Multiscale modeling of materials: (3) Discrete → continuum

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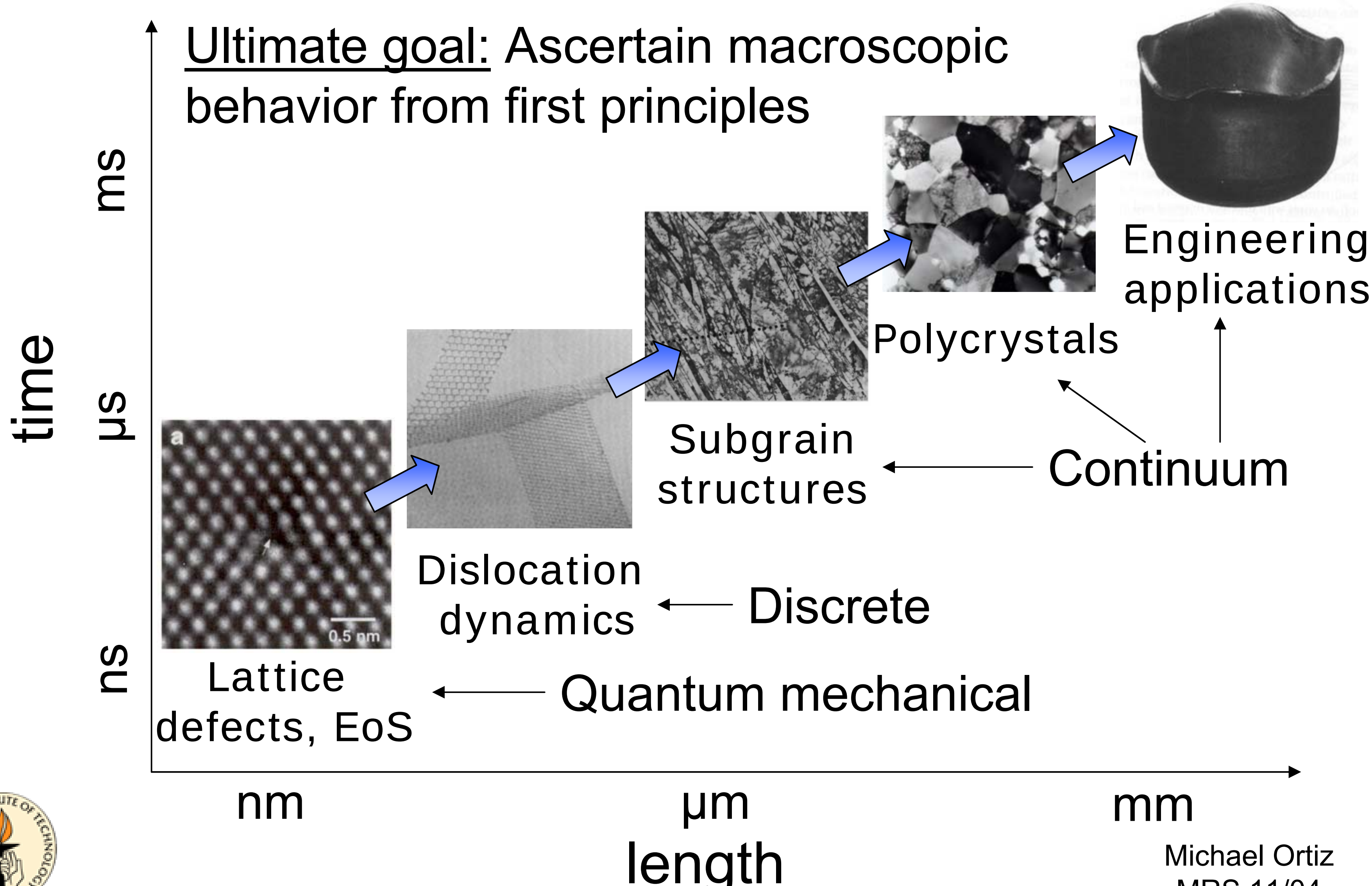
Metal plasticity − Multiscale hierarchy



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The standard continuum model

- Standard model: $E(u,\gamma) =$

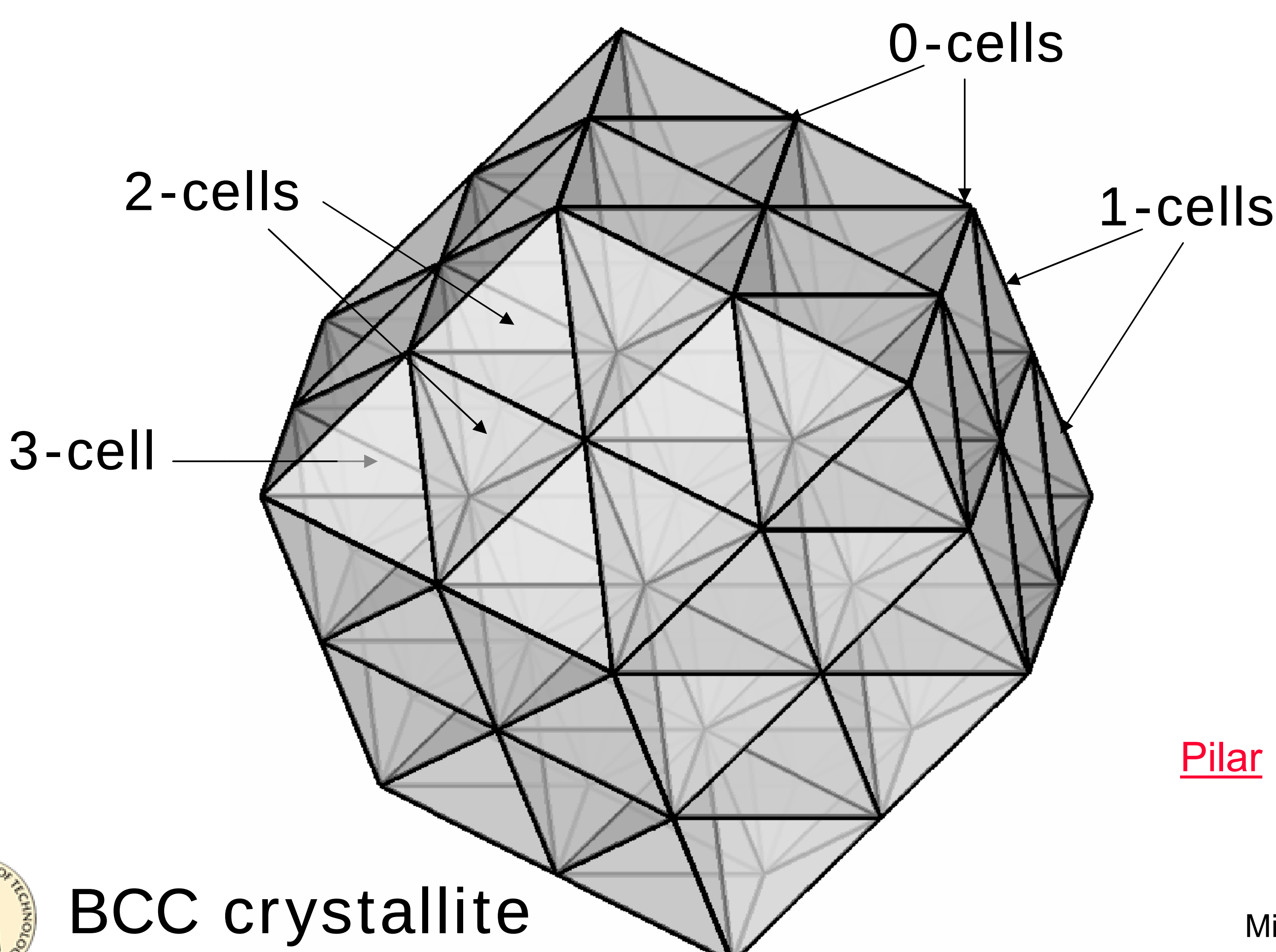
$$\int_\Omega \Big(\underbrace{\frac{1}{2}|\epsilon(u) - \overline{\epsilon}^p(\gamma)|^2}_{\text{strain energy}} + \underbrace{W^p(\gamma)}_{\text{plastic work}} + \underbrace{(T/b)|\mathrm{curl}\,\overline{\beta}^p(\gamma)|}_{\text{core energy}} \Big)\, dx$$

- Plastic work (infinite latent hardening):

$$W^p(\gamma) = \begin{cases} \tau_i|\gamma_i| & \text{if } \gamma_j = 0, \quad \forall j \neq i \\ \infty & \text{otherwise,} \end{cases}$$

- Core energy: $T/b \sim Gb \sim O(\epsilon)$
- **Question**: Is (elastic + core) energy a Γ-limit of a lattice model?

