DFG - Schwerpunktprogram 1095
Analysis
Modeling &
Simulation of
Multiscale Problems

Marie Curie Research Training Network MULTIMAT

Workshop on Multiscale Numerical Methods for Advanced Materials

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Numerical relaxation of nonconvex functionals in phase transitions of solids and finite strain elastoplasticity

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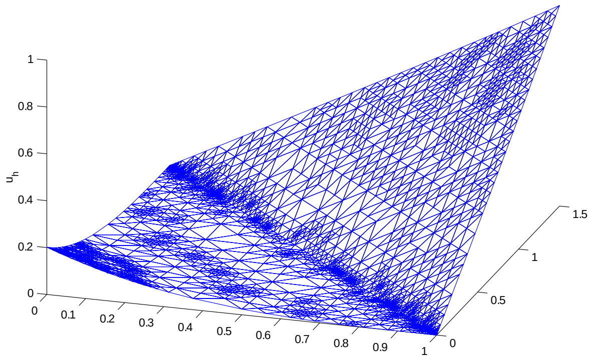
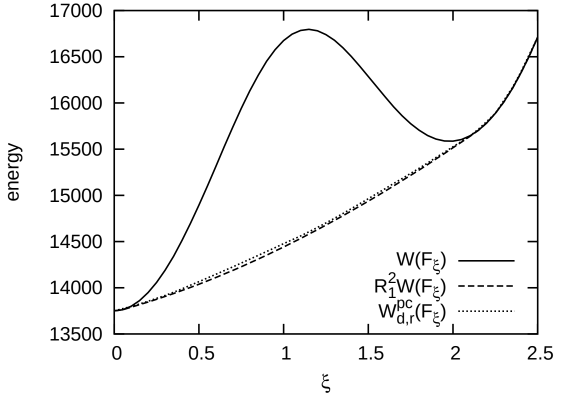
Overview

Computational Microstructures in $2D$



Scientific computing in

vector nonconvex variational problem



Concluding Remarks

A $2D$ scalar benchmark problem

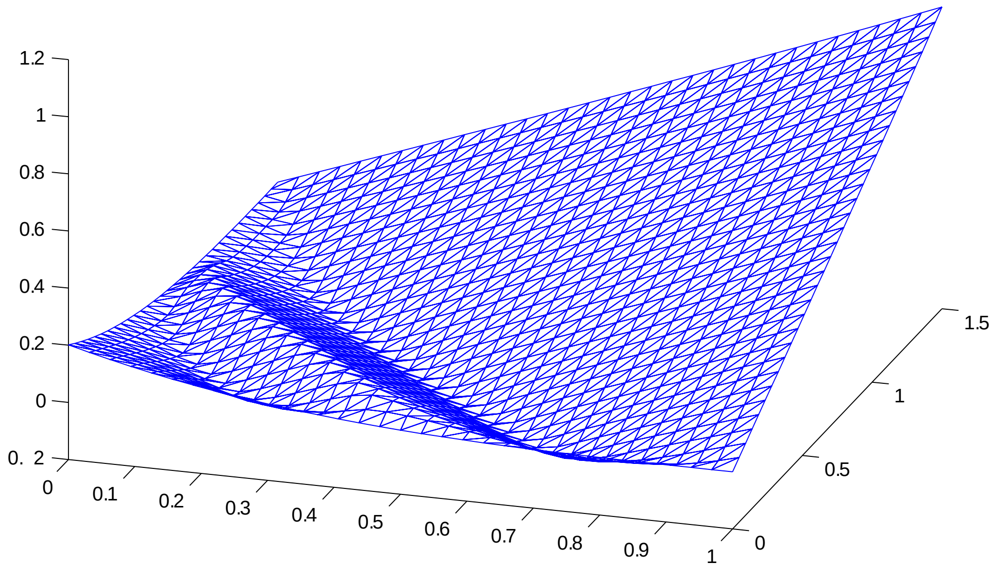
- Ericksen-James density energy in antiplane shear conditions $(m = 1, n = 2)$ motivates

$$W(F) := |F - (3,2)/\sqrt{13}|^2 |F + (3,2)/\sqrt{13}|^2$$

> (P) Minimize $E(u) := \int_\Omega W(Du)\,dx + \int_\Omega |u - f|^2\,dx$ over $u \in \mathcal{A} = u_D + W_0^{1,4}(\Omega)$
> with $\Omega = (0,1) \times (0, 3/2)$, $f(x,y) := -3t^5/128 - t^3/3$ for $t = (3(x-1) + 2y)(\sqrt{13})$

- inf $E(\mathcal{A}) < E(u)$ for all $u \in \mathcal{A}$
- All the weakly converging infimising sequences (u_j) of (P) have the same weak limit u

Finite element solution $u_h(x,y)$ for (P_h)



- Oscillations mesh sensitive
- Difficult numerics

$\Rightarrow$ Why don't we relax?

Relax FE minimization for the benchmark problem

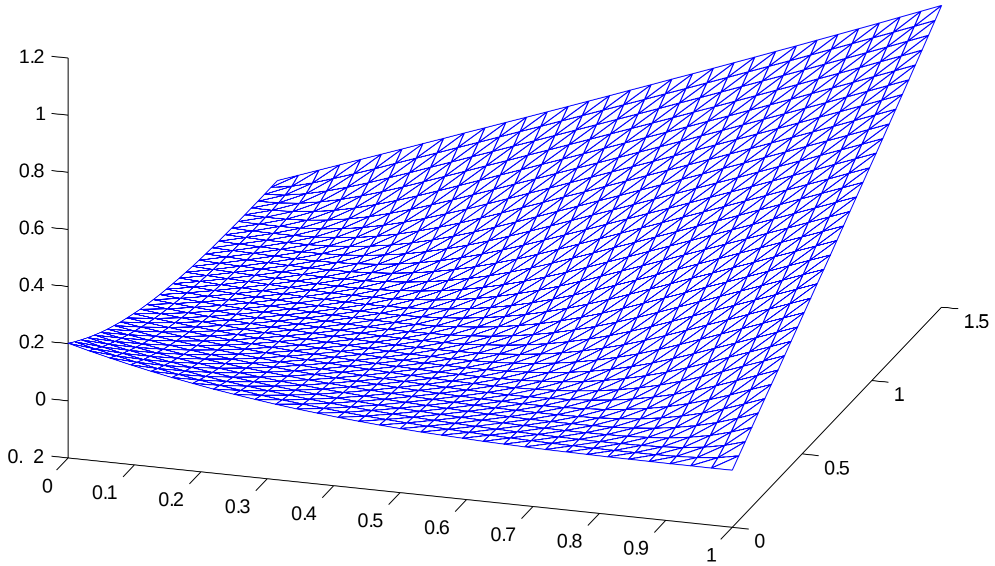
(RP) Minimize

$$RE(u) := \int_\Omega W^{**}(Du)\,dx + \int_\Omega |u-f|^2\,dx$$

with $W^{**}(F) = (((|F|^2-1)_+)^2 + 4(|F|^2 - ((3,2)\cdot F)^2/\sqrt{13})$.

- (RP) has a unique solution $u \in \mathcal{A}$ equals to the weak limit u
- $E(u_j) \to \inf E(\mathcal{A}) \Rightarrow \sigma_j := DW(Du_j) \to \sigma := DW^{**}(Du)$ in measure

Finite element solution $u_h(x,y)$ for (RP_h)



- No oscillations and interface no sharp
- Simple numerics

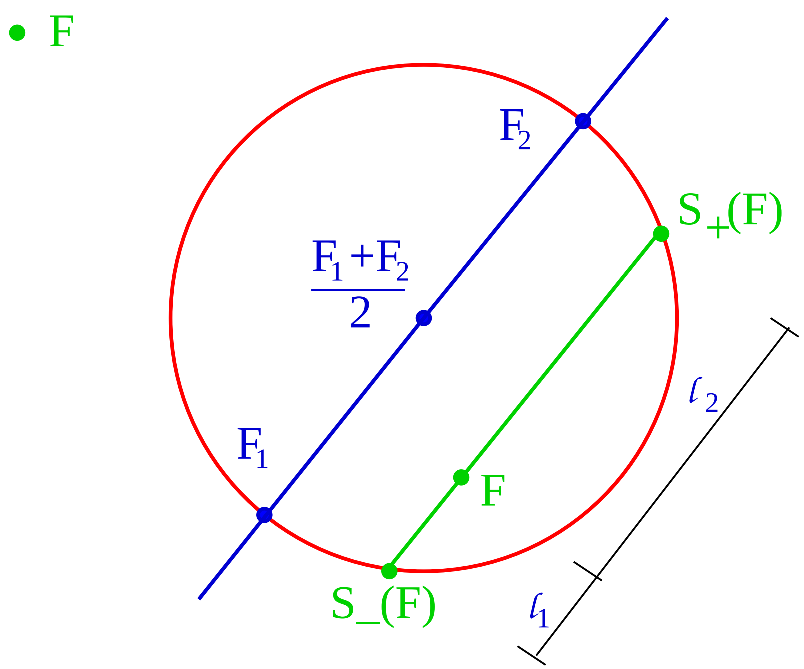
$\Rightarrow$ Where is the microstructure?

