Modeling of dislocations: from discrete models to the line-tension limit

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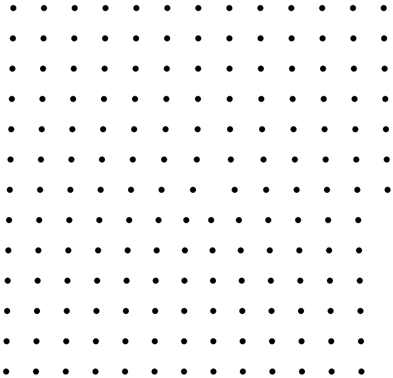
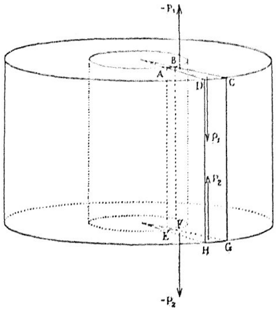
Based on joint work with Pilar Ariza (Sevilla), Adriana Garroni (Roma), Stefan Müller (Bonn), Michael Ortiz (Bonn/Caltech)

Roma, 07.02.2023

Dislocations in crystals





Vito Volterra, 1907

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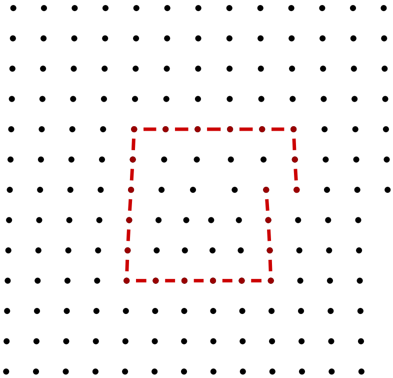

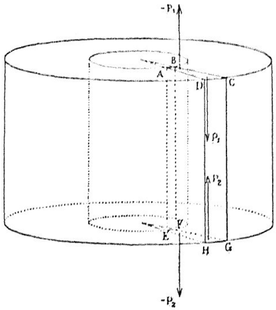

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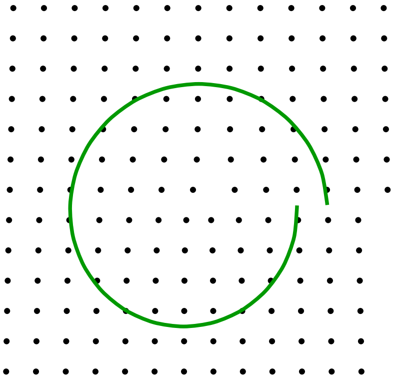

$$\int_{\partial B_r} |\beta| d\mathcal{H}^1 \geq \left| \int_{\partial B_r} \beta \cdot t d\mathcal{H}^1 \right| = |b|, \qquad \int_{\partial B_r} |\beta|^2 d\mathcal{H}^1 \geq \frac{|b|^2}{2\pi r}$$

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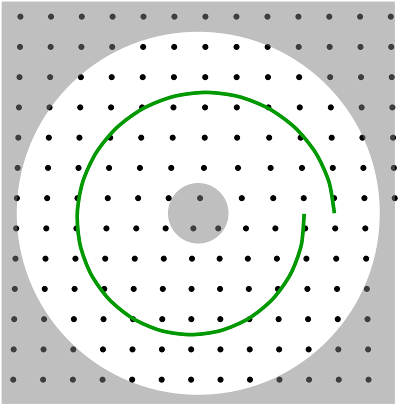

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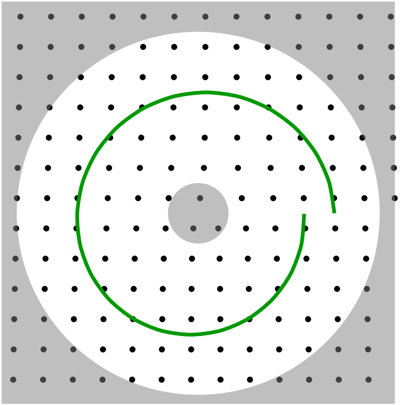