Crystals as discrete differential complexes



BCC crystallite

Pilar

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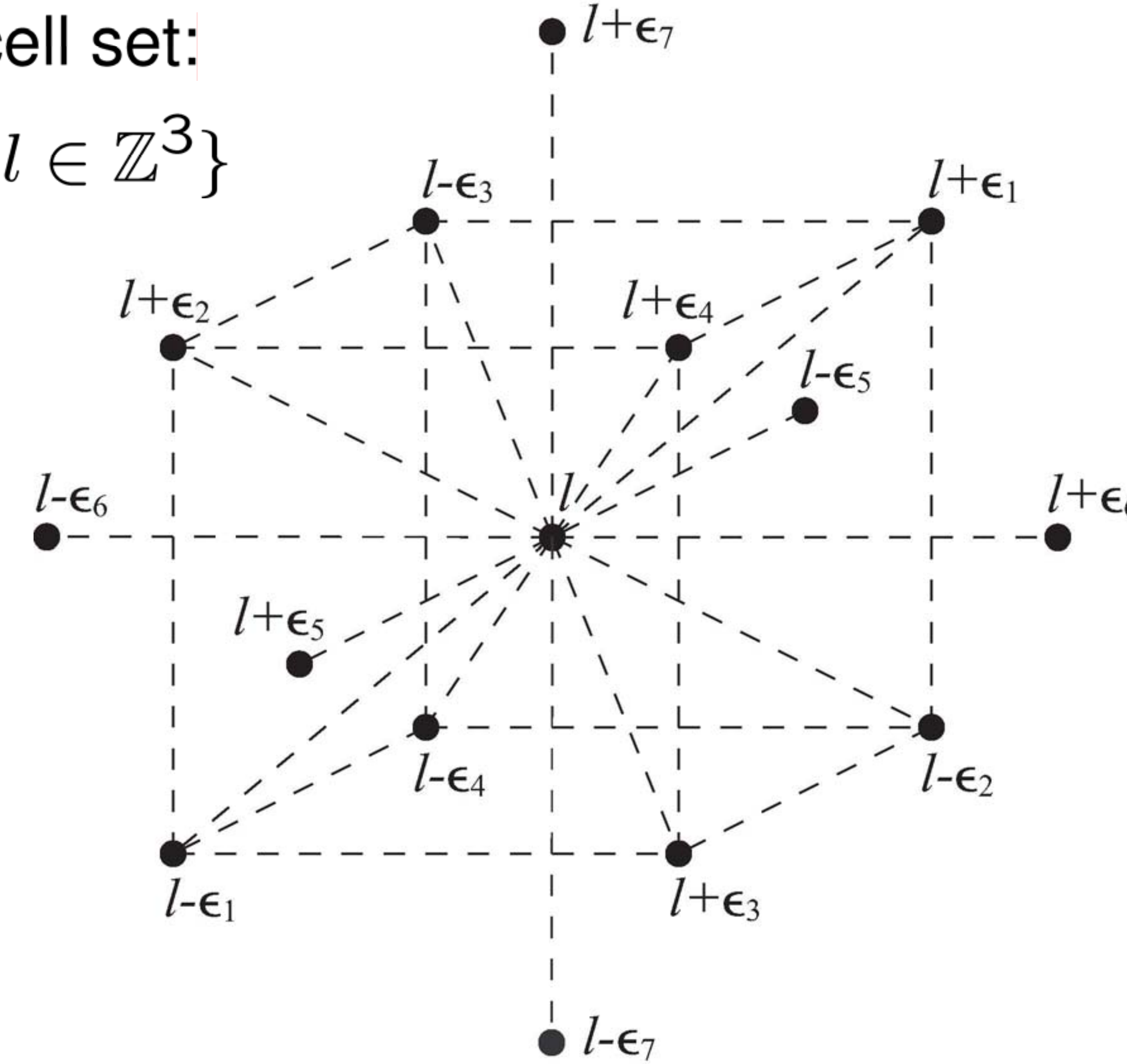
BCC lattice complex: 0-cells

- Indexing of 0-cell set:

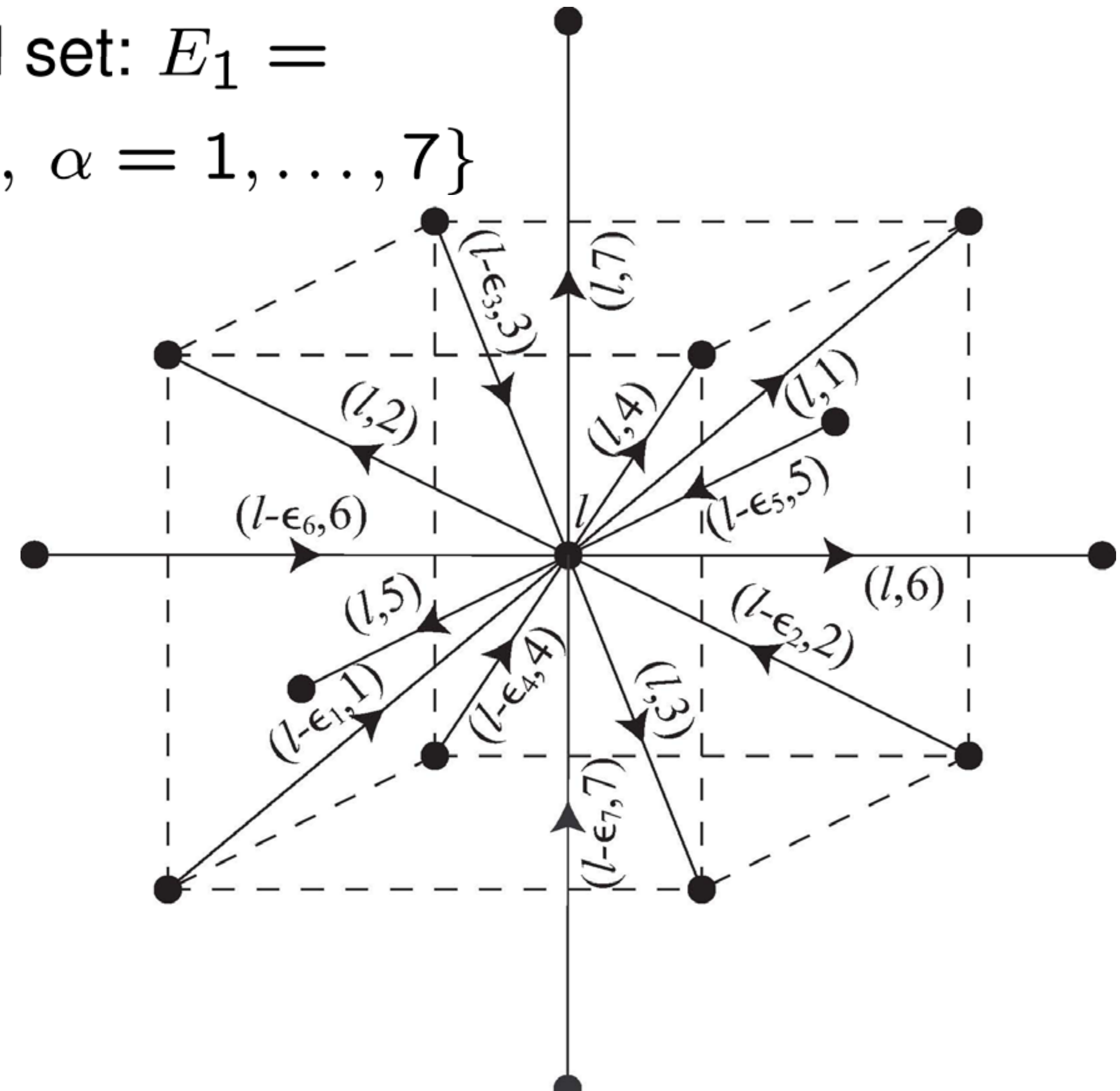
$$E_0 = \{e_0(l),\ l \in \mathbb{Z}^3\}$$

$$\left.\begin{aligned}
\epsilon_1 &= (1,0,0) \\
\epsilon_2 &= (0,1,0) \\
\epsilon_3 &= (0,0,1) \\
\epsilon_4 &= (1,1,1) \\
\epsilon_5 &= (0,1,1) \\
\epsilon_6 &= (1,0,1) \\
\epsilon_7 &= (1,1,0)
\end{aligned}\right\}$$