GYM for $2D$ scalar benchmark problem

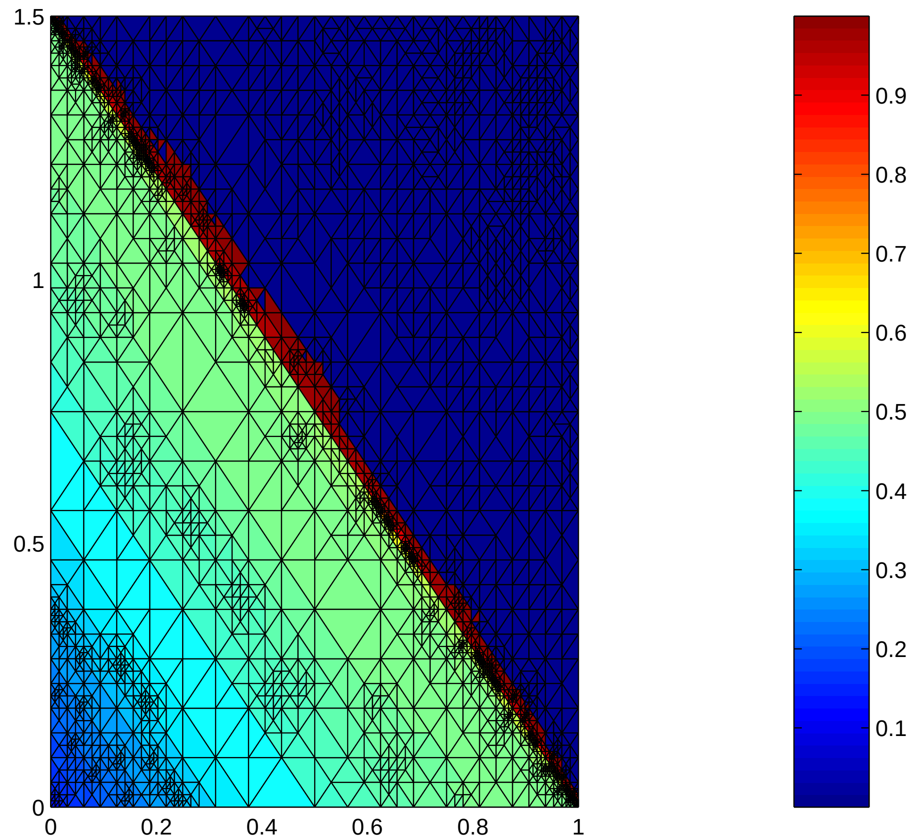
There exists a unique gradient Young measure (C & Plecháč '97)

$$\nu_x = \lambda(F)\delta_{S_+(F)} + (1-\lambda(F))\delta_{S_-(F)}$$

with $\mathbb{P} = \mathbb{I} - F_2 \otimes F_2$, $\lambda(F) = \frac{\ell_1}{\ell_1+\ell_2}$, and $S_\pm(F) = \begin{cases} \mathbb{P}F \pm F_2(1-|\mathbb{P}F|^2)^{-1/2} \text{ if } |F| \leq 1; \\ F \text{ if } 1 < |F|. \end{cases}$



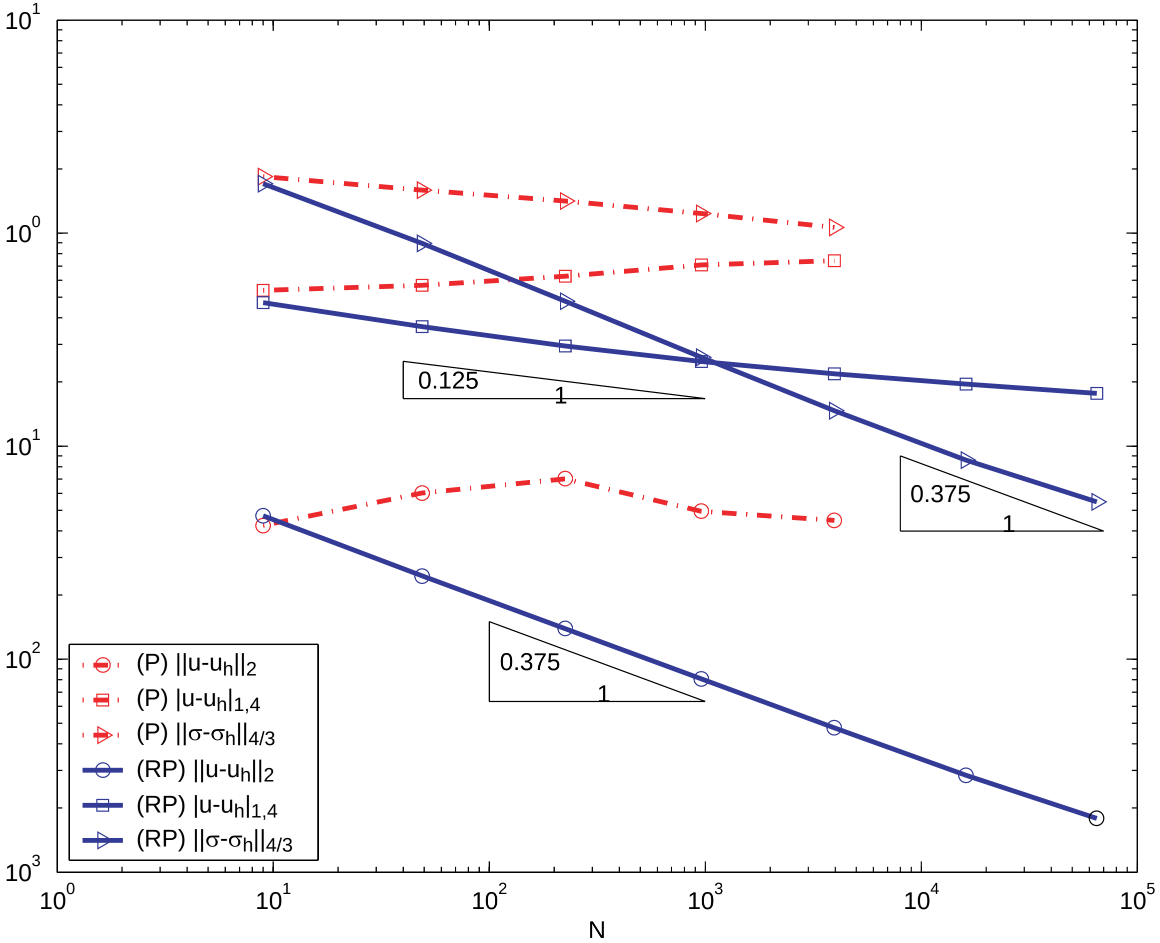
Volume fraction from u_h of (RP) on $(\mathcal{T}_{15}, N = 2485)$



Convergence rate on uniform meshes for (P) & (RP)

A priori error analysis for (RP_h)

$$\|u-u_h\|_{L^2}+\|\sigma-\sigma_h\|_{L^{4/3}} \lesssim \inf_{v_h\in\mathcal{A}_h}\|D(u-v_h)\|_{L^4(\Omega)} \lesssim |u-Iu|_{W^{1,4}(\Omega)}$$



- a priori bounds of limitate use in error control (lack of regularity for u) $\Rightarrow$ use a posteriori error estimate

