Effective density energy: Quasiconvex envelope

- For vector nonconvex variational problems

quasiconvexity of $W(x, u, Du) \Leftrightarrow$ seq. w.l.s.c. of $E(u) = \int_\Omega W(Du(x))\,dx$

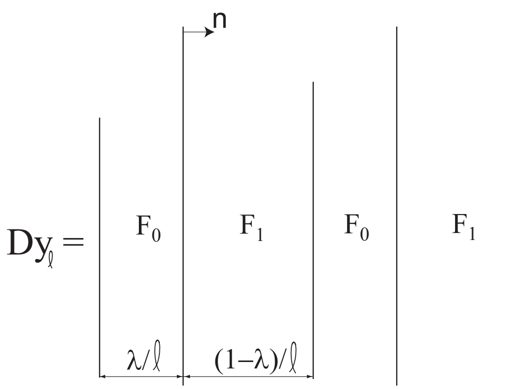
- Quasiconvex envelope

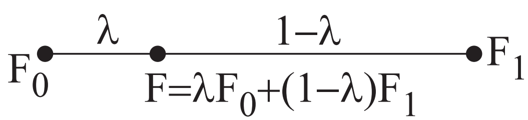
$$W^{qc}(F) = \inf_{\substack{y \in W^{1,\infty} \\ y = Fx \text{ on } \partial\omega}} \frac{1}{|\omega|} \int_\omega W(Dy(x))\,dx$$

- Quasiconvex envelope known only for few energy densities
- Restrict $y = y(x)$ only to some microstructural patterns $\Rightarrow$ Laminates