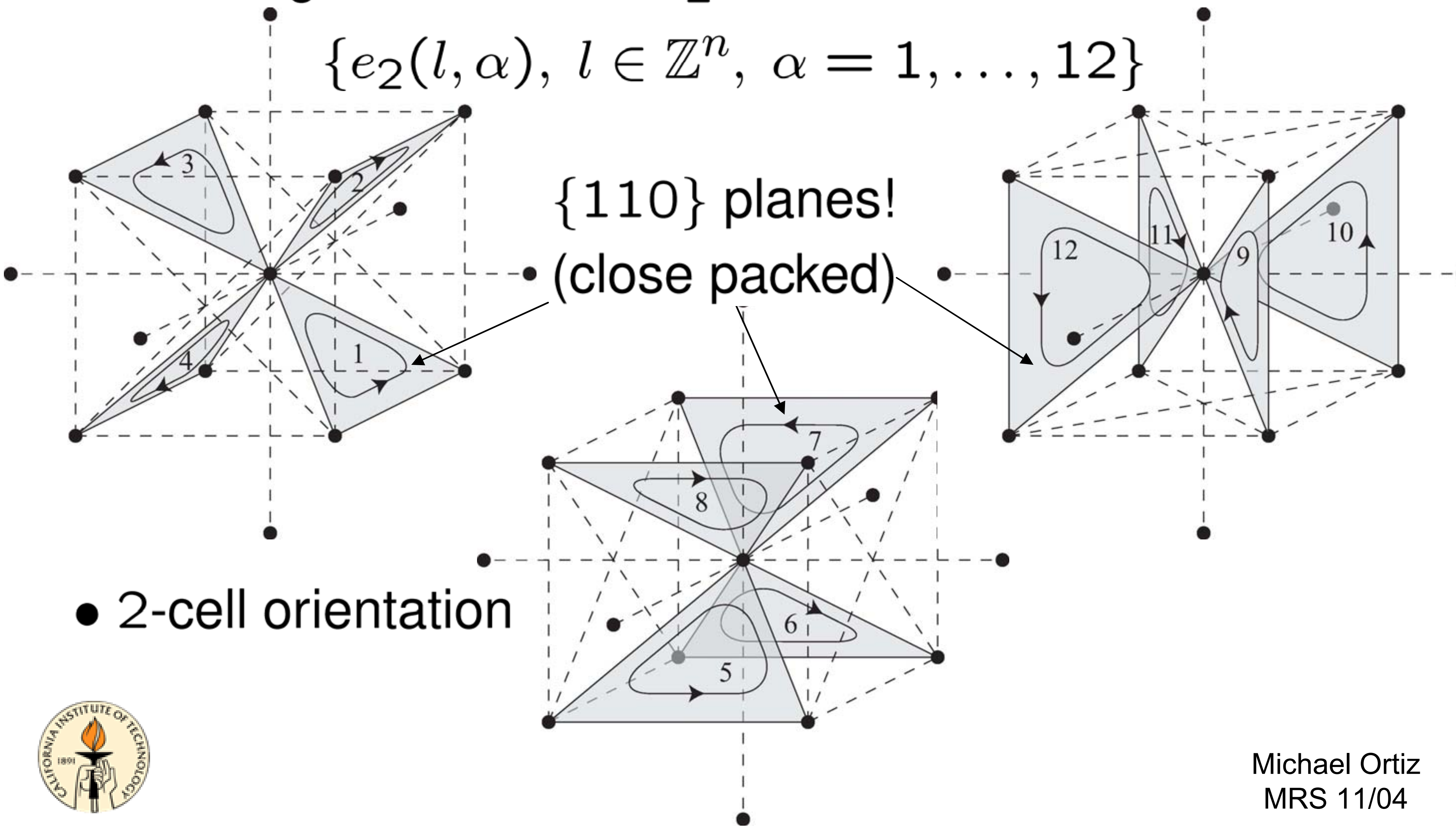
BCC lattice complex: 1-cells

- Indexing of 1-cell set: $E_1 = \{e_1(l, \alpha),\ l \in \mathbb{Z}^n,\ \alpha = 1, \ldots, 7\}$
- 1-cell orientation



BCC lattice complex: 2-cells

- Indexing of 2-cell set: $E_2 = \{e_2(l, \alpha),\ l \in \mathbb{Z}^n,\ \alpha = 1, \dots, 12\}$

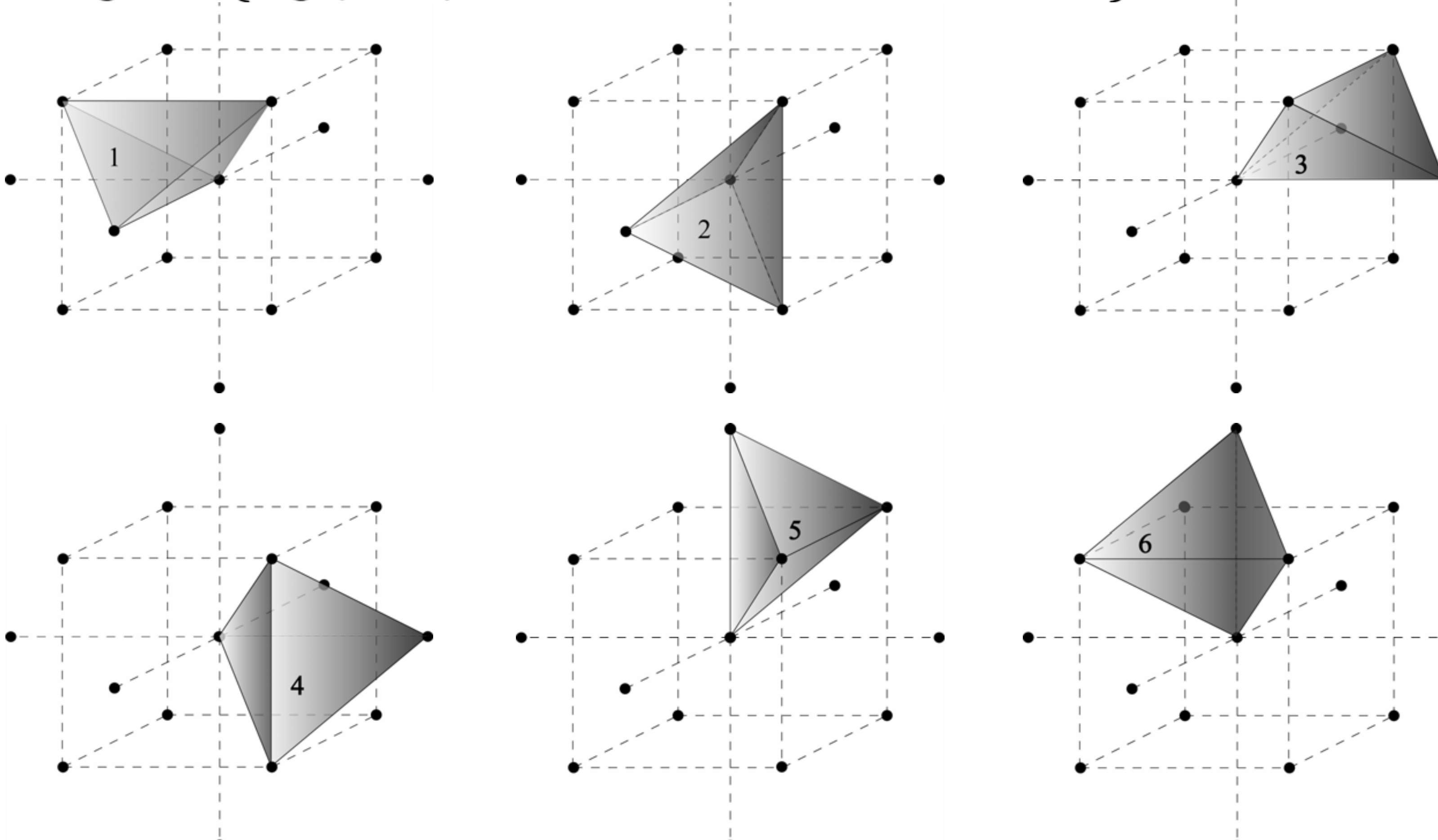


- 2-cell orientation

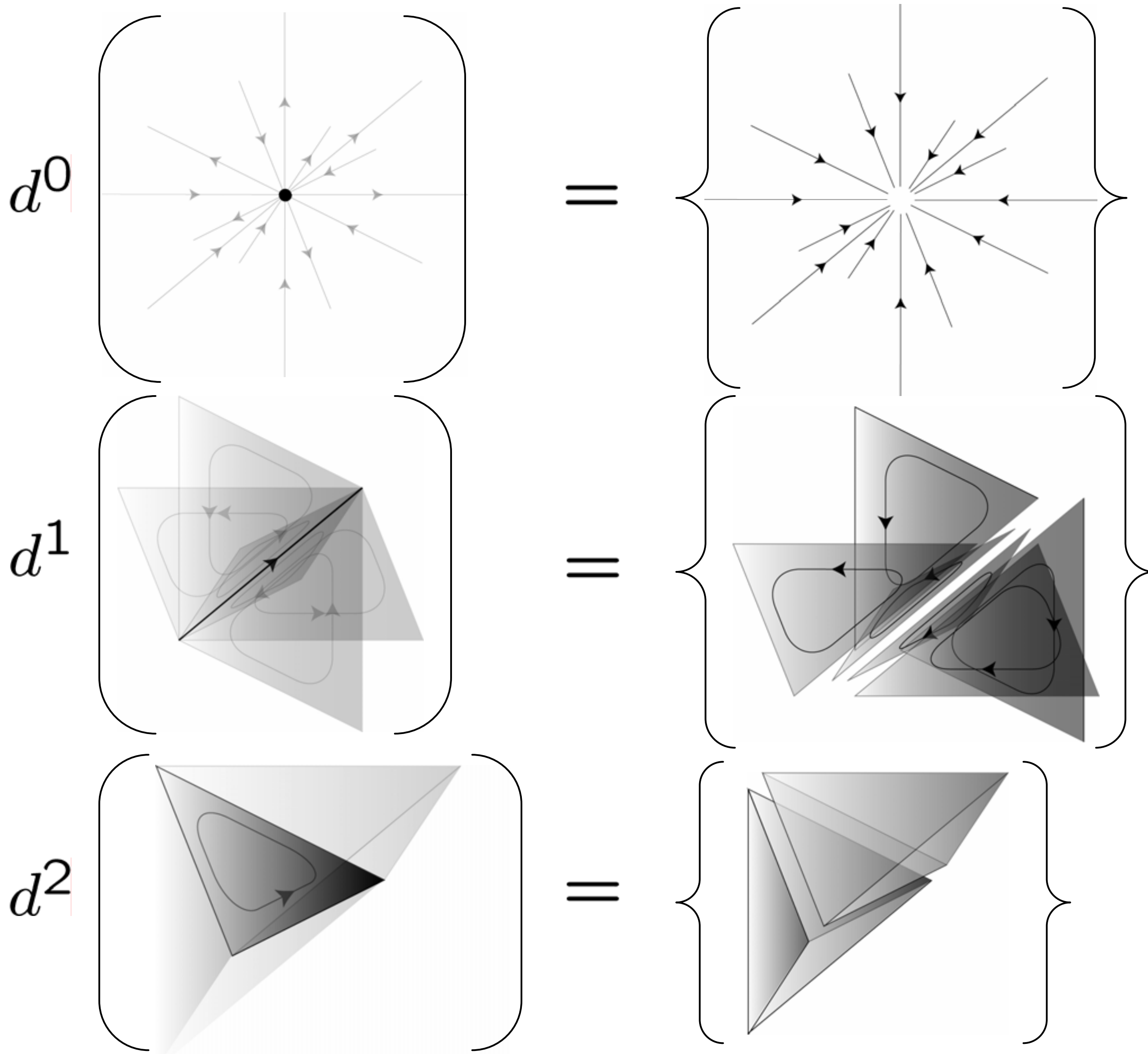
BCC lattice: Lattice complex

- Indexing of 3-cell set (+ outward orientation):