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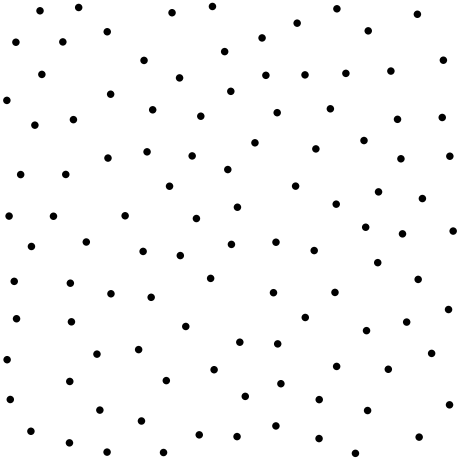
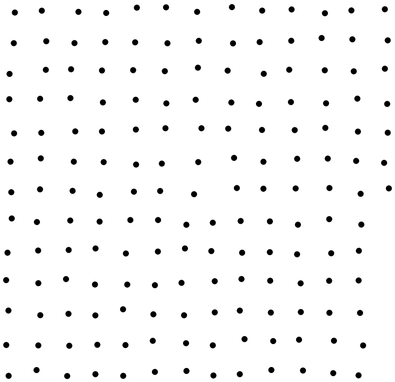
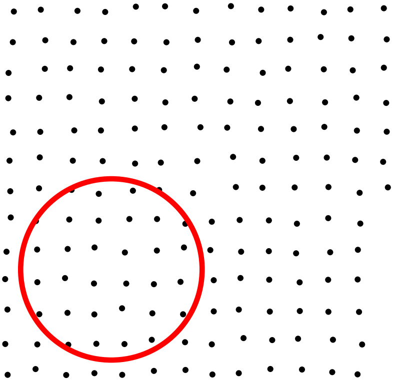
$$\frac{1}{c} \int_{B_R \setminus B_\epsilon} |\beta + \beta^T|^2 \geq \int_{B_R \setminus B_\epsilon} |\beta|^2 \geq \frac{|b|^2}{2\pi} \ln \frac{R}{\epsilon}$$

1.





$$\sum_{i \neq j} V(|x_i - x_j|)?$$



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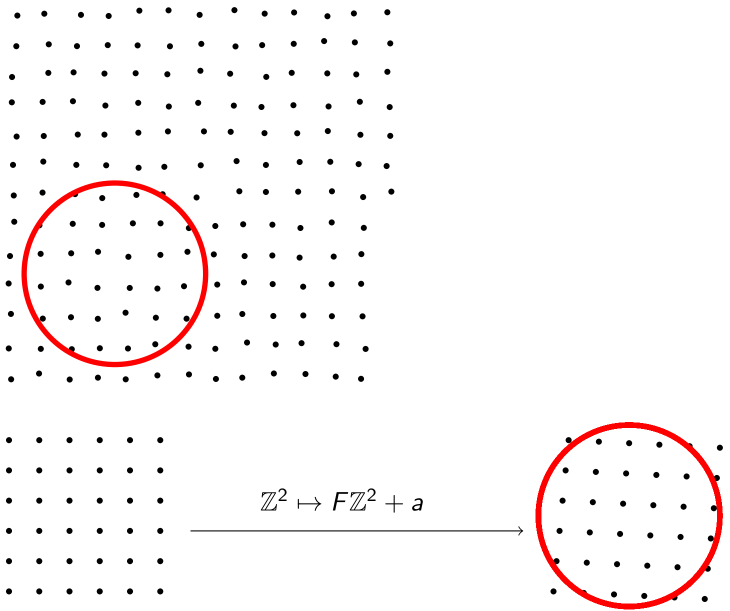
$\mathbb{Z}^2 \mapsto F\mathbb{Z}^2 + a$

$P \subset \mathbb{R}^3$

$x \in \mathbb{R}^3,\ r > 0$

$$\min_{a \in \mathbb{R}^3, F \in \mathbb{R}^{3\times 3}} D(P \cap B_r(x), (F\mathbb{Z}^3 + a) \cap B_r(x))$$

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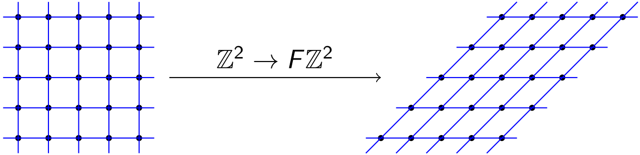
$F\mathbb{Z}^3 + a = G\mathbb{Z}^3 + b$ iff $G^{-1}F \in \mathrm{GL}(3, \mathbb{Z}),\ G^{-1}(b-a) \in \mathbb{Z}^3$



$$F = \begin{pmatrix} 1 & 1 \\ 0 & 1 \end{pmatrix} \in GL(2, \mathbb{Z})$$

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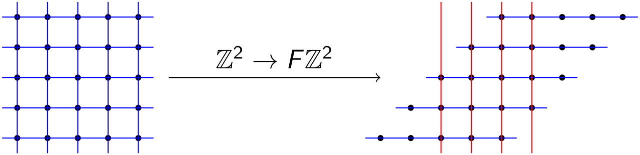