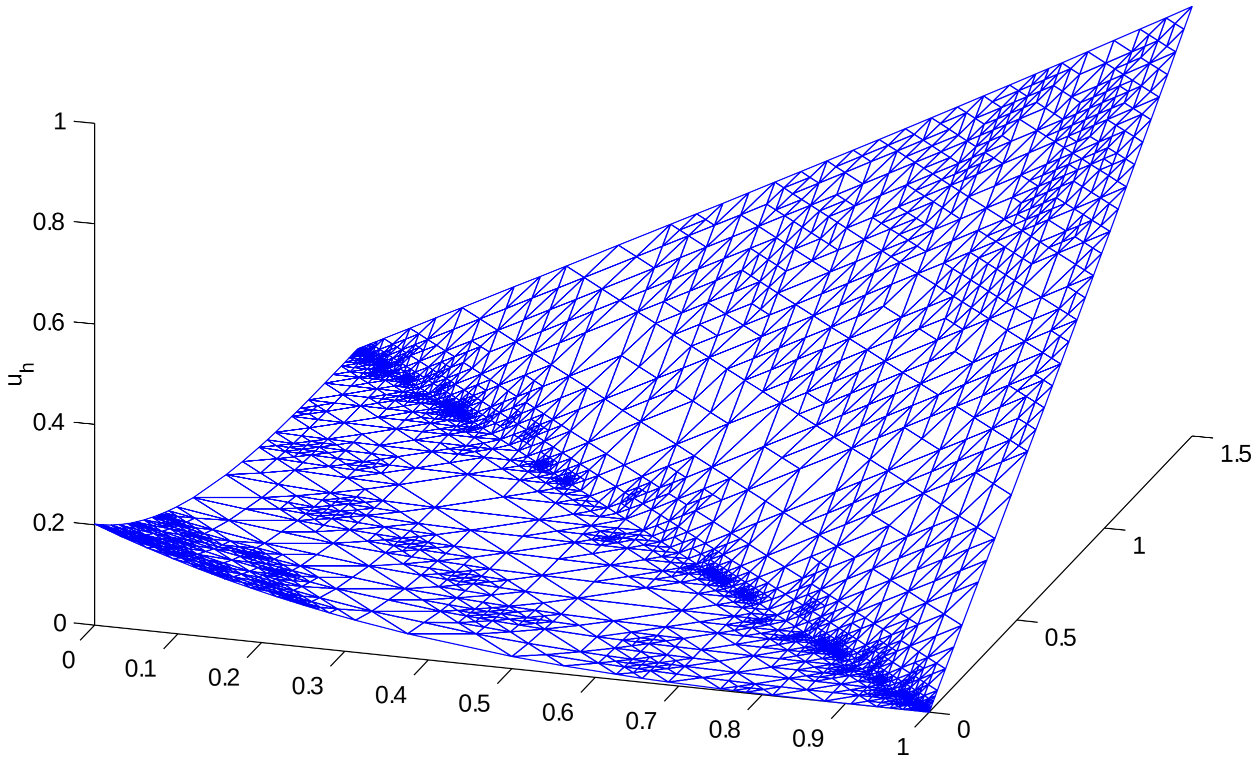
A posteriori error estimate and adaptivity for (RP)

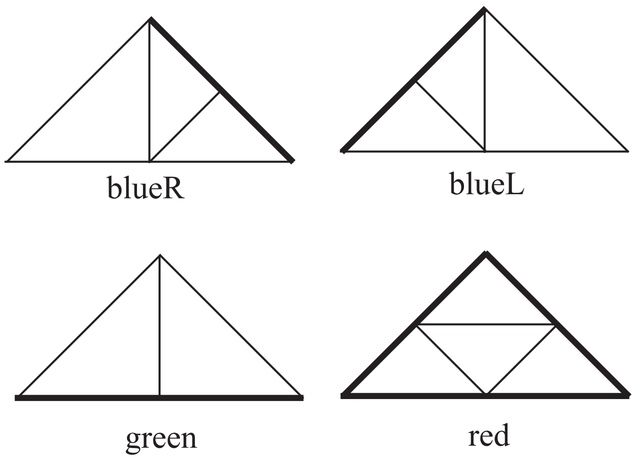
Averaging a posteriori error estimate for (RP_h)

$$\eta_M - h.o.t. \leq \|\sigma - \sigma_h\|_{L^{4/3}} \leq c\eta_M^{1/2} + h.o.t.$$

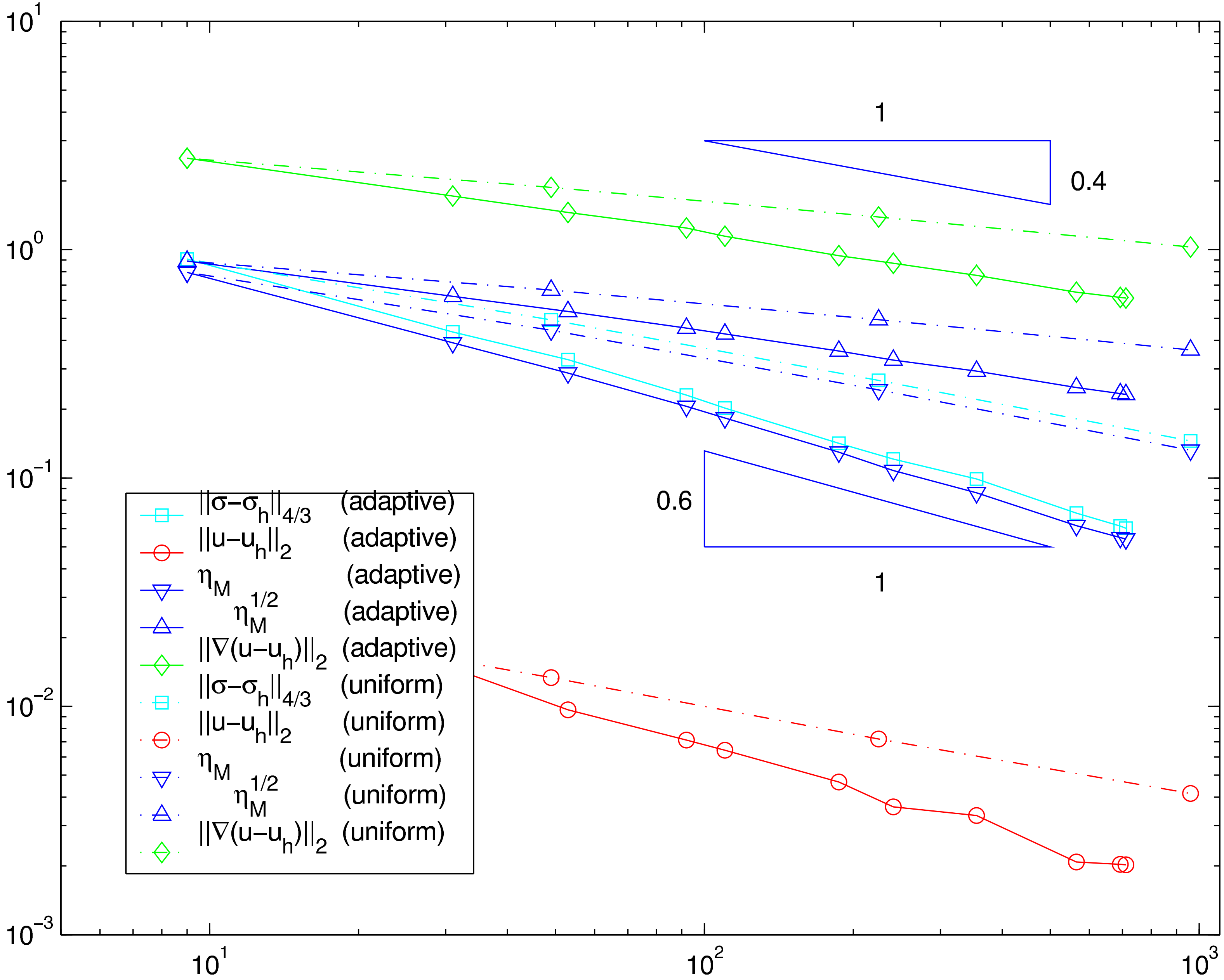
with $\eta_M = (\sum_{T\in\mathcal{T}} \eta_T^{4/3})^{3/4}$, $\eta_T = \|\sigma_h - \mathcal{A}\sigma_h\|_{L^{4/3}(T)}$, $\mathcal{A}$ averaging operator

$\Rightarrow$ Efficiency-reliability gap (C & Jochimsen '03)





Experimental Convergence Rates for (RP)



Convexification ⦶ Stabilization

- In general, $E^c(u)$ with multipla minima and D^2E^c positive semidefinite
- Need for stabilization $\Rightarrow E^c_\gamma(v) = E^c(v) + \gamma\|\nabla v\|^2_{L^2(\Omega)}$

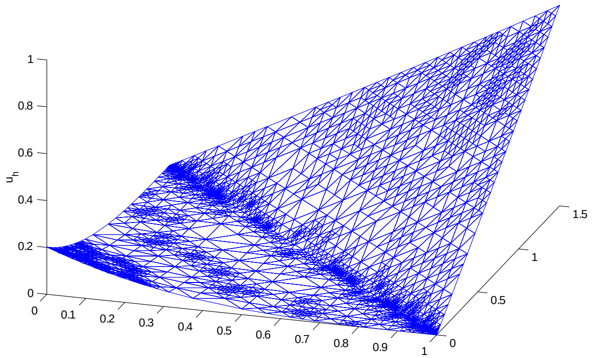
> Proof in (C et al '04) of global convergence for a damped Quasi-Newton scheme applied to the minimization of E^c_γ.