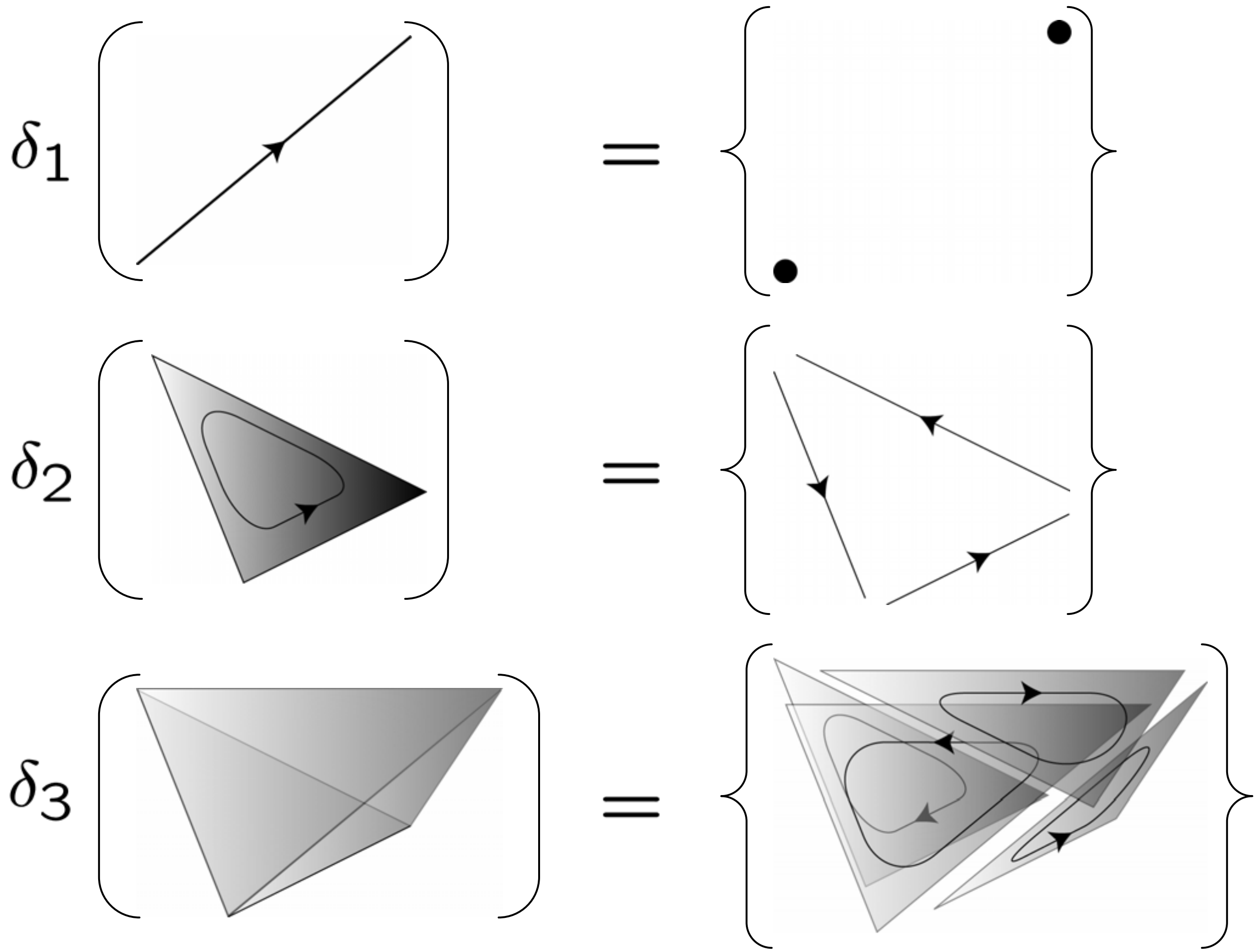
$$E_3 = \{e_3(l,\alpha),\ l \in \mathbb{Z}^n,\ \alpha = 1,\ldots,6\}$$



BCC lattice – Differential operators



BCC lattice – Codifferential operators



Differential calculus and integration

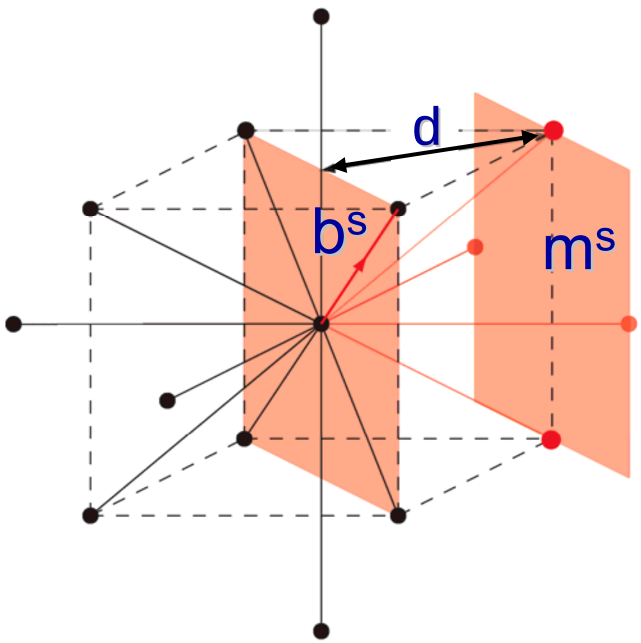
- Forms: $\Omega^p \ni \omega^p : E_p \longrightarrow \mathbb{R}^m$
- $d^2 = 0, \delta^2 = 0 \Rightarrow \{\Omega^p, d^p\}, \{\Omega_p, \delta_p\} \equiv$ lattice differential complexes.
- $H^p \equiv \underbrace{\text{ker}\delta^p}/\underbrace{\text{im}\delta^{p-1}} \equiv p$th cohomology group

  $B^p \equiv$ group of p-coboundaries

  $Z^p \equiv$ group of p-cocycles
- BCC lattice: $H^p = 0 \Rightarrow$ discrete Poincare lemma
- Integral of a form: $\int_A \alpha = \langle \alpha, \chi_A \rangle$
- Discrete Stoke's theorem:

$$\langle d\omega, \chi_A \rangle = \langle \omega, \partial \chi_A \rangle \Longleftrightarrow \int_A d\omega = \int_{\partial A} \omega$$

Discrete crystal plasticity



- Displacements: $u : E_0 \to \mathbb{R}^3$
- Slip fields: $\underbrace{\xi : E_1 \to \mathbb{Z}^N}$

integer-valued!

- Eigendeformations:

$$\beta(e_1) = \sum_{s=1}^{N} \xi^s(e_1)\, b^s \underbrace{\frac{dx(e_1)\cdot m^s}{d}}$$

lattice-preserving shears

- Elastic energy:

$$E(u,\xi) = \frac{1}{2}\langle \Psi * (du-\beta), (du-\beta)\rangle$$

force constants

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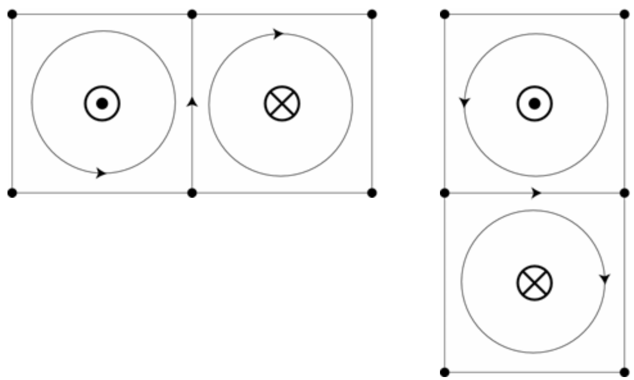
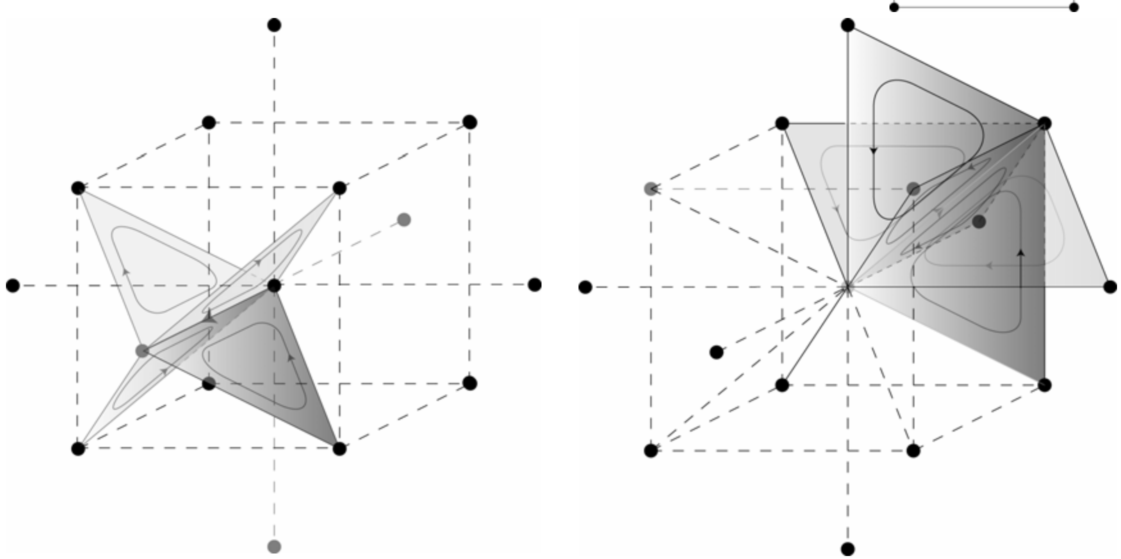
Discrete dislocations