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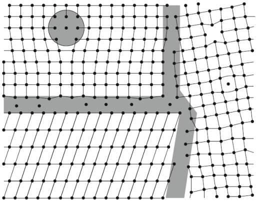
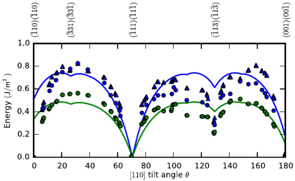
Models for D?

– Luckhaus-Mugnai 2010

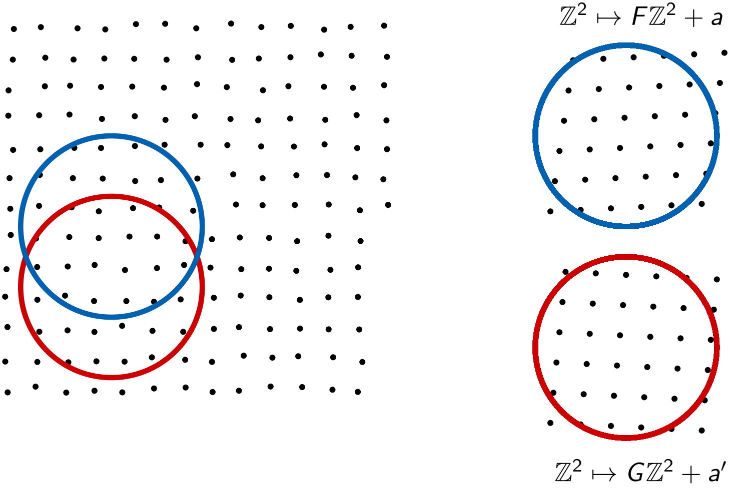


– Runnels-Beyerlein-SC-Ortiz 2016



Grain boundary energy, Cu and Au (fcc)

– ....


$\mathbb{Z}^2 \mapsto F\mathbb{Z}^2 + a$
$\mathbb{Z}^2 \mapsto G\mathbb{Z}^2 + a'$

“Lemma”. Choose “minimal” F. If $D \ll 1$ in ω, then $\operatorname{curl} F = 0$ in ω

Elasticity: $F = \nabla u$, $E[u] = \int W(\nabla u) dx$

$(W(QFR) = W(F),\ Q \in SO(3),\ R \in \mathrm{GL}(3, \mathbb{Z}))$

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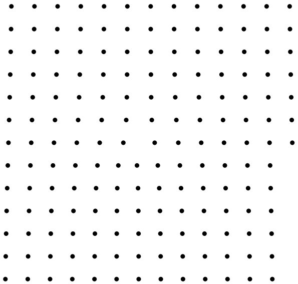

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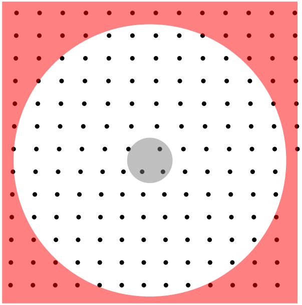

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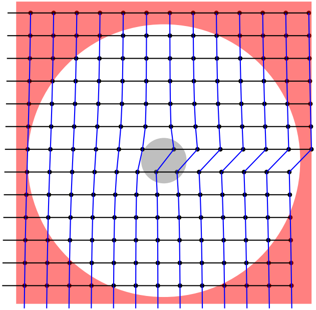
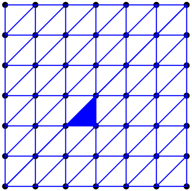
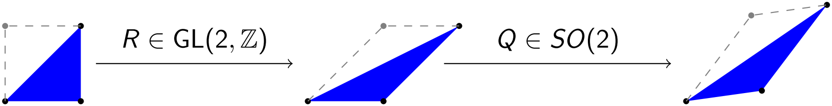


Atomic-scale finite elements for reconstructive phase transformations



$$E = \sum_{t \in T} \min_{R \in GL(2,\mathbb{Z}),\, Q \in SO(2)} |\nabla u(t) - QR|^2$$