Finite laminates and microstructures

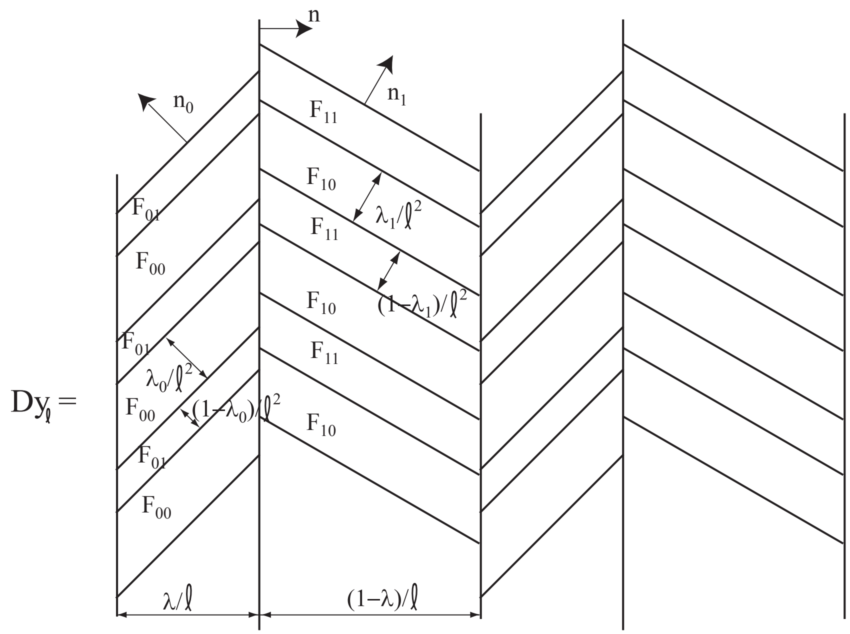
$1st$ order laminate

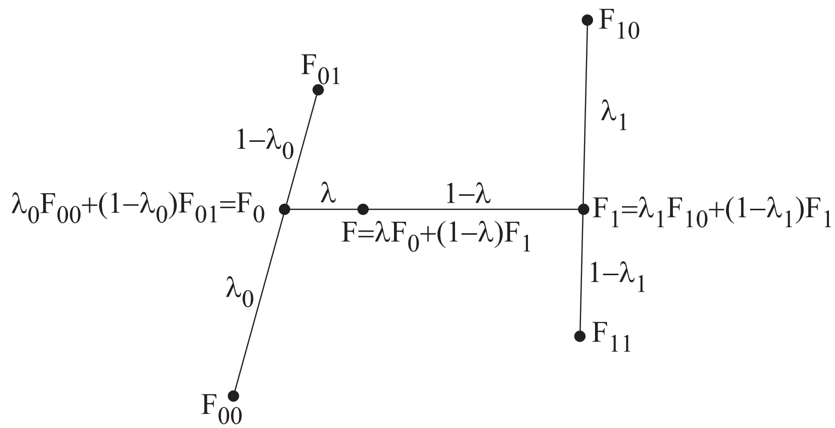




$$F_0 - F_1 = a \otimes n$$

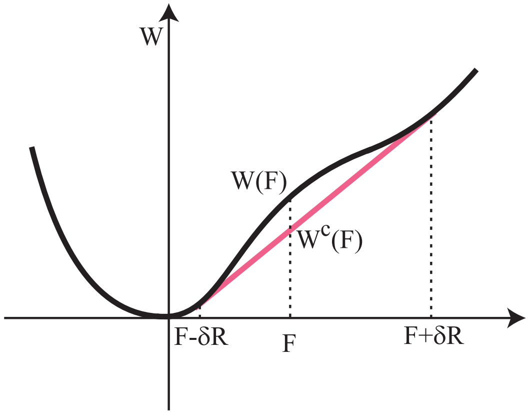
$2nd$ order laminate

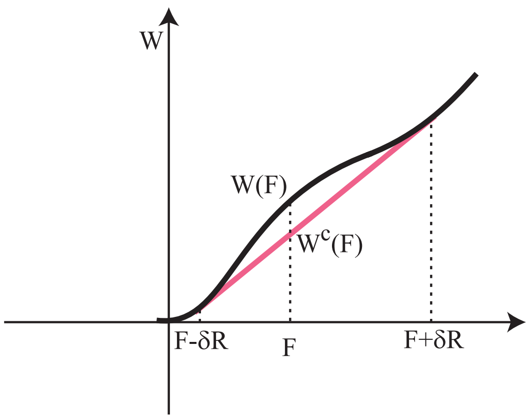




$$F_0 - F_1 = a \otimes n,\ F_{00} - F_{01} = a_0 \otimes n_0,$$
$$F_{10} - F_{11} = a_1 \otimes n_1$$

Numerical lamination: algorithm





Algorithm 2 (Numerical lamination) *[Bartels 04, Dolzmann 99]*

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

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

(c) $R^{(k+1)}W = g$, *compare with* $R^{(k)}W$ *to stop, else* $k = k+1 \longrightarrow$*(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
  $\mathcal{R}^1_\delta = \{\delta R \in \mathbb{R}^{3\times 3} : R = a \otimes b, \text{ with } a, b \in \mathbb{Z}^3\}$
- Define $\ell_{R,\delta} := \{\ell \in \mathbb{Z} : F + \ell\delta R \in \overline{\text{co}\mathcal{N}_{\delta,r}}\}$

Solve

$$R^{(k+1)}_{\delta,r}W(F) = \inf_{R \in \mathcal{R}^1_\delta} \inf_{\theta \in \mathbb{R}^{\#\ell_{R,\delta}}} \Big\{ \sum_{\ell \in \ell_{R,\delta}} \theta_\ell R^{(k)}_{\delta,r} W(F + \delta\ell R) \,:\, \theta_\ell \geq 0, \sum_{\ell \in \ell_{R,\delta}} \theta_\ell = 1 \Big\}$$

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

Numerical Example: Single-slip elastoplasticity

Kinematic assumption: $F = F_e F_p,\ F_p = I + \gamma s_0 \otimes q_0,\ s = F s_0,\ q = F q_0$

Reduced density energy [C, Hackl & Mielke 02]:

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

$$R^{(1)} W^{red}_{\gamma_0, p_0}(x, F) = \text{inf}\{(1-\lambda) W^{red}_{\gamma_0, p_0}(F - \lambda a \otimes n) + \lambda W^{red}_{\gamma_0, p_0}(F + (1-\lambda) a \otimes n)\}$$

$$a = \rho(\text{cos}\alpha,\ \text{sin}\alpha),\ n = (\text{cos}\beta,\ \text{sin}\beta)$$

$$x = (\lambda, \rho, \alpha, \beta)$$

Algorithm 3 (Clustering method) *[Neumaier 04]*

Input F, initial starting points, tolerance

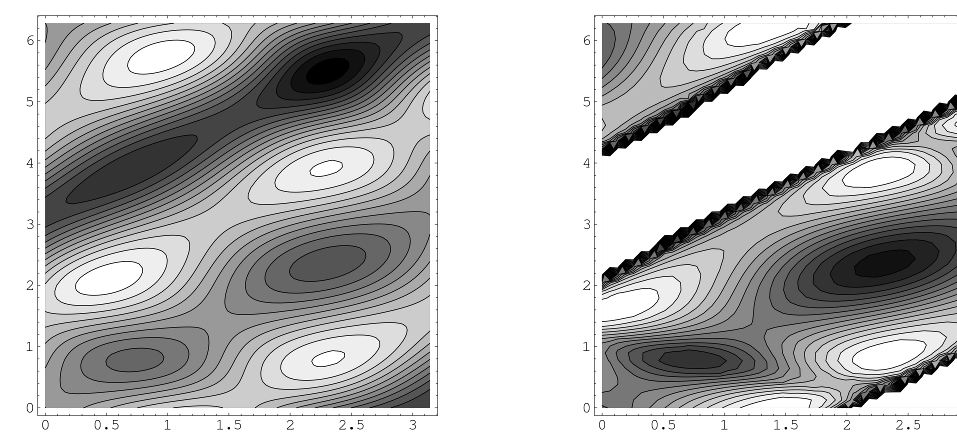
(a) Sampling and reduction

(b) Clustering

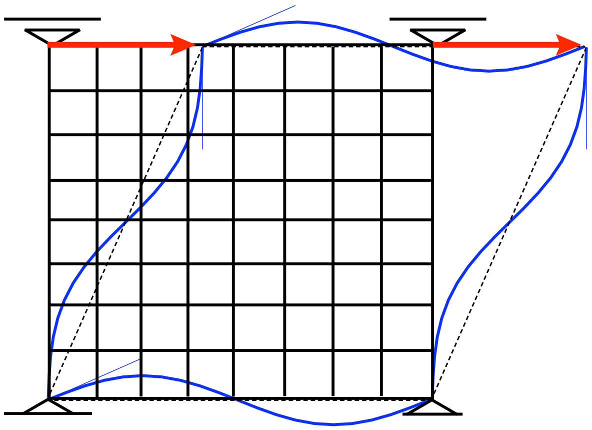
(c) Center of attraction

(d) Local search

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

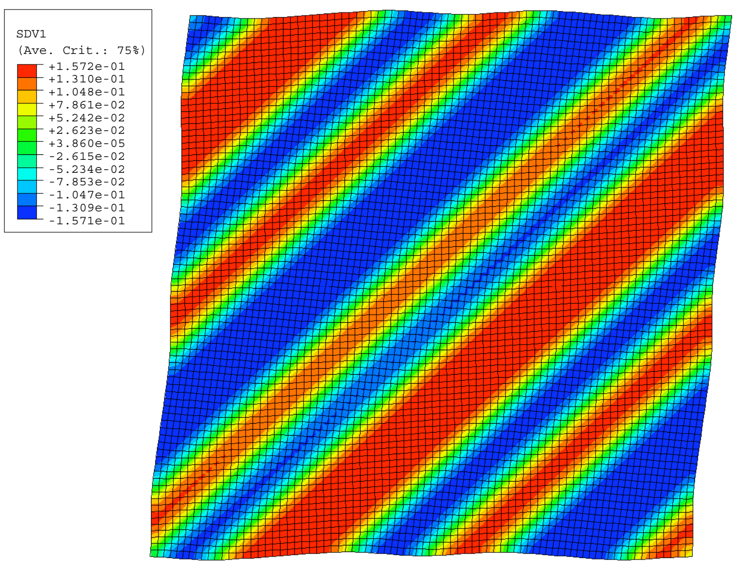


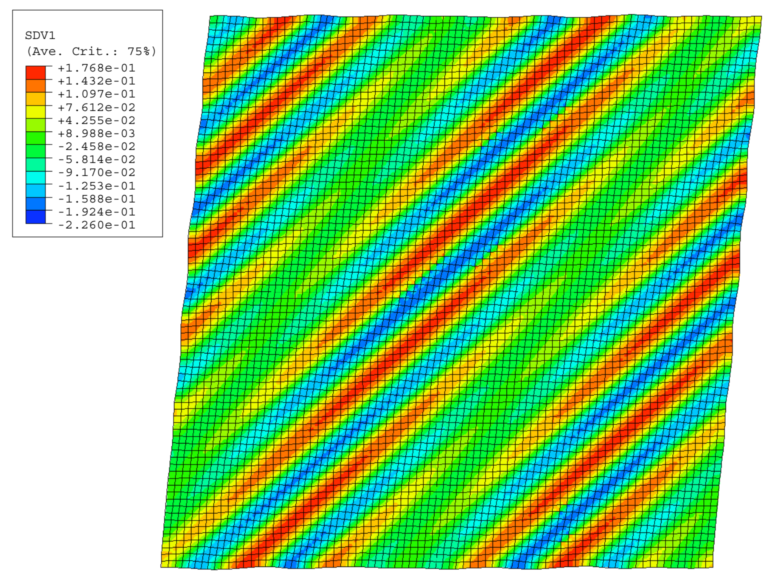
Numerical Example: Single-slip elastoplasticity



Plane strain elements
Periodic BCs

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





- Orientation not sensitive to FE mesh
- Volume fractions not sensitive to FE mesh