- Discrete dislocation density: $Z^2 = B^2 \ni \alpha = d\beta$
- Conservation of Burgers vector: $d\alpha = 0$
- Square lattice:



- BCC lattice:



Elementary (generating) dislocation loops and Burgers circuits

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Continuum limit of harmonic lattices

- Discrete Fourier transform:

$$\hat{u}(k) = \Omega \sum_{l \in \mathbb{Z}^n} u(l) \mathrm{e}^{-ik\cdot x(l)}$$

- $\mathrm{supp}(\hat{u}) = B \equiv$ Brillouin zone of dual lattice.
- Define the functionals over $H^1(\mathbb{R}^n)$:

$$F_\epsilon(u) = \begin{cases} \frac{\epsilon^{n-2}}{2}\langle \Psi * du, du \rangle & \textit{if}\ \mathrm{supp}(\hat{u}) \subset B/\epsilon \\ +\infty & \textit{otherwise} \end{cases}$$

$$F_0(u) = \int_{\mathbb{R}^n} \frac{1}{2} C_{ijkl} u_{i,j} u_{k,l}\, dx \equiv \text{linear elasticity}$$

Theorem. $\Gamma - \lim_{\epsilon \to 0} F_\epsilon = F_0$ *weakly in* $H^1(\mathbb{R}^n)$.

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Continuum limit of stored energy – 2D

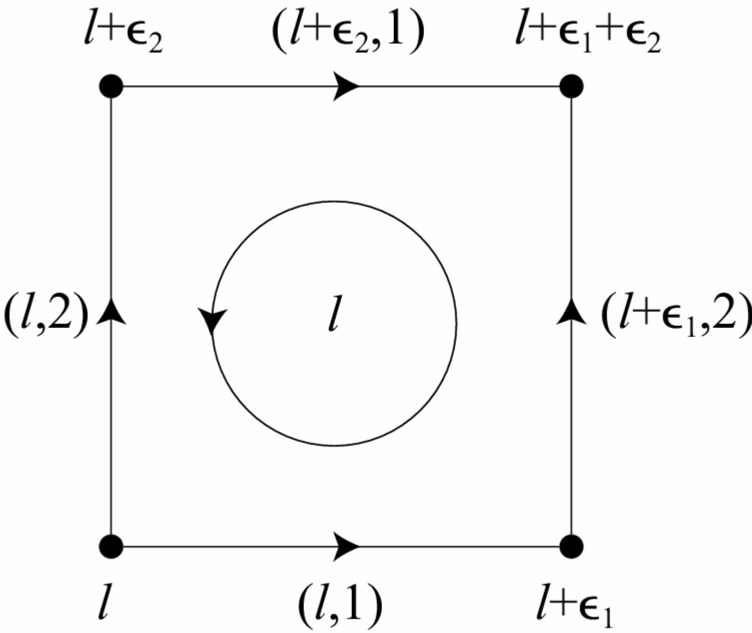
- Nearest-neighbor interactions:

$$E(u) = \int_{E_1} \frac{\mu a}{2} |du(e_1)|^2$$

- Stored energy:

$$E(\alpha) = \frac{\mu b^2}{2} \langle \Delta^{-1} \alpha, \alpha \rangle =$$

$$\int_{-\pi}^{\pi} \int_{-\pi}^{\pi} \frac{\mu b^2}{2} \frac{|\hat{\alpha}(\theta)|^2}{\sin^2 \frac{\theta_1}{2} + \sin^2 \frac{\theta_2}{2}} \frac{d\theta_1 d\theta_2}{(2\pi)^2}$$



Square lattice complex

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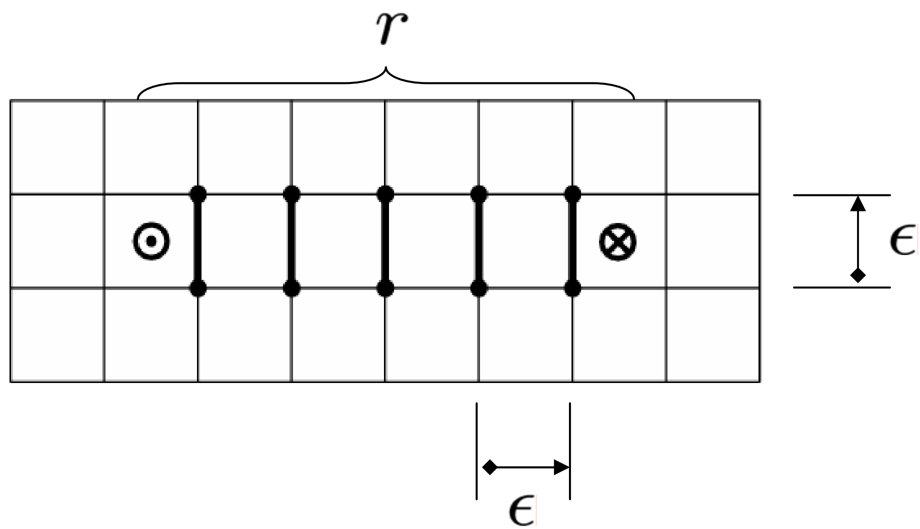
Continuum limit of stored energy – 2D



Screw dipole of size *r* in square lattice

- Dipole energy, $\epsilon \to 0$, r fixed:

$$E_\epsilon \sim \frac{G\epsilon^2}{2\pi}\left(\log\frac{r}{\epsilon} + C\right) = \frac{G\epsilon^2}{2\pi}\left(\log r + \log\frac{1}{\epsilon} + C\right)$$

- Limiting scaled energy: $\lim_{\epsilon\to 0} \frac{E_\epsilon}{\epsilon^2 \log(1/\epsilon)} = \frac{G}{2\pi}$

independent of r! $\Rightarrow$ scales with total dislocation mass

Continuum limit of stored energy – 2D

- Analysis of Marcello Ponsiglione:
- Dislocation measure: $$\hat{\mu}(\alpha) := \sum_{Q \in \Omega_\varepsilon^2} \alpha(Q) \delta_{x(Q)},$$
- Space: $X \equiv$

$$\{\mu \in \mathcal{M}(\Omega) : \mu = \sum_{i=1}^{M} z_i \delta_{x_i},\ M \in \mathbb{N},\ x_i \in \Omega,\ z_i \in \mathbb{Z}\}.$$

- Space: $X_\varepsilon \equiv$ measures μ s. t. $\mu = \widehat{\mu}(\alpha)$ for some discrete dislocation density on an ε-lattice
- Scaling: $$\mathcal{F}_\varepsilon^{\mathrm{d}}(\mu) := \begin{cases} \frac{1}{|\log \varepsilon|} \mathcal{E}_\varepsilon(\tilde{\alpha}(\mu)) & \text{if } \mu \in X_\varepsilon; \\ +\infty & \text{in } X \setminus X_\varepsilon. \end{cases}$$
- Limiting energy: $$\mathcal{F}(\mu) := \frac{1}{2\pi} |\mu|(\Omega)$$

Continuum limit of stored energy – 2D

- Analysis of Marcello Ponsiglione:

Theorem 3.4. *The following* Γ*-convergence result holds.*

i) *Equi-coercivity. Let* $\varepsilon_n \to 0$*, and let* $\{\mu_n\}$ *be a sequence in* X *such that* $\mathcal{F}^d_{\varepsilon_n}(\mu_n) \le E$ *for some positive constant* E *independent of* n*. Then (up to a subsequence)* $\mu_n \xrightarrow{f} \mu$ *for some* $\mu \in X$.

ii) Γ*-convergence. The functionals* $\mathcal{F}^d_{\varepsilon_n}$ Γ*-converge to* $\mathcal{F}$ *as* $\varepsilon_n \to 0$ *with respect to the flat norm, i.e., the following inequalities hold.*

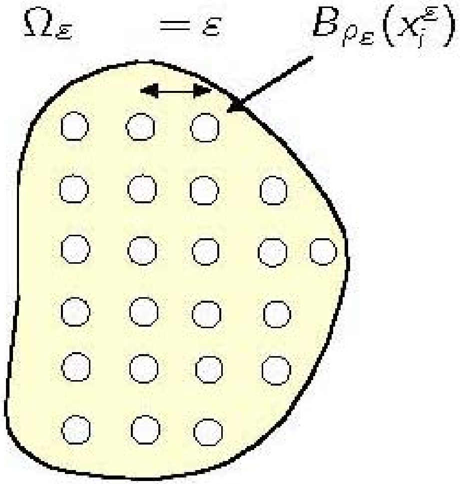
Γ*-liminf inequality:* $\mathcal{F}(\mu) \le \liminf \mathcal{F}^d_{\varepsilon_n}(\mu_n)$ *for every* $\mu \in X$, $\mu_n \xrightarrow{f} \mu$ *in* X.