SC, Zanzotto ARMA 2004

Baggio, Arbib, Biscari, SC, Truskinovski, Zanzotto, Salman PRL 2019

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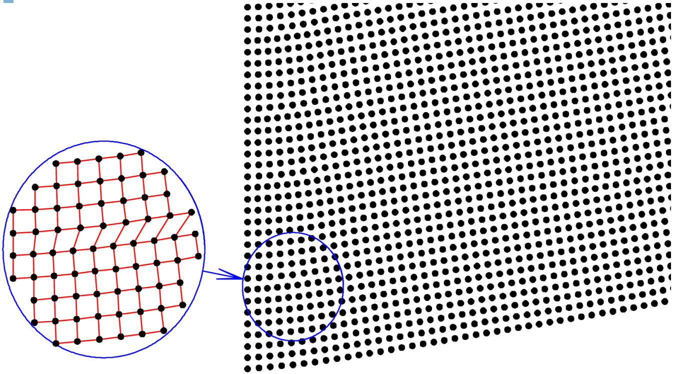

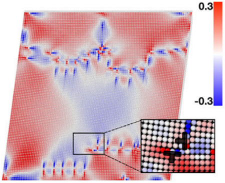

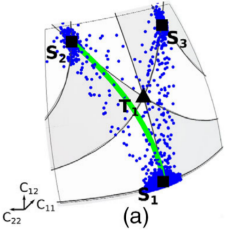

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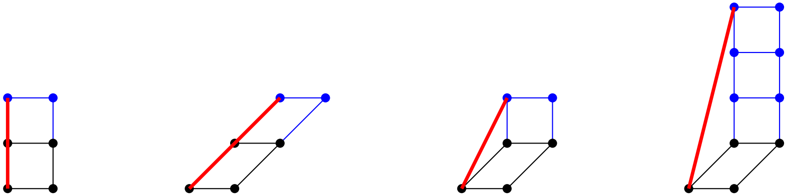
Linearize!!

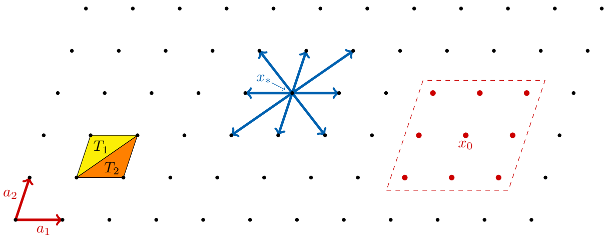
$$\varphi(x) = QFRx,\ Q \in SO(2),\ F \in GL^+(2,\mathbb{R}),\ R \in GL(2,\mathbb{Z})$$

$$\begin{aligned}\varphi(x+h) - \varphi(x) = QFRh &= h + QF(R - Id)h + (QF - Id)h \\ &\simeq h + (R - Id)h + (QF - Id)h \\ &=: h + \xi^{pl}(x,h) + \xi^{el}(x,h)\end{aligned}$$



Basis: Ariza-Ortiz ARMA 2005, Related: Giuliani-Theil JEMS 2022

$\mathcal{L} = F\mathbb{Z}^n$ lattice, $\mathcal{N} \subset \mathcal{L}$ bonds, $\mathcal{C} \subset \mathcal{L}$ cluster



Elastic kinematics:

$u : \Omega \cap \epsilon\mathcal{L} \to \mathbb{R}^n$, $du(x, h) := \frac{u(x+\epsilon h)-u(x)}{\epsilon}$ $(x \in \Omega \cap \epsilon\mathcal{L},\ h \in \mathcal{N})$

$\mathcal{C}_\mathcal{N} := \{(x, h) : x, x + h \in \mathcal{C}, h \in \mathcal{N}\}$

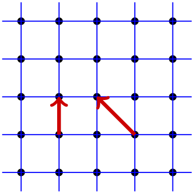
$\xi_{x_0}[u] : \mathcal{C}_\mathcal{N} \to \mathbb{R}^n$, e.g., $\xi_{x_0}(y, h) := du(x_0 + \epsilon y, h)$

Compatibility: $\xi(x, h) = -\xi(x + \epsilon h, -h)$

Linear Ariza-Ortiz model

Ariza-Ortiz:

$$\sum_{x,y,h,h'} B_{x,y,h,h'}(\xi - \xi^{pl})(x,h)(\xi - \xi^{pl})(y,h')$$



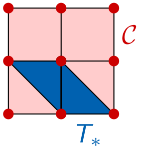
Boundary conditions?

