{I} \subset \mathbb{N}} \mathcal{L}_i$ ($\mathcal{L}_i$: integer-multiplicity 1-currents).
- $\mathcal{L}_i \Rightarrow b^i \in \mathcal{B}_{\mathcal{I}}$ countable
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- The *density* of $\mathcal{L}_{\mathcal{I}}$ is the linear functional $\Lambda_{\mathcal{L}}$:

$$\langle \Lambda_{\mathcal{L}}, w \rangle := \sum_{i \in \mathcal{I} \subset \mathbb{N}} \mathcal{L}_i((wb^i)^*)$$

for every $w \in C_c^\infty(\Omega, \mathbb{R}^{3\times 3})$ ($(wb)^* := w_{kj} b_j dx_k$).

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  for every $w \in C_c^\infty(\Omega, \mathbb{R}^{3\times3})$ ($(wb)^* := w_{kj} b_j dx_k$).
- Two dislocations $\mathcal{L}_\mathcal{I}$ and $\mathcal{L}'_\mathcal{I}$ are geometrically equivalent if

$$\Lambda_\mathcal{L} = \Lambda_{\mathcal{L}'}.$$

- Geometric necessary dislocation set $L^\star$ is the support of $\Lambda_\mathcal{L}$

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- Projections on the crystallocraphic basis: $b = (\beta_1, \beta_2, \beta_3)$ and

$$\mathcal{L}^{b,i} := \{L^b, \tau^b, \beta_i \theta^b\}$$

$$L := \bigcup_{b \in \mathcal{B}} L^b, \quad \theta_i := \sum_{b \in \mathcal{B}} \mathrm{sg}(\tau^b) \beta_i \theta^b \quad \Rightarrow \mathcal{L}_i := \{L, \tau, \theta_i\}$$

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$$|\hat{\mathcal{L}}| \leq C \|\Lambda_{\mathcal{L}}\|_{\mathcal{M}(\bar{\Omega})}$$

Class of admissible deformations

EXISTENCE RESULT FOR

$$\inf_{\substack{(F,\Lambda_{\mathcal{L}})\in\mathcal{F}\times\mathcal{MD}\\ -\mathrm{curl}F=\Lambda_{\mathcal{L}}^{\mathrm{T}}}} \mathcal{W}(F,\Lambda_{\mathcal{L}}), \tag{2}$$

ADMISSIBLE CLASS

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(i) The dislocation current $\mathcal{L} = \{L,\tau,\theta\}$ satisfies the boundary condition and there exists $\hat{F} \in L^p(\hat{\Omega},\mathbb{R}^{3\times 3})$ with $\hat{F}\llcorner\Omega = F$ such that $-\mathrm{curl}\hat{F} = \Lambda_{\mathcal{L}}^{\mathrm{T}}$ in $\bar{\Omega}$.

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(ii) $\det F > 0$ almost everywhere in Ω.

Existence result for mesoscopic dislocations

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SUFFICIENT CONDITIONS TO APPLY THE DIRECT METHOD

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    (see SCALA talk)

Thank you for the attention!