Γ*-limsup inequality: given* $\mu \in X$*, there exists* $\{\mu_n\} \subset X$ *with* $\mu_n \xrightarrow{f} \mu$ *such that* $\limsup \mathcal{F}^d_{\varepsilon_n}(\mu_n) \le \mathcal{F}(\mu)$.

Continuum limit of stored energy – 2D

- Approach of A. Garroni and G. Leone:

Fix $\varepsilon > 0$ and $\rho_\varepsilon \to 0$ as $\varepsilon \to 0$, and the points x_i such that



- $N_\varepsilon := \sharp\{x_i^\varepsilon\} \sim \frac{1}{\varepsilon^2}$
- $\mathrm{dist}\,(x_i^\varepsilon, x_j^\varepsilon) \sim \varepsilon$ for $i \neq j$ (ε is the average distance)
- $\{x_i^\varepsilon\}$ are "uniformly distributed"

For simplicity we assume that the points x_i^ε are periodically distributed (on a lattice of period ε)

Continuum limit of stored energy – 2D

- Approach of A. Garroni and G. Leone:

- Energy: $F_\varepsilon(\mathbf{H},\mathbf{b}) := \int_{\Omega_\varepsilon} \mathbf{C}(E(\mathbf{H}))E(\mathbf{H})\,dx$

- Space: $(\mathbf{H},\mathbf{b}) \in X_\varepsilon$

$$= \left\{ L^2(\Omega_\varepsilon,\mathbb{R}^{2\times 2}) \times PC_\varepsilon(\Omega,S) \;:\; \text{“Curl}\,\mathbf{H} = \sum_{\mathrm{i}} \mathbf{b}(\mathrm{x}_\mathrm{i}^\varepsilon)\delta_{\mathrm{x}_\mathrm{i}^\varepsilon}\text{”} \right\}$$

- $PC_\epsilon(\Omega,\mathcal{S}) \equiv$ functions piecewise constant on squares of size ε.

Continuum limit of stored energy – 2D

- Approach of A. Garroni and G. Leone:
- Regimes: $$\lim_{\varepsilon \to 0} \varepsilon^2 |\log \rho_\varepsilon| = L$$
  - Subcritical: $L = +\infty$
    Very diluted regimes $\longrightarrow$ only self interaction
  - Critical: $L \in (0, +\infty)$
    Self interaction $\sim$ Long range interaction
  - Super critical: $L = 0$
    Dense regime
- Scaling: $$\mathcal{F}_\varepsilon(\mathbf{H}, \mathbf{b}) := \frac{\varepsilon^2}{|\log \rho_\varepsilon|} F_\varepsilon(\mathbf{H}, \mathbf{b})$$

Continuum limit of stored energy – 2D

- Approach of A. Garroni and G. Leone:

- ("Compactness") If $\mathcal{F}_\varepsilon(\mathbf{H}_\varepsilon, \mathbf{b}_\varepsilon) \le C$ then, up to a subsequence, there exist $\mathbf{H} \in L^2(\Omega, \mathbb{R}^{2\times 2})$ and $\mathbf{b} \in L^2(\Omega, \overline{\mathrm{co}S})$ such that

$$\begin{cases} \varepsilon^2 \chi_{\Omega_\varepsilon} \mathbf{H}_\varepsilon \rightharpoonup \mathbf{H} \\ \mathbf{b}_\varepsilon \rightharpoonup \mathbf{b} \end{cases} \quad \text{in } L^2 \quad \text{and} \quad \mathrm{Curl}\, \mathbf{H} = \mathbf{b}$$

- (Γ-convergence) $\mathcal{F}_\varepsilon$ Γ-converges to

$$\mathcal{F}(\mathbf{H}) = \int_\Omega \varphi^{**}(\mathrm{Curl}\, \mathbf{H})\, \mathrm{dx} + \frac{1}{L} \int_\Omega \mathbf{C}(E(\mathbf{H}))E(\mathbf{H})\, dx$$

with the constraint $\mathrm{Curl}\, \mathbf{H} \in \mathrm{L}^2(\Omega, \overline{\mathrm{co}S})$ where φ^{**} is the convex envelope of

$$\varphi(\mathbf{b}) = \begin{cases} \frac{\mu(\lambda+\mu)}{4\pi(\lambda+2\mu)} |\mathbf{b}|^2 & \text{if } \mathbf{b} \in S \\ +\infty & \text{otherwise} \end{cases}$$

Continuum limit of stored energy – 2D

- Approach of A. Garroni and G. Leone:

THE CASE $L = 0$

$$\mathcal{F}_L(\mathbf{H}) := L\mathcal{F}(L\mathbf{H}) = \int_\Omega \frac{1}{L}\varphi^{**}(L\,\mathrm{Curl}\,\mathbf{H})\,\mathrm{dx} + \int_\Omega \mathbf{C}(\mathrm{E}(\mathbf{H}))\mathrm{E}(\mathbf{H})\,\mathrm{dx}$$

Theorem 3. $\mathcal{F}_L(\mathbf{H})$ Γ-converges to

$$\mathcal{F}_0(\mathbf{H}) = \int_\Omega \varphi_0\left(\frac{\mathrm{Curl}\,\mathbf{H}}{|\mathrm{Curl}\,\mathbf{H}|}\right)|\mathrm{Curl}\,\mathbf{H}| + \int_\Omega \mathbf{C}(\mathrm{E}(\mathbf{H}))\mathrm{E}(\mathbf{H})\,\mathrm{dx}$$

with $\mathbf{H} \in \{\mathbf{K} \in L^2 : \mathrm{Curl}\,\mathbf{K}$ is a measure with bounded variation$\}$ where φ_0 is the 1-homogeneous function defined by

$$\varphi_0(\mathbf{b}) = \lim_{t\to 0} \frac{1}{t}\varphi(t\mathbf{b})$$

Note: φ_0 always exists when $\mathbf{0}$ is isolated in S.

Continuum limit of stored energy – 2D

- Approach of A. Garroni and G. Leone, examples:

1) If $S = S^1 \cup \{\mathbf{0}\}$, then

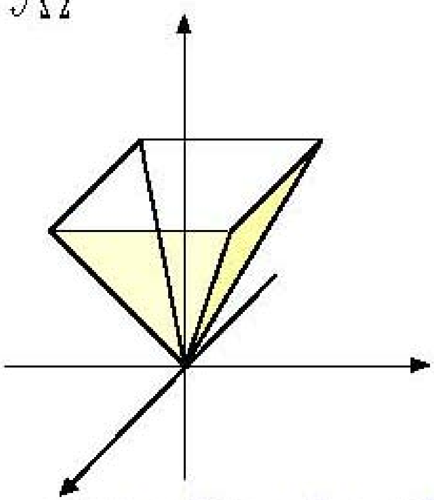
$$\mathcal{F}_0(\mathbf{H}) = \|\mathrm{Curl}\,\mathbf{H}\| + \int_\Omega \mathbf{C}(\mathrm{E}(\mathbf{H}))\mathrm{E}(\mathbf{H})\,\mathrm{dx}$$

2) In the cubic case; i.e., $S = \{\mathbf{e}_1, \mathbf{e}_2, -\mathbf{e}_1, -\mathbf{e}_2, \mathbf{0}\}$ we get

$$\mathcal{F}_0(\mathbf{H}) = \int_\Omega \varphi_0\left(\frac{\mathrm{Curl}\,\mathbf{H}}{|\mathrm{Curl}\,\mathbf{H}|}\right) |\mathrm{Curl}\,\mathbf{H}| + \int_\Omega \mathbf{C}(\mathrm{E}(\mathbf{H}))\mathrm{E}(\mathbf{H})\,\mathrm{dx}$$

where

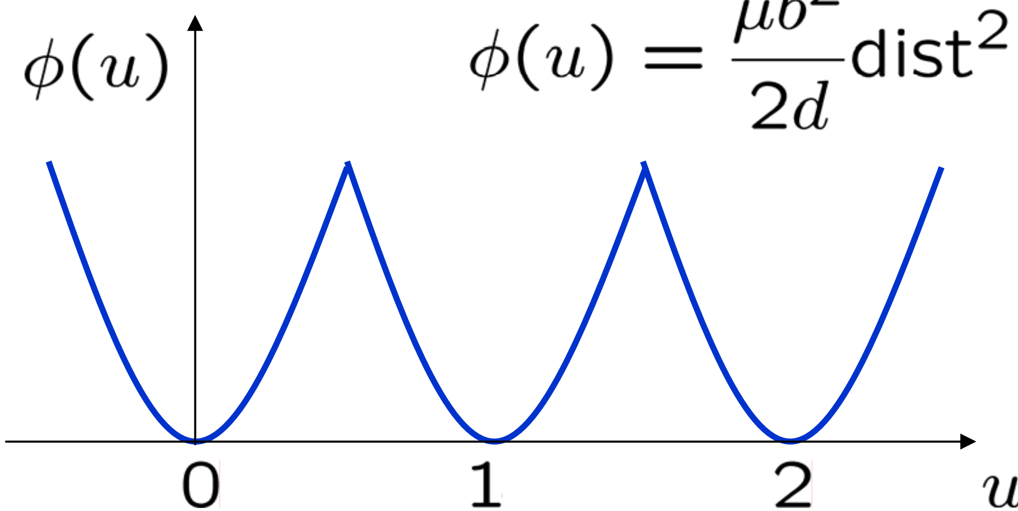
$$\varphi_0(\mathbf{b}) = \frac{\mu(\lambda+\mu)}{4\pi(\lambda+2\mu)}(|b_1| + |b_2|)$$