Giuliani-Theil:

$$\frac{1}{2}\sum_{x\sim y}[(u(y) - u(x) - \xi^{pl}(x, y-x)) \cdot (y-x)]^2, \qquad \xi^{pl}(x, y-x) \in \mathcal{L}$$

$$E_C : D_C \to \mathbb{R}_{\geq 0}, \text{ quadratic, } E_C[\xi] = E_C[\xi + F] \text{ for } F \in \mathbb{R}^{n\times n}_{\text{skew}}$$

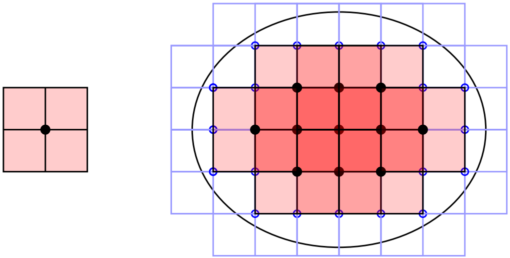
$$\alpha \min_F \sum_{(x,h)\in T_*} |\xi(x,h) - Fh|^2 \leq E_C[\xi]$$



Example: $E^0_C[\xi] := \min_F \sum_{(x,h)\in \mathcal{C}_\mathcal{N}} |\xi(x,h) - Fh|^2.$

Elastic constants: $\frac{1}{2}\mathbb{C}A \cdot A := |T_*|\, E_C[A]$

Total energy: $E_\epsilon[u_\epsilon, \Omega] = \sum_{x+\epsilon\mathcal{C}\subset\Omega\cap\epsilon\mathcal{L}} \epsilon^3 E_C[\xi_x[u_\epsilon]]$



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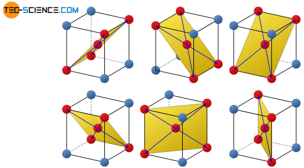
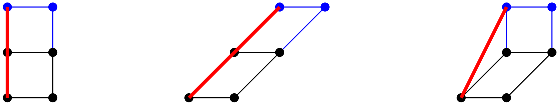
$$(b_1, m_1), \dots, (b_{N_s}, m_{N_s}) \in \mathcal{L} \times \mathcal{L}^*$$

Slip systems



$$\xi^{pl}(x,h) = \sum_{\ell=1}^{N_s} b_\ell \zeta_\ell(x,h)(m_\ell \cdot h), \qquad \zeta_\ell(x,h) m_\ell \cdot h \in \mathbb{Z}$$

$$\xi = \xi^{el} + \xi^{pl}$$



Plastic slip

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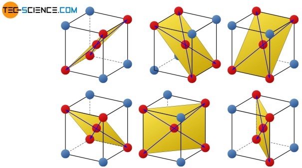
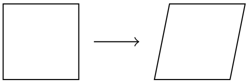


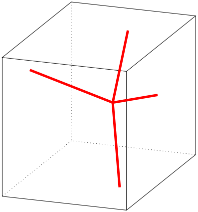
$$\xi^{pl}(x,h) = \textstyle\sum_{\ell=1}^{N_s} b_\ell \zeta_\ell(x,h)(m_\ell \cdot h), \qquad \zeta_\ell(x,h) m_\ell \cdot h \in \mathbb{Z}$$

$$F = \textstyle\sum_\ell \gamma_\ell b_\ell \otimes m_\ell \qquad Fh = \textstyle\sum_\ell \gamma_\ell b_\ell (m_\ell \cdot h)$$



Dilute dislocations

$\gamma = \cup\gamma_i \subset \Omega$, γ_i segments, $|\gamma_i| \geq \alpha_\epsilon$,
similar bound for angles, $\alpha_\epsilon \to 0$ slowly.