A sufficient condition for quasiconvexity: polyconvexity

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

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

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

Polyconvex envelope of W

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

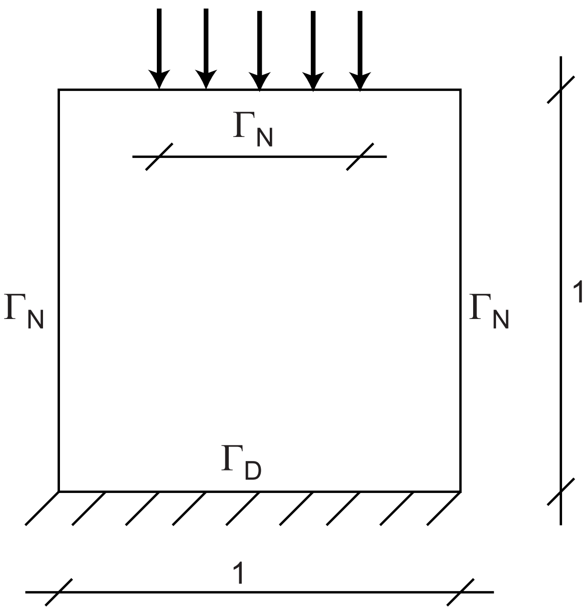
Numerical Polyconvexification[Roubíček 96, Bartels 04]

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

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

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

Numerical Example: Ericksen-James energy density



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

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 $\mathcal{A}$

Algorithm 4 (Steepest descent method)

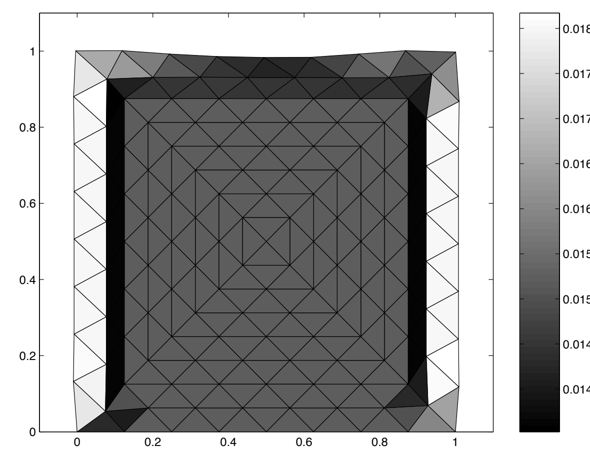
Input $u_h^{(0)}$; ε; δ; *set* $j=0$.

(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 $t_j \;:\; E_\delta^{pc}(u_h^{(j)} + t_j r_h^{(j)}) < E_\delta^{pc}(u_h^{(j)})$

(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