Continuum limit of stored energy – 2.5D

- Consider the special case (Koslowski et al ’02):
  - i) Activity on single slip system, single slip plane.
  - iii) Approximate lattice elasticity by continuum elasticity outside the slip plane.
  - iv) Peierls potential: $u \equiv$ displacement jump,

$$\phi(u) = \frac{\mu b^2}{2d} \text{dist}^2(u, \mathbb{Z})$$



Continuum limit of stored energy – 2.5D

- Total energy: $E(u) =$

$$\underbrace{\int_{\mathbb{R}^2} \frac{\mu b^2}{2d} \text{dist}^2(u, \mathbb{Z}) dx}_{\text{Core energy}} + \underbrace{\frac{1}{(2\pi)^2} \int_{\mathbb{R}^2} \frac{\mu b^2}{4} K |\hat{u}|^2 dk}_{\text{Elastic energy}} - \underbrace{\int_{\mathbb{R}^2} b\tau u dx}_{\text{External}}$$

where $K = \dfrac{k_2^2}{\sqrt{k_1^2 + k_2^2}} + \dfrac{1}{1-\nu} \dfrac{k_1^2}{\sqrt{k_1^2 + k_2^2}}$

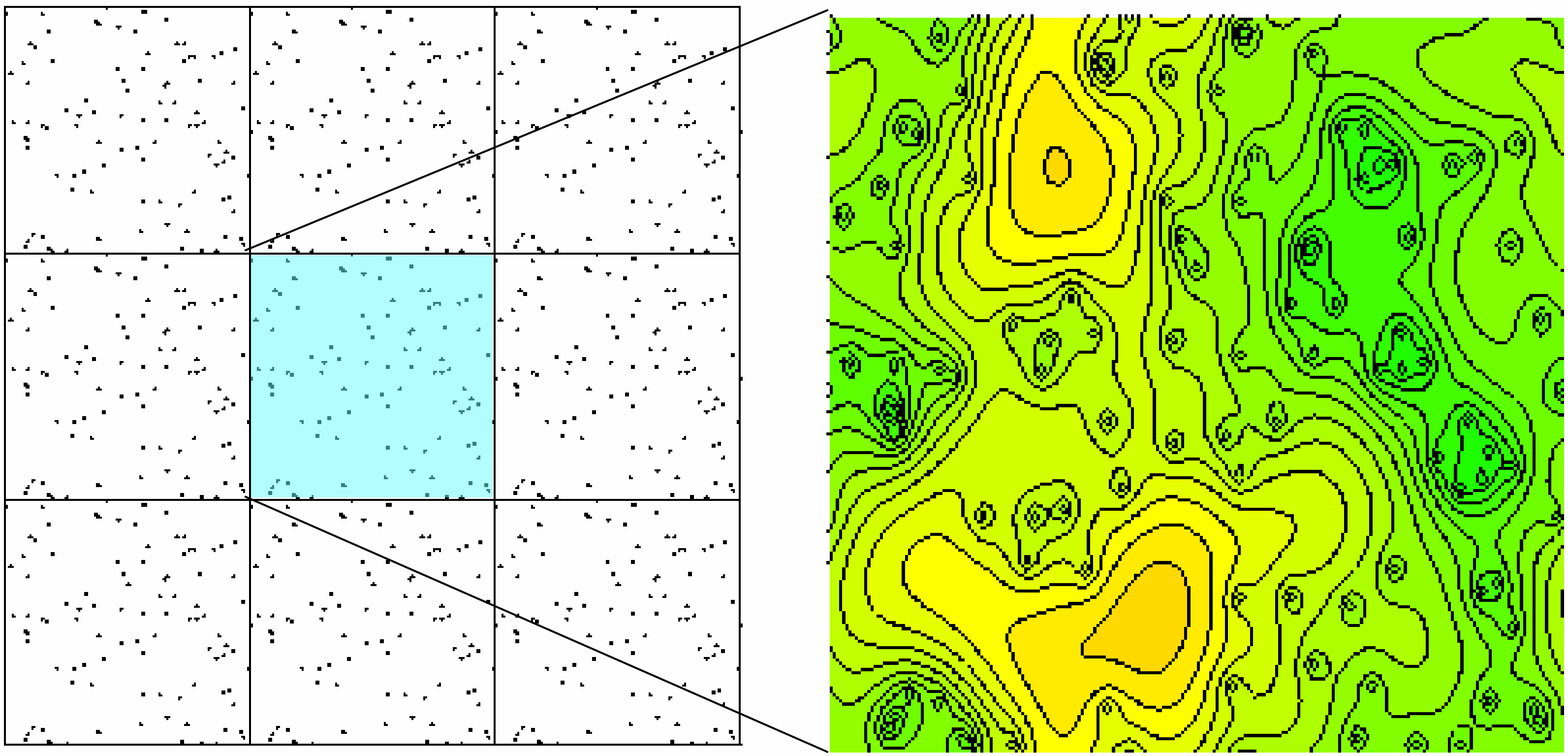
- Structure of the energy:

$$E_\epsilon(u) = \frac{1}{2\epsilon} \int_{\mathbb{R}^2} \text{dist}^2(u, \mathbb{Z}) dx + |u|^2_{H^{1/2}} + \text{linear term}$$

(cf Alberti, Bouchitte and Seppecher ’98)

Dislocation-obstacle interaction

- Problem geometry: i) Periodic square cell.
  ii) Random array of obstacles.



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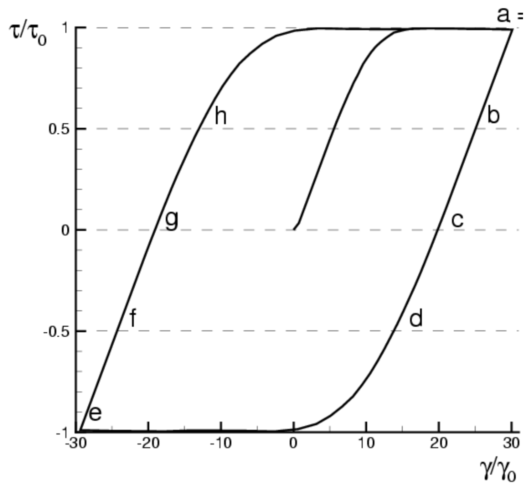
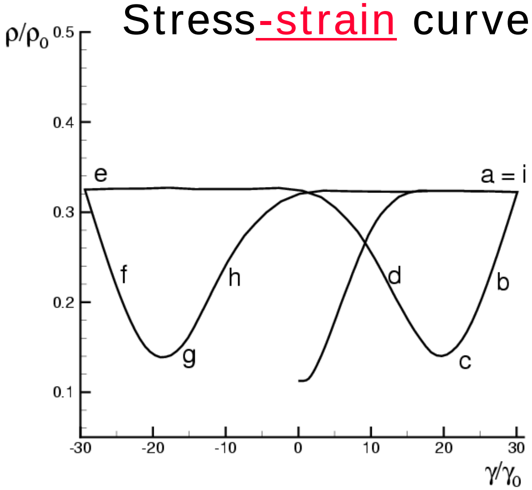
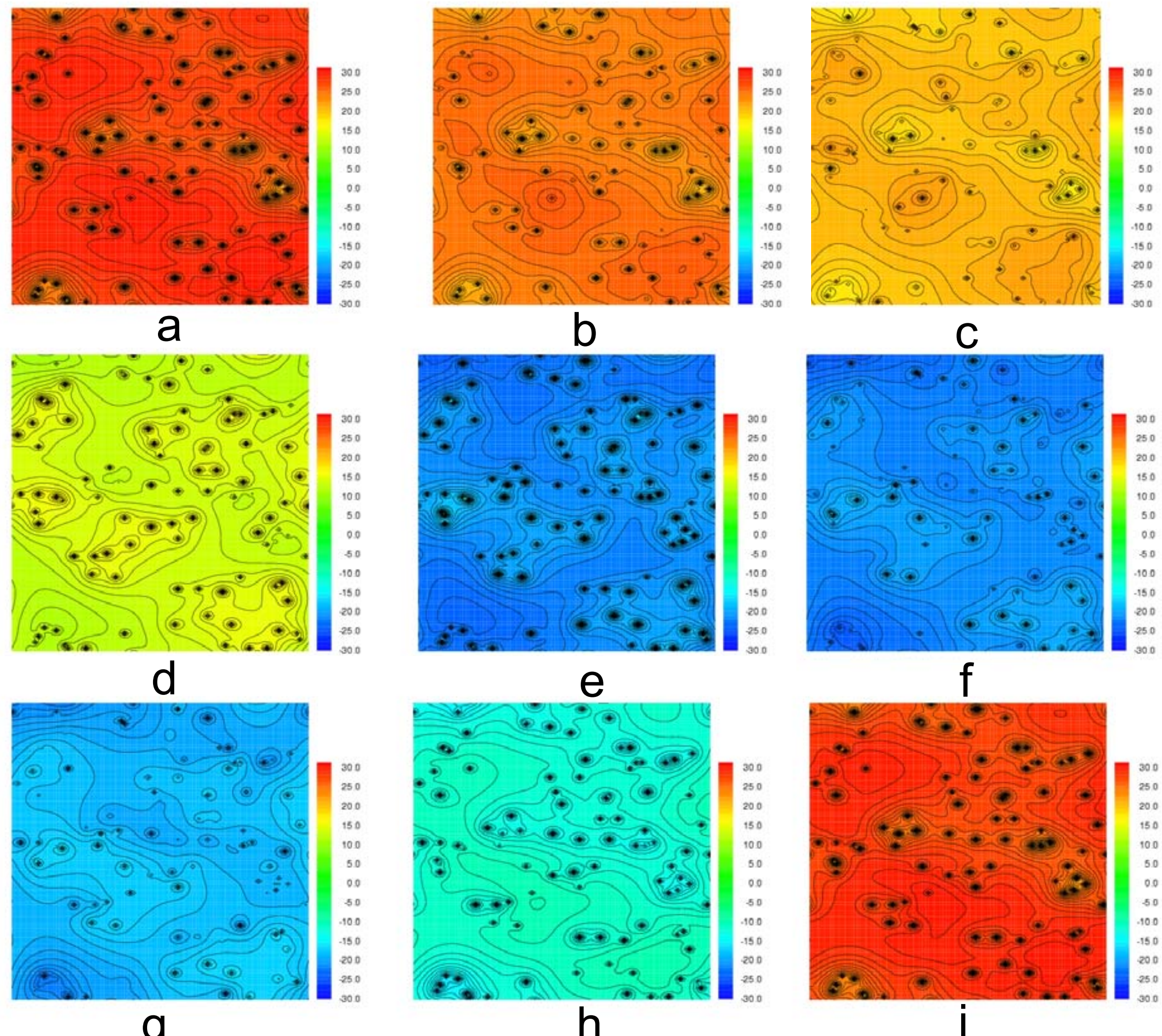
Dislocation-obstacle interaction