ξ "curl-free" on $\Omega \setminus B_{\rho_\epsilon}(\gamma_\epsilon)$

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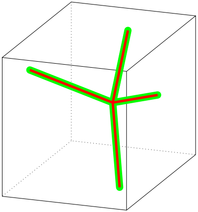

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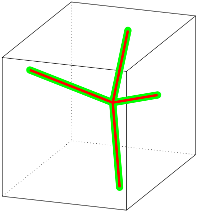

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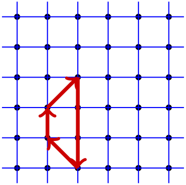
$$\mathrm{circ}(\xi, \{x_0, \ldots, x_K = x_0\}) := \sum_i \xi(x_i, x_{i+1} - x_i)$$



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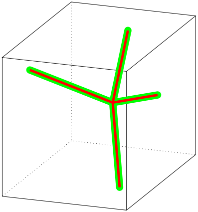

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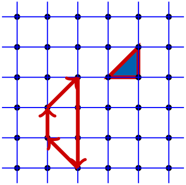
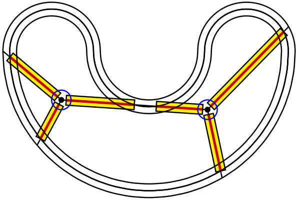
t simplex, $\mathrm{circ}(\xi, \cdot) = 0$ on t: $\xi(x,h) = F_t h$ on t.



Interpolate:

$$(L\xi)(t) := \operatorname*{argmin}_{F \in \mathbb{R}^{3\times 3}} \sum_{(x, x+h) \in t} |Fh - \xi(x,h)|^2$$

Extension: If $\mathrm{circ} L\xi = 0$ in $\Omega \setminus B_\rho(\cup_i \gamma_i)$,
$\exists$ extension $\beta \in L^1(\Omega'; \mathbb{R}^{3\times 3})$
with $\mathrm{curl}\, \beta = \sum_i \theta_i \otimes t_i \mathcal{H}^1 \llcorner \gamma_i \cap \Omega'$,
$\|\beta\|_{3/2} \le \|L\xi\|_{3/2}$.



Theorem [SC-Garroni 2021]:
For any $\beta \in L^1(\Omega; \mathbb{R}^{n\times n})$ there is $R \in \mathbb{R}^{n\times n}_{\mathrm{skw}}$ such that

$$\|\beta - R\|_{L^{1^*}} \le C\|\beta + \beta^T\|_{L^{1^*}} + C|\mathrm{curl}\, \beta|(\Omega)$$

+ the corresponding nonlinear estimate, with $1^* = n/(n-1)$

$n = 2$, linear: Garroni-Leoni-Ponsiglione 2010
$n = 2$, nonlinear: Müller-Scardia-Zeppieri 2014

Let $E_\epsilon : X_\epsilon \to [0,\infty]$, $E_0 : X_0 \to [0,\infty]$.
Fix a convergence criterion $x_\epsilon \to x_0$ ($x_\epsilon \in X_\epsilon$, $x_0 \in X_0$).

$E_\epsilon \xrightarrow{\Gamma} E_0$ iff:

a) $E_0[x_0] \leq \liminf E_\epsilon[x_\epsilon]$ for all sequences $u_\epsilon \to x_0$;

b) $\forall x_0$, $\exists x_\epsilon \to x_0$ with $E_0[x_0] \geq \limsup E_\epsilon[x_\epsilon]$.

Compactness: If $\sup_\epsilon E_\epsilon[x_\epsilon] < \infty$, then there is a convergent subsequence.

Here: $\xi_\epsilon \to \beta$ if the interpolations converge weakly in L^p

Discrete-to-continuum, elasticity

Theorem [SC-Garroni-Ortiz 2022]: $E_\epsilon[u_\epsilon, \Omega] \xrightarrow{\Gamma} \int_\Omega \frac{1}{2}\mathbb{C}Du \cdot Dudx.$

Key estimate: $E_\epsilon[\psi_\delta * u_\epsilon, \omega'] \leq E_\epsilon[u_\epsilon, B_\delta(\omega')]$

$\int_{\omega'} \frac{1}{2}\mathbb{C}F_\delta \cdot F_\delta dx \leq (1 + c\frac{\epsilon}{\delta})E_\epsilon[u_\epsilon, \omega]$, where $F_\delta := \psi_\delta * DJ_\epsilon u_\epsilon$

Continuum-to-continuum, dilute dislocations

$$E_\epsilon^c = \int_{\Omega \setminus B_\epsilon(\gamma_\epsilon)} \frac{1}{2}\mathbb{C}\beta \cdot \beta, \qquad \operatorname{curl}\beta = \epsilon b \otimes t\mathcal{H}^1 \llcorner \gamma$$

Theorem [SC-Garroni-Ortiz 2015, SC-Garroni-Marziani 2022]