- FEs (u_h) form infimizing sequence for $E^c := \int_\Omega W^{**}(Du)\,dx + \mathcal{L}(u)$ such that

  $u_h \rightharpoonup u$ in $W^{1,p}$ with $u_h \to u$ in L^p and $Du_h \rightharpoonup Du$ in L^p
- For each $h > 0$, let u_h minimize $E^c + J_h$ over $\mathcal{A}_h$

> Proof in (B et al '04) of
>
> $$Du_h \to Du \text{ in } L^p$$
>
> for the following stabilization terms for standard low-order FEM
>
> - $J_h(v_h) = \sum_{E\in\mathcal{E}_\Omega} h_E^\gamma \int_E |[Dv_h]|^2\,ds$
> - $J_h(v_h) = \int_\Omega h_\mathcal{T}^{\gamma-1}|Dv_h - \mathcal{A}Dv_h|^2\,dx$
> - $J_h(v_h) = h^\gamma \int_\Omega |Dv_h|^2\,dx$

Computational Microstructures in $2D$



Scientific computing in

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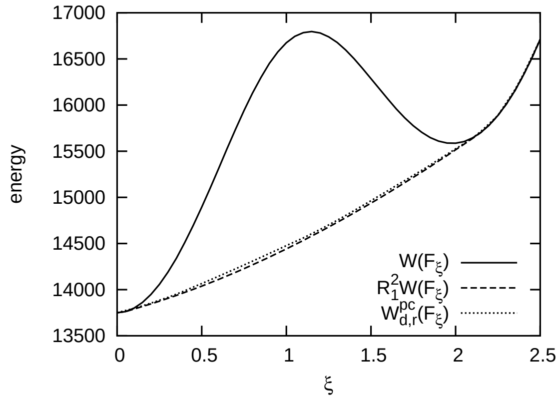


Concluding Remarks

Effective density energy: Quasiconvex envelope

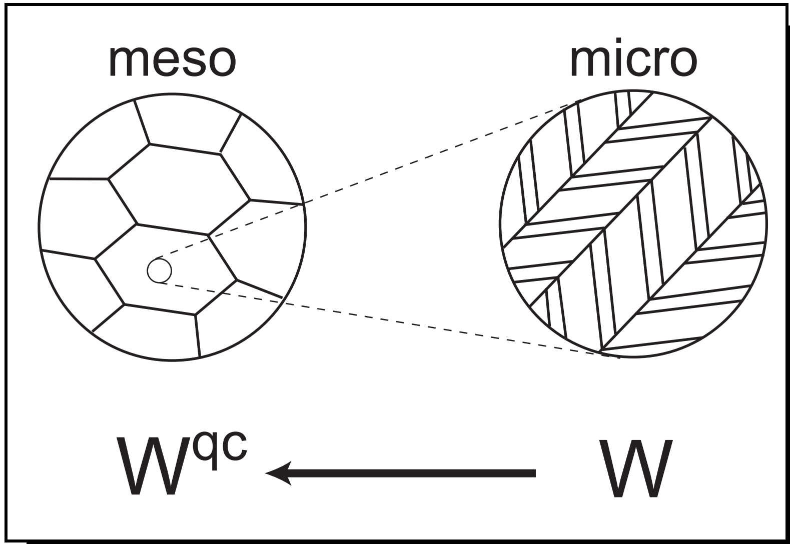
- For vector nonconvex variational problems, the relaxed formulation reads

$$\min_{u \in \mathcal{A}} \int_\Omega W^{qc}(Du(x))\,dx \quad \left(= \inf_{u \in \mathcal{A}} \int_\Omega W(Du(x))\,dx\right)$$

Quasiconvex envelope W^{qc} of W

$$W^{qc}(F) = \inf_{\substack{y \in W^{1,\infty} \\ y = Fx \text{ on } \partial\omega}} \frac{1}{|\omega|} \int_\omega W(Dy(x))\,dx$$

$\Longleftrightarrow$



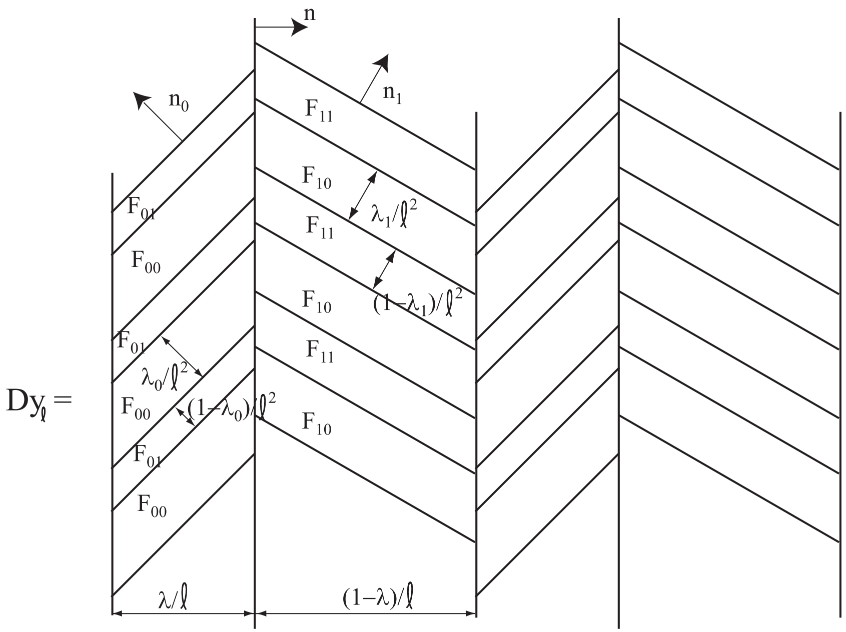
- W^{qc} known only for few energy densities W
- Simpler notions are Polyconvexity and Rank-1-convexity with

$$W^c \le W^{pc} \le W^{qc} \le W^{rc} \le W$$

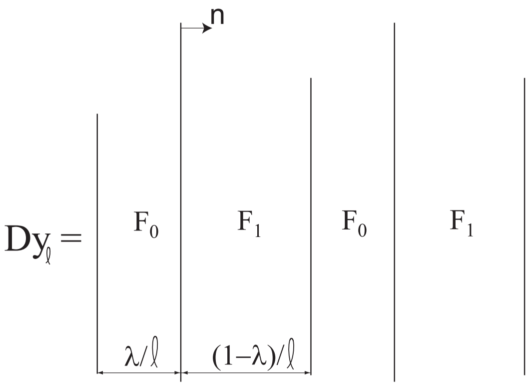
- Restrict $y = y(x)$ only to some microstructural patterns $\Rightarrow$ Laminates

