Upscaling and spatial localization of non-local energies with applications to crystal plasticity

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Structured deformations

First order (Del Piero, Owen)

The model sets a basis to address problems in non-classical deformations of continua (for instance, study of equilibrium configurations of crystals with defects) where an analysis at macroscopic and microscopic levels is required, dividing the study of deformations in two parts: the part arising from smooth changes and the part due to slips and separations (disarrangements) at smaller length scales.

- $$\text{StD pair}(g, G)$$

  with $f_n \xrightarrow{L^\infty} g$, $\nabla f_n \xrightarrow{L^\infty} G$, and with f_n injective.

- g accounts for the *macroscopic change in geometry*.

$$M := \nabla g - G$$

is attained through *slips* and *separations* (disarrangements) that take place at a smaller length scale.

Structured deformations

More precisely:

1. Simple deformations are pairs (K, g) where $K \subset \Omega$ consists of a finite union of Lipschitz sets of Hausdorff dimension $N-1$ and $g\lfloor\Omega\backslash K$ is a one-to-one differentiable function.
2. A triple (K, g, G) is a limit of simple deformations if $K \subset \Omega, g \in L^\infty(\Omega; \mathbb{R}^N)$ and $G \in L^\infty(\Omega; \mathbb{R}^{N\times N})$ and there exists a sequence of simple deformations (K_n, f_n) such that $K := \cup_{p=1}^{\infty} \cap_{n=p}^{\infty} K_n,\ f_n \xrightarrow{L^\infty} g,\ \nabla f_n \xrightarrow{L^\infty} G.$
3. A triple (K, g, G) is a structured deformation if (K, g) is a simple deformation, $G : \Omega\backslash K \to \mathbb{R}^{N\times N}$ is continuous and there exists $m > 0$ such that, for all $x \in \Omega\backslash K,\ m < \det G(x) \leq \det \nabla g(x).$
4. Approximation Theorem: there exists f_n injective and piecewise smooth such that $f_n \xrightarrow{L^\infty} g$, $\nabla f_n \overset{L^\infty}{\rightharpoonup} G$, $K = \cup_{n=1}^{\infty} \cap_{p=n}^{\infty} K_p.$

Example *Deck of cards*

$$N = 2,\ \Omega = (0,1)^2,$$

$$g(x_1, x_2) = (x_1 + x_2, x_2),\ \text{(simple shear)}\ G = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

$$f_n(x) = (x_1 + \frac{k}{n}, x_2),\ \frac{k}{n} \leq x_2 < \frac{k+1}{n},\ k = 0, \ldots n-1$$