If γ_ϵ dilute,

$$\frac{1}{\epsilon^2 \ln \frac{1}{\epsilon}} E_\epsilon^c[\beta_\epsilon] \xrightarrow{\Gamma} E_0[\eta, \mu] := \int_\Omega \frac{1}{2}\mathbb{C}\eta \cdot \eta dx + \int_\gamma \psi_{\mathbb{C}}^{rel}(b, t) d\mathcal{H}^1$$

Topology:

- $\beta_\epsilon \to S$ in L^1, $S \in \mathbb{R}^{3\times 3}_{\mathrm{skw}}$
- $\mu_\epsilon := \dfrac{1}{\epsilon}\operatorname{curl}\beta_\epsilon \rightharpoonup \mu = b \otimes t\mathcal{H}^1 \llcorner \gamma$
- $\dfrac{\beta_\epsilon - S_\epsilon}{\epsilon \ln^{1/2} \frac{1}{\epsilon}} \rightharpoonup \eta$ in $L^{\frac{3}{2}}$; $\operatorname{curl}\eta = 0$

Discrete-to-continuum, dilute dislocations

Theorem [SC-Garroni-Ortiz 2023+]

If γ_ϵ dilute and ξ_ϵ curl-free on $\Omega \setminus B_{m\epsilon}(\gamma_\epsilon)$,

$$\frac{1}{\epsilon^2 \ln \frac{1}{\epsilon}} E_\epsilon[\xi_\epsilon] \xrightarrow{\Gamma} E_0[\eta, \mu] = \int_\Omega \frac{1}{2} \mathbb{C}\eta \cdot \eta + \int_\gamma \psi_{\mathbb{C}}^{rel}(b, t) d\mathcal{H}^1$$

Topology:

- $\frac{1}{\epsilon} \text{curl}\, L\xi_\epsilon \rightharpoonup \mu = b \otimes t \mathcal{H}^1 \llcorner \gamma$ in $\mathcal{D}'$
- $\frac{L\xi_\epsilon - S_\epsilon}{\epsilon \ln^{1/2} \epsilon} \chi_{\Omega \setminus B_{m\epsilon}(\gamma_\epsilon)} \rightharpoonup \eta$ in $L^{3/2}_{loc}$

Discrete-to-continuum, dilute dislocations

Theorem [SC-Garroni-Ortiz 2023+]

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$$\left[\frac{1}{\epsilon}\int_\Omega L\xi_\epsilon \cdot \mathrm{curl}\,\varphi dx \to \int_\gamma b\varphi \cdot t d\mathcal{H}^1 \qquad \forall \varphi \in C_c^\infty(\Omega; \mathbb{R}^3)\right]$$

- $\frac{L\xi_\epsilon - S_\epsilon}{\epsilon \ln^{1/2} \epsilon} \chi_{\Omega \setminus B_{m\epsilon}(\gamma_\epsilon)} \rightharpoonup \eta$ in $L^{3/2}_{loc}$

Straight dislocations: from $\mathbb{C}$ to $\psi_{\mathbb{C}}$

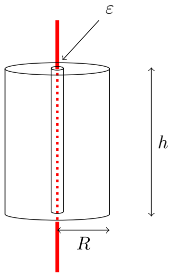
Theorem [SC-Garroni-Ortiz 2015]:

$$\lim_{h\to\infty}\lim_{\epsilon\to 0}\frac{1}{h\ln(R/\epsilon)}\inf\int_{T^h_{\epsilon,R}}\frac{1}{2}\mathbb{C}\beta\cdot\beta=\psi_{\mathbb{C}}(b,t)$$

with curl $\beta = b\otimes t\mathcal{H}^1 \llcorner (\mathbb{R}t)$,

$T^h_{\epsilon,R} = (B_R \setminus B_\epsilon)\times(0,h)$,

$\psi_{\mathbb{C}}(b,t)$ the energy of the 1d solution



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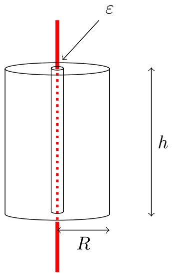

Proof strategy:
Uniform Korn's inequality
Average in direction t, reduce to 2D
Again Korn, affine inside and outside
Uniqueness of the solution to $\operatorname{div}\mathbb{C}\beta=0$, $\operatorname{curl}\beta=\mu$