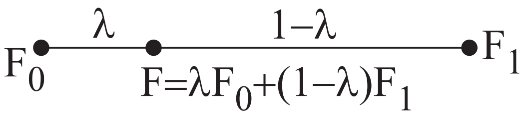
Finite laminates and microstructures

$2nd$ order laminate

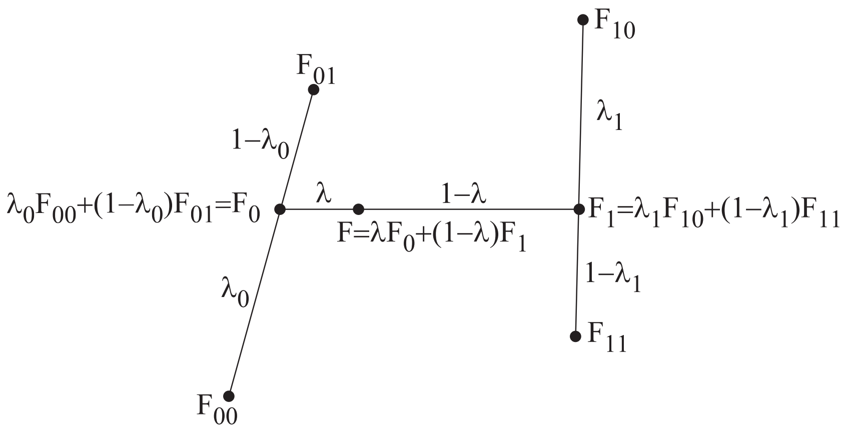


$1st$ order laminate





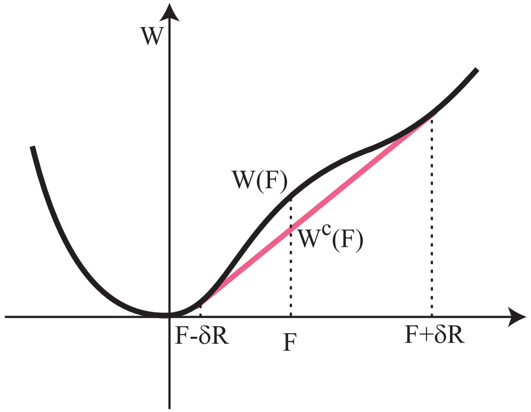
$$F_0 - F_1 = a \otimes n$$

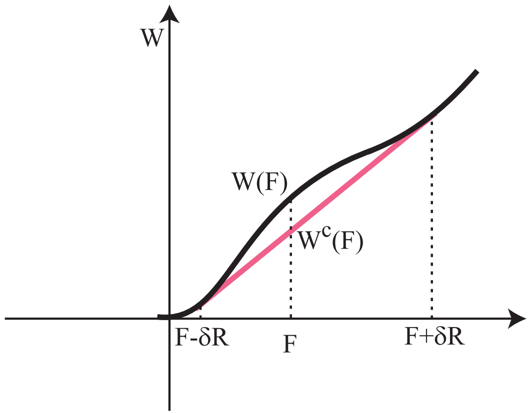


$$F_0 - F_1 = a \otimes n,\; F_{00} - F_{01} = a_0 \otimes n_0,$$

$$F_{10} - F_{11} = a_1 \otimes n_1$$

Numerical lamination: algorithm





Numerical lamination (B ’04, Dolzmann ’99)

(a) $k = 0$; $R^{(k)}W = W$

(b) $g = R^{(k)}W$.

(c) For each F, for each $a, b \in I\!R^3$, $g =$convexify $R^{(k)}W(F + ta \otimes b)$.

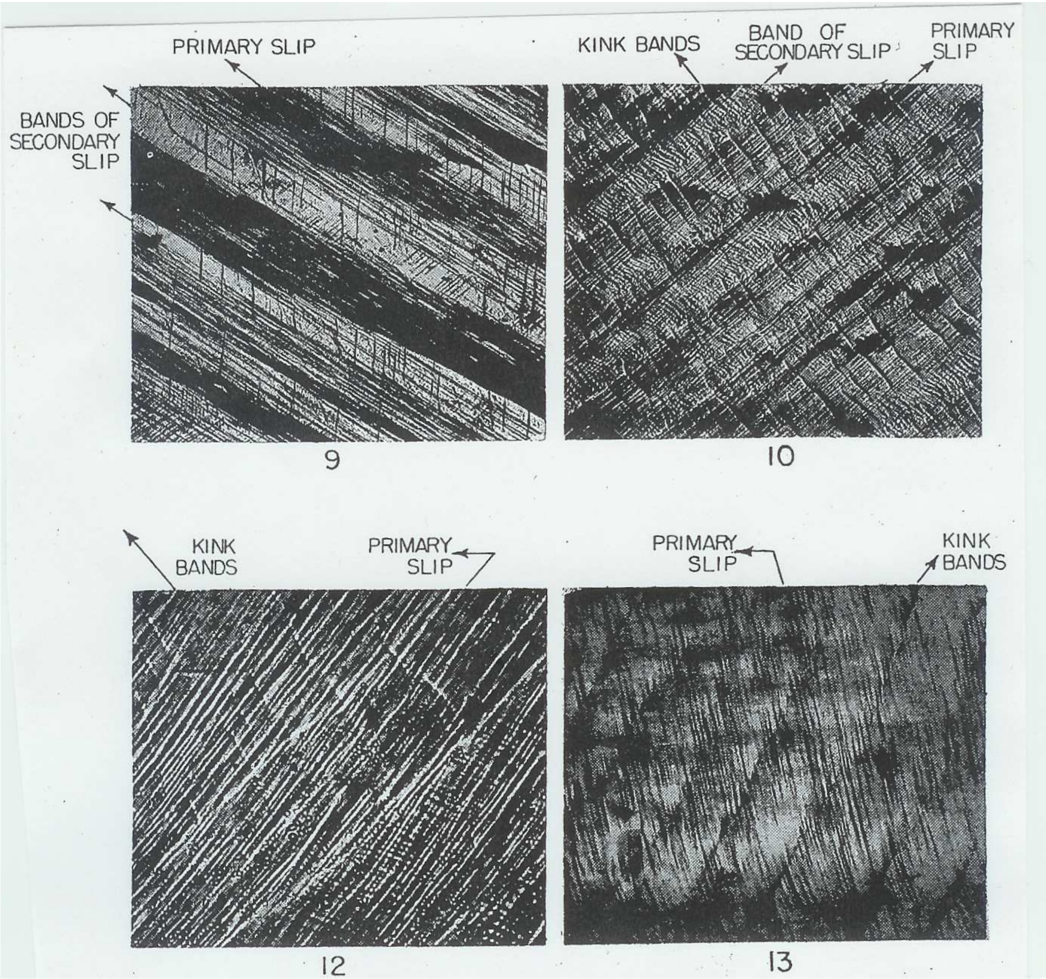
(d) $R^{(k+1)}W = g$, compare with $R^{(k)}W$ to stop, otherwise $k := k+1$ and goto (b).

- Define discrete set of matrices $\mathcal{N}_{\delta,r} = \delta\mathbb{Z}^{3\times 3} \cap \overline{B_r(0)}$
- Define discrete set of rank-one directions $\mathcal{R}^1_\delta = \left\{\delta R \in I\!R^{3\times 3} : R = a \otimes b, \text{ with } a, b \in \mathbb{Z}^3\right\}$
- Define $\ell_{R,\delta} := \{\ell \in \mathbb{Z} : F + \ell\delta R \in \overline{\text{co}\mathcal{N}_{\delta,r}}\}$

Solve $\quad R^{(k+1)}_{\delta,r}W(F) = \inf\limits_{R \in \mathcal{R}^1_\delta} \inf\limits_{\substack{\theta_\ell \in I\!R^{\#\ell_{R,\delta}} \ \theta_\ell \geq 0 \\ \sum_{\ell \in \ell_{R,\delta}} \theta_\ell = 1}} \sum_{\ell \in \ell_{R,\delta}} \theta_\ell R^{(k)}_{\delta,r} W(F + \delta\ell R)$

Convergence if: W Lipschitz, $\quad W = W^{rc}$ on $I\!R^{3\times 3} \setminus B_r(0)$, $\quad \exists\, L \in \mathbb{N} : R^{(L)}_{\delta,r}W = W^{rc}(F)$