Stress-strain curve



Dislocation density



(Movie)

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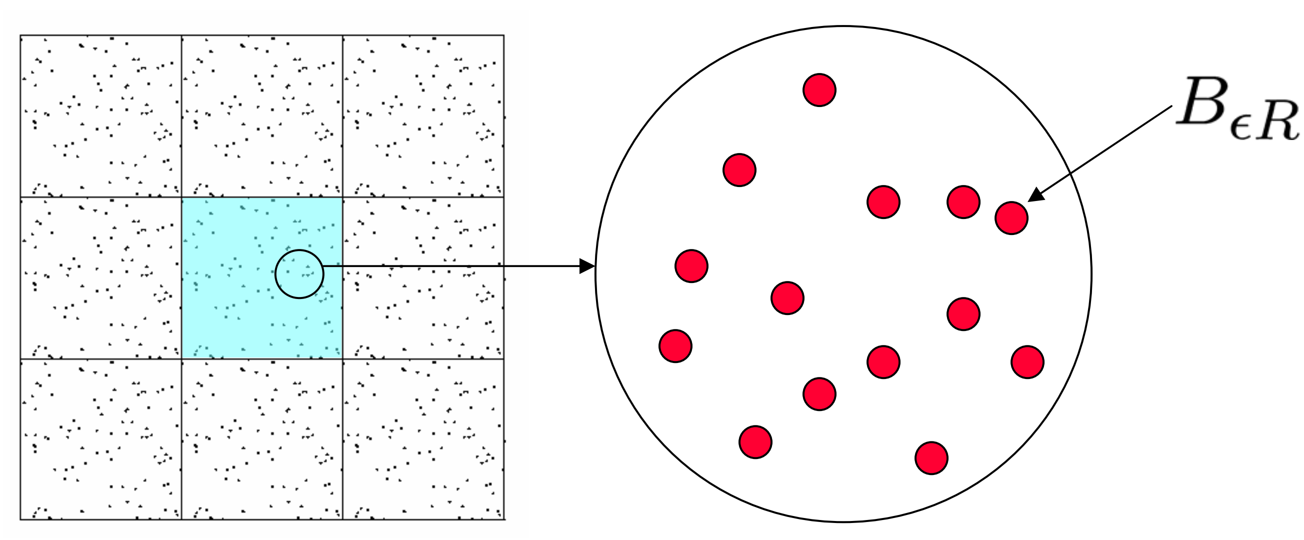
Γ-limit analysis – Impenetrable obstacles

- Energy (Garroni and Müller ’03): $E_\epsilon(u) =$

$$\frac{1}{2\epsilon}\int_{T^2} \text{dist}^2(u,\mathbb{Z})dx + \int_{T^2\times T^2} K_\nu(x-y)|u(x)-u(y)|^2 dxdy$$

if $u \in H^{1/2}(T^2)$ and $u = 0$ on N_ϵ obstables.

- Two regimes: i) $\epsilon N_\epsilon \to 1$; ii) $\epsilon N_\epsilon / \log(1/\epsilon) \to 1$.

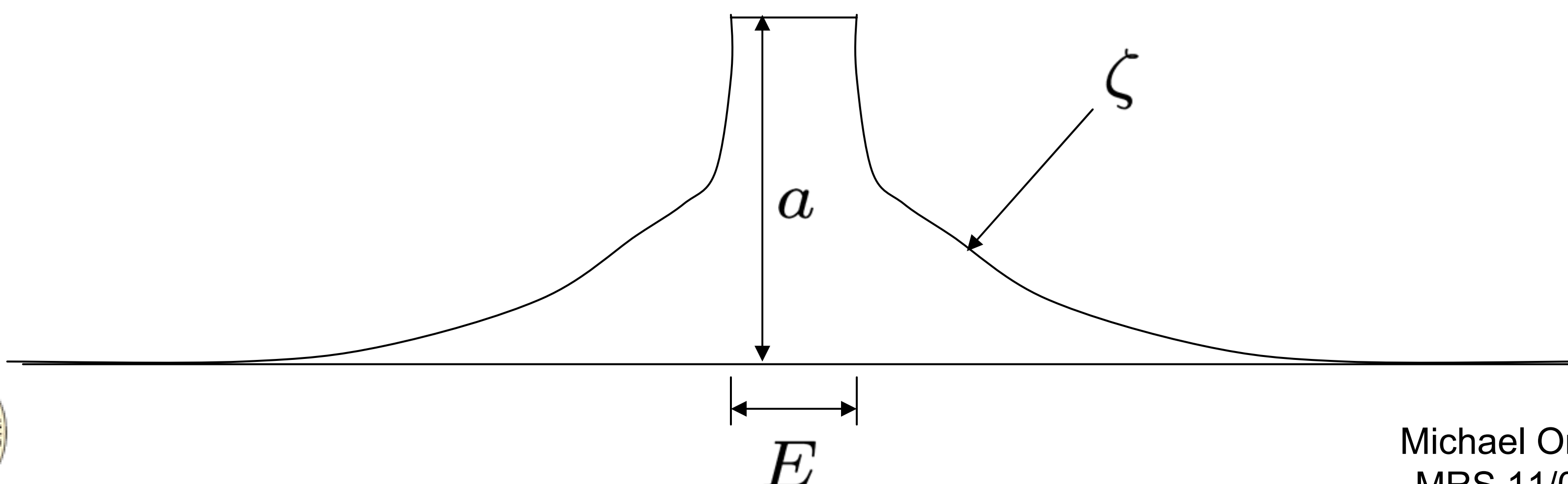


Γ-limit analysis – Impenetrable obstacles

- Dislocation capacity of an open set:

$$D^{\nu}_{\frac{1}{2}}(a, E) = \inf \Big\{ \int_{\mathbb{R}^2} \text{dist}^2(\zeta, \mathbb{Z}) dx + \int_{\mathbb{R}^2 \times \mathbb{R}^2} \Gamma_\nu(x-y) |\zeta(x) - \zeta(y)|^2 dx dy \Big\}$$

subject to $\zeta = a$ on E, $\zeta \in L^4(\mathbb{R}^2)$.



Γ-limit analysis – Impenetrable obstacles

Theorem (Garroni and Müller '03) *The scaled energy* $F_\epsilon(u) = E_\epsilon(u)/N_\epsilon \epsilon$ Γ*-converges with respect to the strong* L^2 *topology to the functional:*

$$F(u) = \begin{cases} D^\nu_{\frac{1}{2}}(u, B_R), & \text{if } u = \text{constant} \in \mathbb{Z} \\ +\infty & \text{otherwise} \end{cases}$$

Theorem (Garroni and Müller '03) *The scaled energy* $F_\epsilon(u) = E_\epsilon(u)/N_\epsilon \epsilon / \log(1/\epsilon)$ Γ*-converges with respect to the strong* L^2 *topology to the functional:*

$$F(u) = \int \gamma(\nabla u/|\nabla u|)|\nabla u| dx + \int D^\nu_{\frac{1}{2}}(u, B_R) dx$$

if $u \in L^2(T^2, \mathbb{Z})$, $F(u) = +\infty$ *otherwise.*