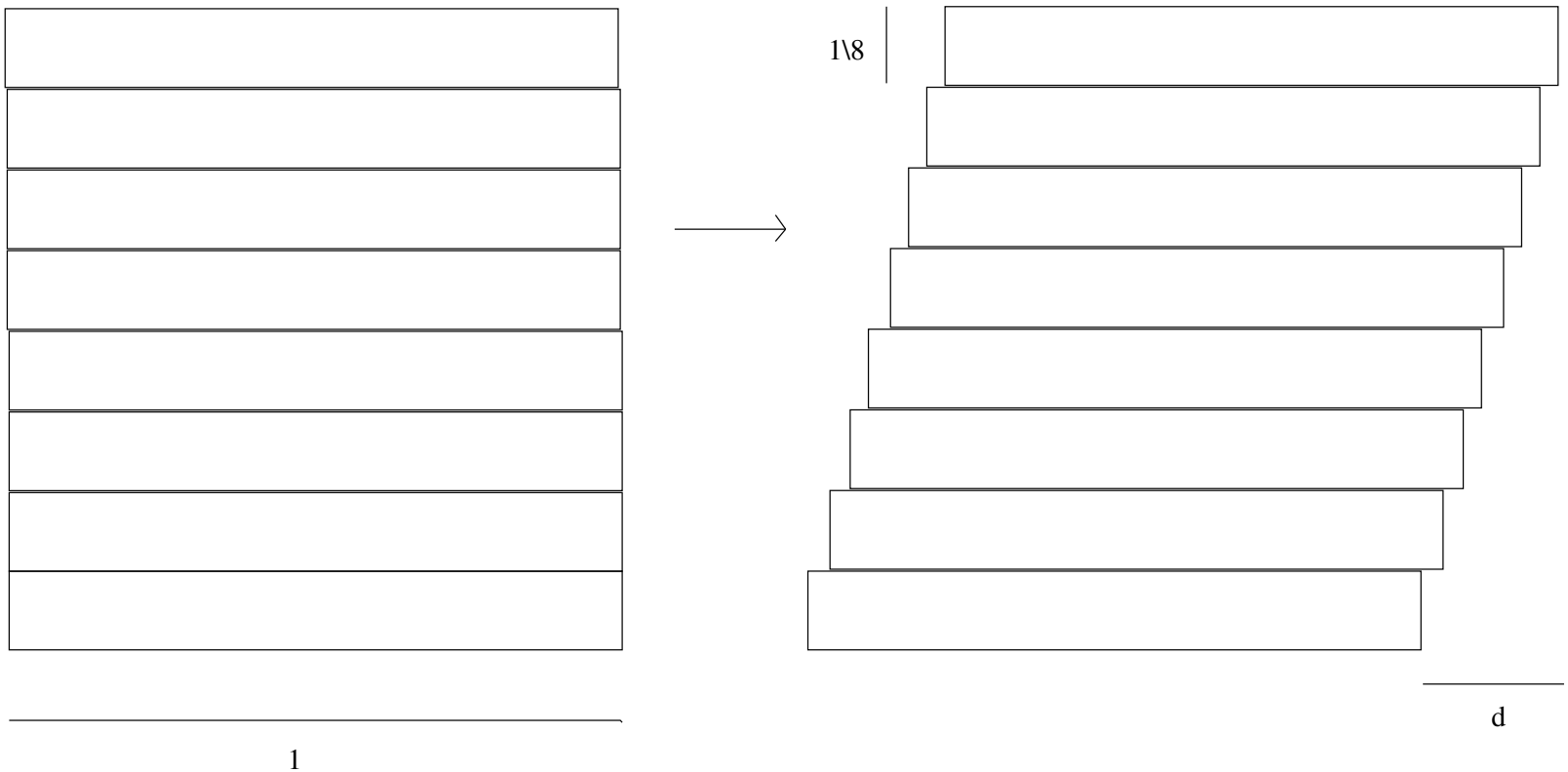
$$f_n \xrightarrow{L^\infty} g,\ \nabla f_n \xrightarrow{L^\infty} G,\ Df_n \rightharpoonup \nabla g = \begin{bmatrix} 1 & 1 \\ 0 & 1 \end{bmatrix}$$

$$M = \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix}$$

Example

Deck of cards

f_8



Structured Deformations (Choksi & Fonseca) by means of BV-SBV spaces

- A function $u \in L^1(\Omega;\mathbb{R}^d)$ $(d \geq 1)$ is of bounded variation, i.e. $u \in BV(\Omega;\mathbb{R}^d)$, if $D_j u_i \in \mathcal{M}(\Omega)$, $i = 1, \dots d$, $j = 1, \dots N$.

$$Du = \nabla u \mathcal{L}^N \lfloor \Omega + ([u] \otimes \nu_{(u)}) \mathcal{H}^{N-1} \lfloor S_{(u)} + D^c u.$$

$$[u] = u^+ - u^-, \quad S_{(u)} \text{ is countably } N-1 \text{ rectifiable}$$

- $$SBV(\Omega;\mathbb{R}^d) = \{u \in BV(\Omega;\mathbb{R}^d) : D^c u = 0\}$$

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BV-SBV spaces

- Theorem (Alberti) Let $F \in L^1(\Omega;\mathbb{R}^{d\times N})$, then there exists $f \in SBV(\Omega;\mathbb{R}^d)$ such that: $\nabla f = F\,\mathcal{L}^N$ a.e. *in* Ω and

$$|D^s f|(\Omega) \leq C||F||_{L^1(\Omega;\mathbb{R}^{d\times N})},\ |f|_{L^1(\Omega;\mathbb{R}^d)} \leq C||F||_{L^1(\Omega;\mathbb{R}^{d\times N})}.$$

- Given $G \in L^1(\Omega;\mathbb{R}^{d\times N})$ and $g \in SBV(\Omega;\mathbb{R}^d)$, there exists $h \in SBV(\Omega;\mathbb{R}^d)$ such that $\nabla h = G - \nabla g$.
  Let h_n be a piecewise constant approximation of h in L^1 norm.
- Define $u_n := g + h - h_n$. Then $u_n \to g$ in L^1 and $\nabla u_n = G$.