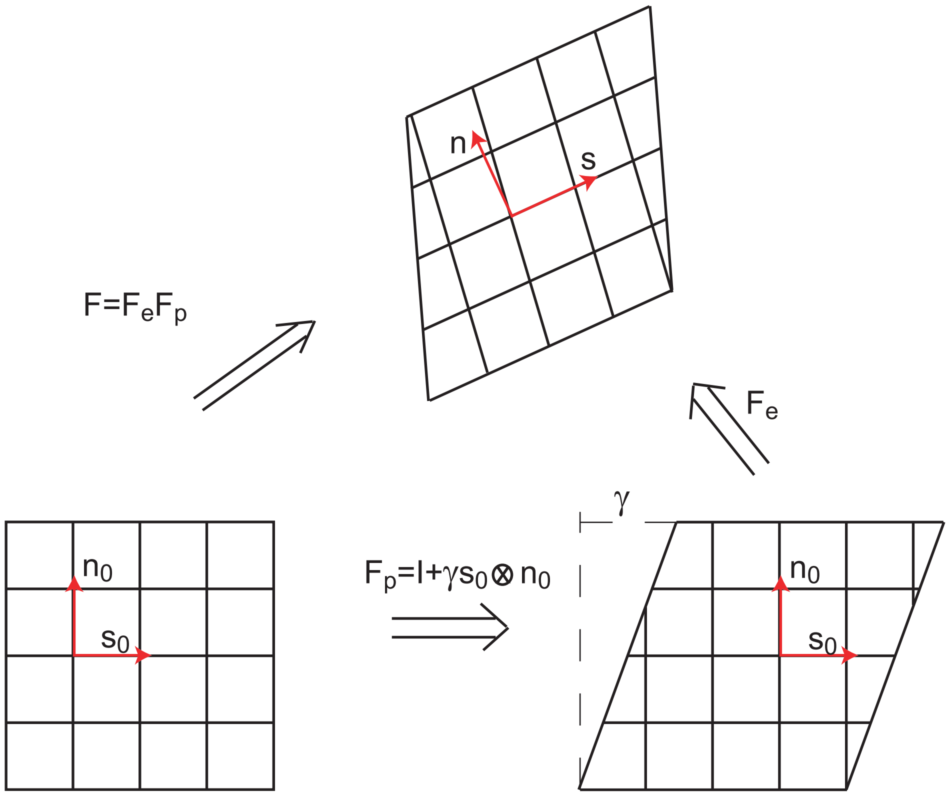
Strain hardening in FCC metal crystals (Experiments)



Optical micrographs of Al single crystal (Fig 9-10) & Au single crystal (Fig 12-13)

in a shear deformation test (Sawkill & Honeycombe)

Modeling crystal plasticity with single slip system



Constitutive modelling assumptions

$$W(F,z) = U(\text{det}F_e) + \frac{\mu}{2}\text{tr}(F_e^T F_e) + \frac{a}{2}p^2$$

$$\Delta = \begin{cases} r|\dot\gamma| & \text{if } |\dot\gamma| + \dot p \le 0 \\ \infty & \text{else} \end{cases} \quad \Rightarrow$$

$$\mathcal{D}(z_0,z_1) = \begin{cases} r|\gamma_1-\gamma_0| & \text{if } |\gamma_1-\gamma_0| \le p_0 - p_1 \\ \infty & \text{else} \end{cases}$$

a, μ, r material constants, U neo-Hookian energy

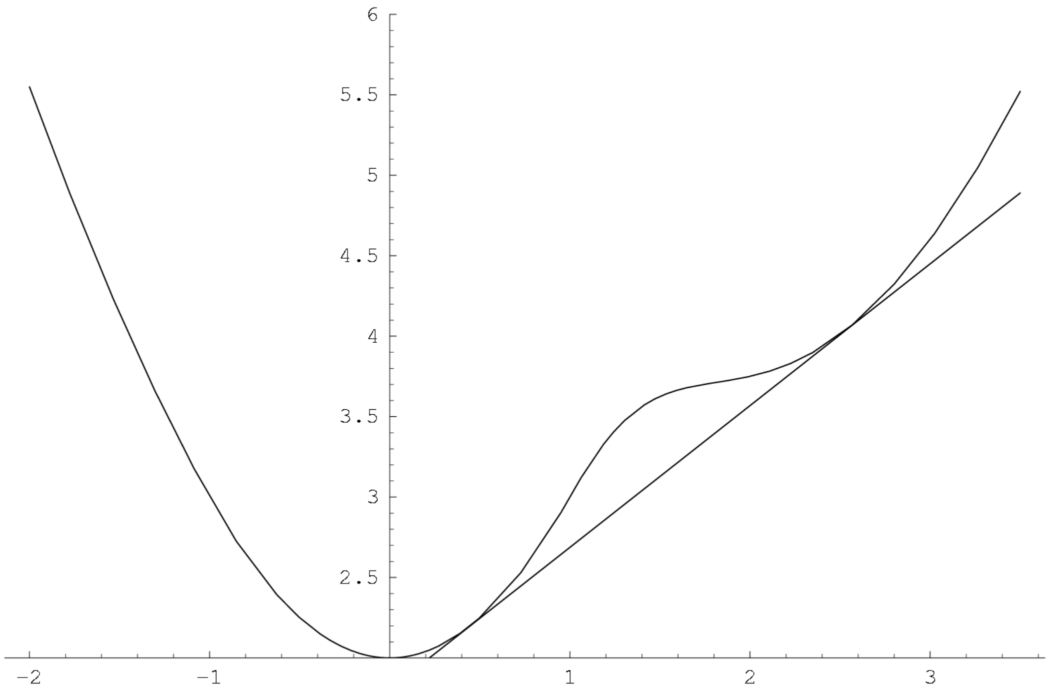
$\Rightarrow$ Closed form for $W^{red}_{\gamma_0,p_0}$ (C et al '02)

$$W^{red}_{\gamma_0,p_0}(F) = U(\text{det}F) + \frac{\mu}{2}\left(\text{tr}F^T F - 2\gamma_0 s\cdot n + \gamma_0^2 s\cdot s - \frac{\left(|s\cdot n - \gamma_0 s\cdot s| - \frac{r-ap_0}{\mu}\right)_+^2}{|s|^2 + \frac{a}{\mu}}\right)$$

Properties of $W^{red}_{\gamma_0,p_0}$

$\Rightarrow$ Examine $W^{red}_{\gamma_0,p_0}(F)$ along the family of rank-one tensors

$$F = I + \frac{1}{2}\alpha(s_0 + n_0) \otimes (n_0 - s_0)$$



$W^{red}(\alpha)$ for $\mu = 2, a = 0, r = 1, z_0 = 0$

$W^{red}(\alpha)$ is not convex $\Rightarrow$ $W^{red}(F)$ is not rank-one convex

$\Rightarrow$ $W^{red}(F)$ is not quasiconvex $\Rightarrow$ microstrctures as minimizers of the energy

Numerical lamination for single-slip elastoplasticity

For $W^{red}_{\gamma_0,p_0}(F)$ the relaxation over the first order laminates is:

$$R^{(1)}W^{red}_{\gamma_0,p_0}(F;z) = \inf_z \{(1-\lambda)W^{red}_{\gamma_0,p_0}(F-\lambda a\otimes n) + \lambda W^{red}_{\gamma_0,p_0}(F+(1-\lambda)a\otimes n)\}$$

with $a = \rho(\cos\alpha,\ \sin\alpha)$, $n = (\cos\beta,\ \sin\beta)$, and $z = (\lambda, \rho, \alpha, \beta)$

Clustering algorithm (C et al. '04)

Input F, initial starting points (z_i), tolerance

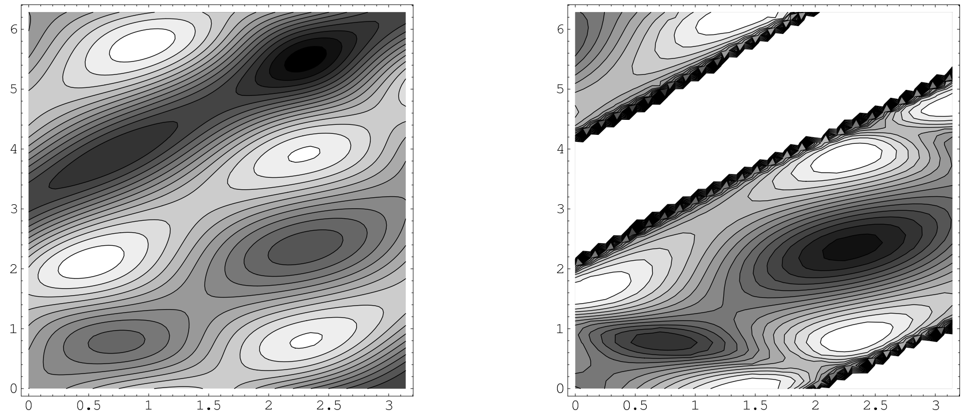
(a) Sampling and reduction

(b) Clustering

(c) Center of attraction

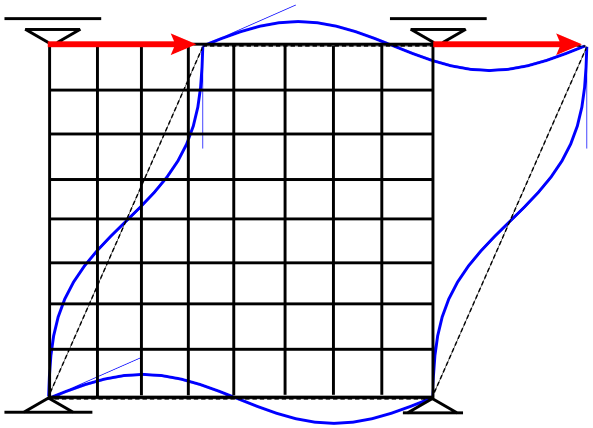
(d) Local search

Output the value of $R^{(1)}W^{red}_{\gamma_0,p_0}(F)$.



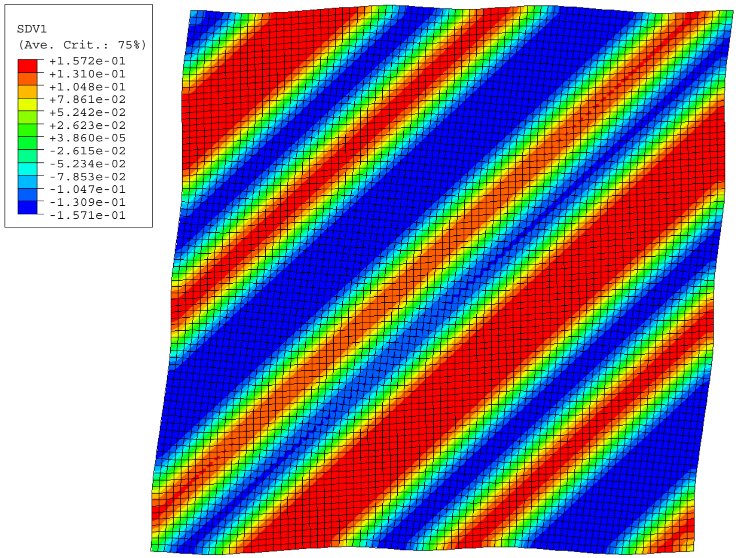
Multiple minima (white) of $R^{(1)}W^{red}_{\gamma_0,p_0}(z)$ projected on the plane $\alpha-\beta$. Left: $\lambda = 0.1\ \rho = 0.6$. Right: $\lambda = 0.1\ \rho = 2.1$.

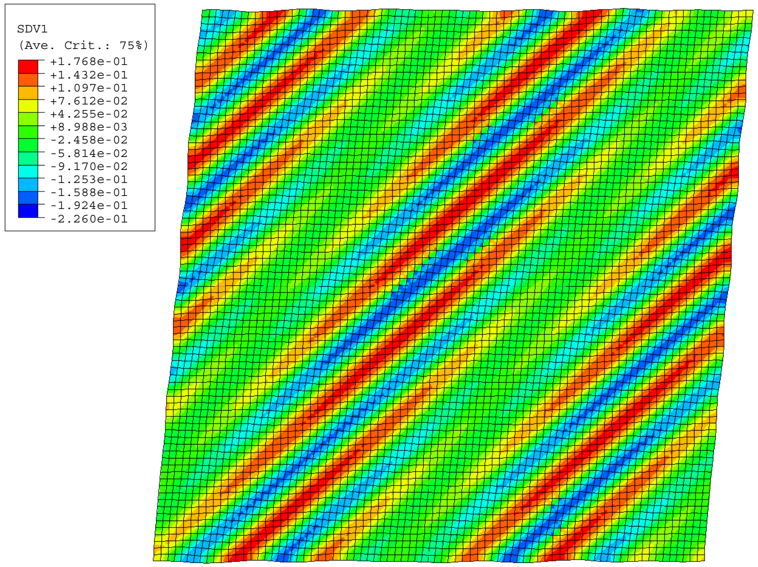
Numerical Example



Plane strain elements
Periodic BCs

Minimize $\int_\Omega R^{(k)} W(Du)\,dx$ over $\mathcal{A}$





$\Rightarrow$ Orientation not sensitive to FE mesh

$\Rightarrow$ Volume fractions not sensitive to FE mesh

A sufficient condition for quasiconvexity: polyconvexity

$$T : F \in I\!R^{3\times 3} \to T(F) = (F, \mathrm{cof}F, \det F) \in I\!R^{3\times 3} \times I\!R^{3\times 3} \times I\!R,$$

$$g : I\!R^{3\times 3} \times I\!R^{3\times 3} \times I\!R \to I\!R \text{ convex}$$

W polyconvex if $W(F) = g(T(F))$ for each $F \in I\!R^{3\times 3}$

Polyconvex envelope of W

$$W^{pc}(F) = \inf_{\substack{A_i \in I\!R^{3\times 3} \\ \lambda_i \in I\!R}} \{\sum_{i=1}^{19} \lambda_i W(A_i) \,:\, \lambda_i \geq 0, \sum_{i=1}^{19} \lambda_i = 1, \sum_{i=1}^{19} \lambda_i T(A_i) = T(F)\}$$

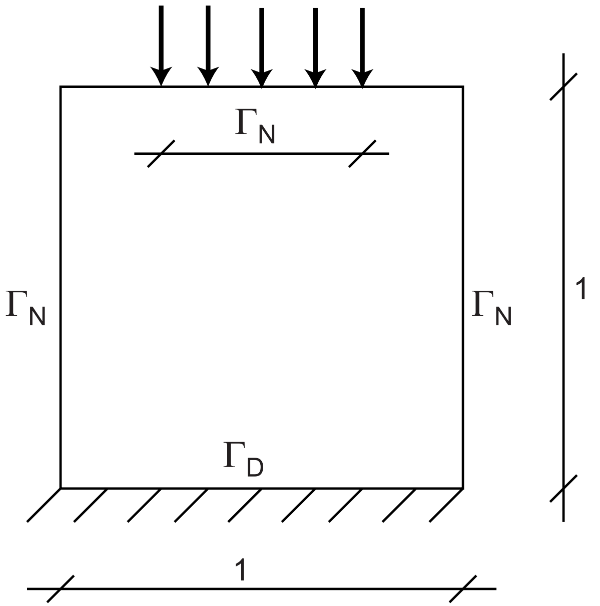
Numerical Polyconvexification (Roubíček '96, B '04)

$$W^{pc}_{\delta,r}(F) = \inf_{\theta_A \in I\!R^{\#\mathcal{N}_{\delta,r}}} \{ \sum_{A \in \mathcal{N}_{\delta,r}} \theta_A W(A) \,:\, \theta_A \geq 0, \sum \theta_A = 1, \sum_{A \in \mathcal{N}_{\delta,r}} \theta_A T(A) = T(F)\}$$

$W \in C^{1,\alpha}_{loc}(I\!R^{3\times 3})$ with $\alpha \in (0,1] \Rightarrow W^{pc}_{\delta,r}(F) \to W^{pc}(F)$ as $\delta \to 0$

$\lambda^F_{\delta,r} \in I\!R^{19}$ Lagrangian multiplier, $\quad \lambda^F_{\delta,r} \circ DT(F) \to \sigma := DW^{pc}(F)$

Numerical Example: Ericksen-James energy density



$$W = k_1(\mathrm{Tr}C-\alpha-\beta)^2+k_2C_{12}+k_3(C_{11}-\alpha)^2(C_{22}-\alpha)^2$$

W no rank-1 convex $\Rightarrow$ W no quasiconvex

Minimize $\int_\Omega W^{pc}_{\delta,r}(Du)\,dx + \int_{\Gamma_N} f u\,dx$ over $\mathcal{A}$

Steepest descent method

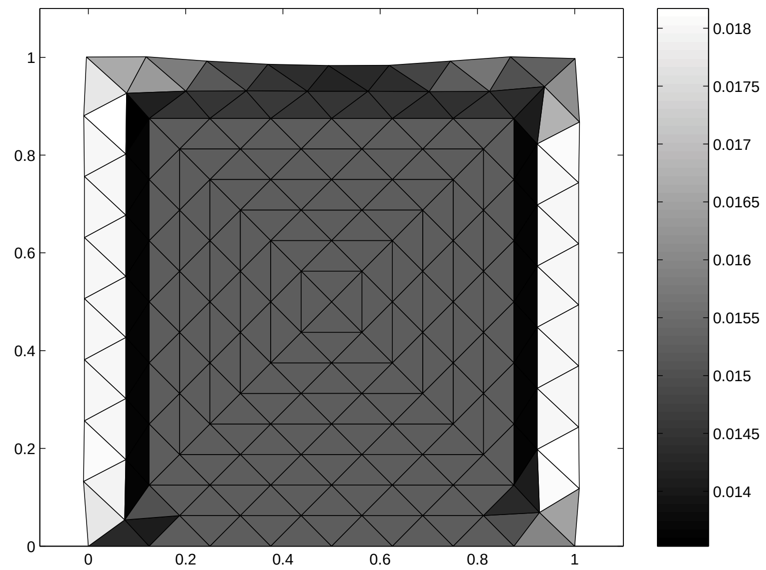
Input $u_h^{(0)}$; ε; δ; set $j=0$.

(a) Evaluate $\langle g_h^{(j)}, v_h\rangle = \int_\Omega \sigma_h^{(j)} \cdot Dv_h\,dx + \mathcal{L}(v_h)$

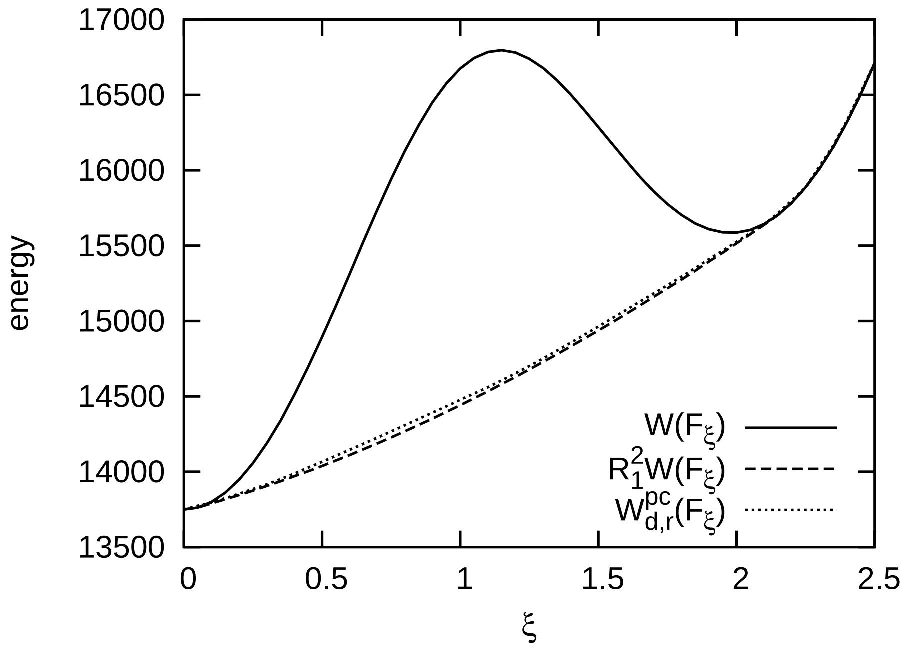
(b) If $\|g_h^{(j)}\| \le \varepsilon$ stop else set $r_h^{(j)} = g_h^{(j)}$.

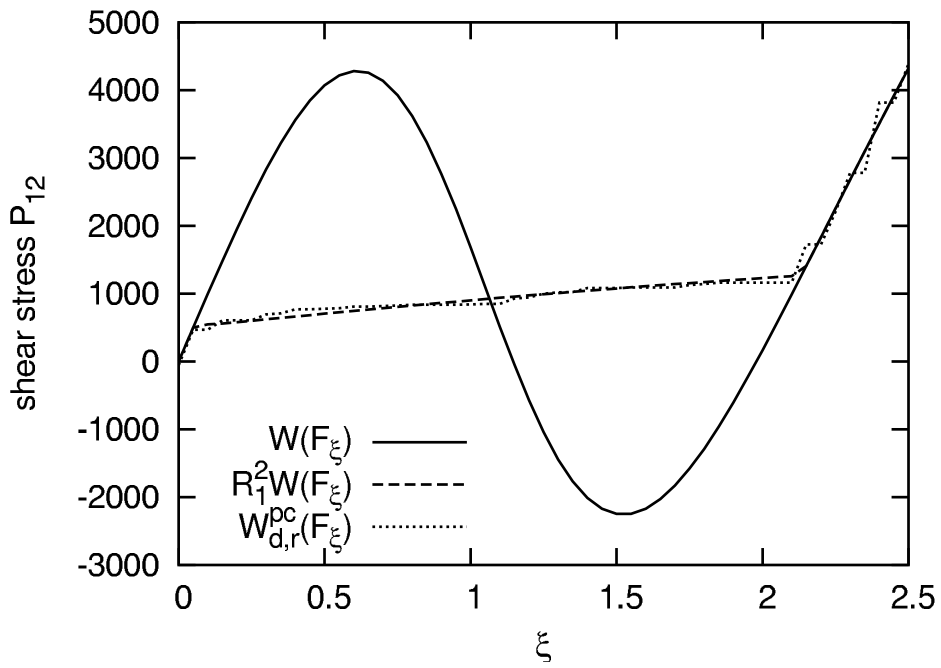
(d) Compute $t_j \,:\, E^{pc}_\delta(u_h^{(j)} + t_j r_h^{(j)}) < E^{pc}_\delta(u_h^{(j)})$

(e) Set $u_h^{(j+1)} = u_h^{(j)} + t_j r_h^{(j)}$; $j = j+1$ and goto (a).

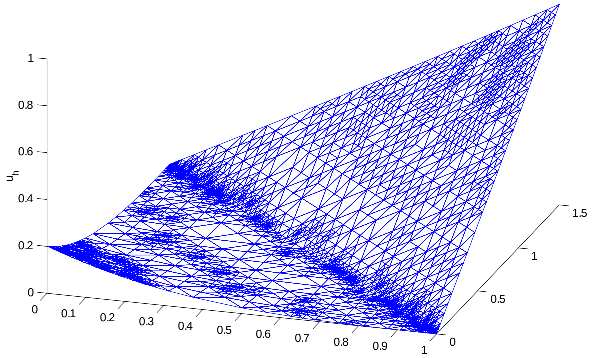


Numerical relaxation for the single-slip elastoplasticity



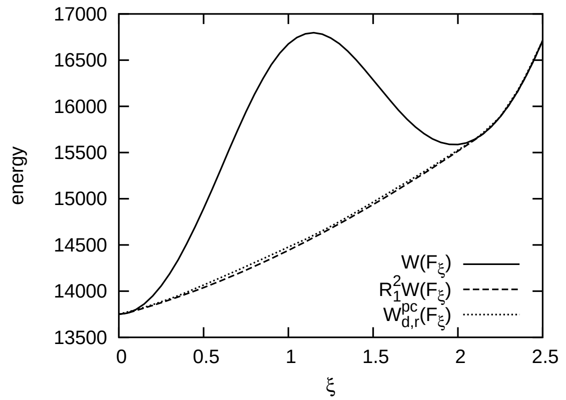


Computational Microstructures in $2D$



Scientific computing in

vector nonconvex variational problem



Concluding Remarks

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Open Tasks:

- Numerical Quasiconvexification. A computational challenge: Compute W^{qc}

- Computational microstructure: Efficient algorithms for efficient numerical relaxation

- Error analysis for vector nonconvex minimisation problems still in their infancy

(C & Dolzmann ’04) establish a priori error estimate for finite element discretizations in nonlinear elasticity for polyconvex materials under small loads

- How to model surface energy in crystal plasticity?

(Ortiz & Repetto ’99, Conti & Ortiz ’04) introduce a dislocation line energy and for latent hardening show competition between different contributions with different energy scaling

- How to analyse evolution of microstructures in finite strain elastoplasticity?