Structured Deformations: an important remark about *SBV*

Assume for simplicity that $g \in W^{1,1}$, i.e. there are no macroscopic "cracks". If $u_n \to g$, then $Du_n \rightharpoonup Dg \equiv \nabla g$ in the sense of distributions and therefore if $\nabla u_n \overset{*}{\rightharpoonup} G$, we have that $D^s u_n \rightharpoonup M = \nabla g - G$ in the sense of distributions. Hence, the difference between macroscopic and microscopic "bulk densities" is achieved by a limit of singular measures.

By Ambrosio's Compactness Theorem in SBV, we have that $\nabla g = G\ \mathcal{L}^N$ a.e. unless $\mathcal{H}^{N-1}(S_{(u_n)}) \to +\infty$, i.e. unless there is a diffusion of cracks whose amplitude is tending to zero.

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Integral representation (SBV framework)

The energy associated with the structured deformation (g, G) can be defined as the most economical way to build up the pair using approximations in SBV:

$$I_L(g,G) = \inf_{u_n \in SBV(\Omega;\mathbb{R}^d)} \left\{ \liminf_{n\to\infty} E_L(u_n),\ u_n \xrightarrow{L^1} g,\ \nabla u_n \xrightarrow{L^p} G \right\} \tag{1}$$

for $(g, G) \in SBV(\Omega;\mathbb{R}^d) \times L^p(\Omega;\mathbb{R}^{d\times N})$, $p \geq 1$, with

$$E_L(v) = \int_\Omega W(x, \nabla v)\, dx + \int_{S_v} \psi(x, [v], \nu_v)\, d\mathcal{H}^{N-1}, \tag{2}$$

$v \in SBV(\Omega;\mathbb{R}^d)$

Integral representation result in CF

- Under appropriate assumptions (among which linear growth of ψ), $I_L(g, G)$ admits an integral representation of the form:

$$I_L(g, G) = \int_\Omega H_p(x, \nabla g, G)\, dx + \int_{S(g)} h_p(x, [g], \nu_{(g)}]\, d\mathcal{H}^{N-1},$$

  with H and h defined through appropriate cell formulae.
- The relaxed bulk energy density H depends both on W and ψ.

Integral representation result in CF

We start by introducing the assumptions on the bulk and interfacial energy densities W and ψ. Let $p > 1$ and let $W\colon \Omega \times \mathbb{R}^{d\times N} \to [0,+\infty)$ and $\psi\colon \Omega \times \mathbb{R}^d \times \mathcal{S}^{N-1} \to [0,+\infty)$ be continuous functions satisfying the following conditions

$(W1)_p$ there exists $C > 0$ such that, for all $x \in \Omega$ and $A, B \in \mathbb{R}^{d\times N}$,

$$|W(x,A) - W(x,B)| \leq C|A-B|\big(1 + |A|^{p-1} + |B|^{p-1}\big);$$

$(W2)$ there exists a continuous function $\omega_W\colon [0,+\infty) \to [0,+\infty)$ with $\omega_W(s) \to 0$ as $s \to 0^+$ such that, for every $x, x_0 \in \Omega$ and $A \in \mathbb{R}^{d\times N}$,

$$|W(x,A) - W(x_0,A)| \leq \omega_W(|x-x_0|)(1+|A|^p);$$

Integral representation result in CF

($\psi 1$) there exist $c, C > 0$ such that, for all $x \in \Omega$, $\lambda \in d$, and $\nu \in \mathcal{S}^{N-1}$,

$$c|\lambda| \leq \psi(x, \lambda, \nu) \leq C|\lambda|;$$

($\psi 2$) (positive 1-homogeneity) for all $x \in \Omega$, $\lambda \in d$, $\nu \in \mathcal{S}^{N-1}$, and $t > 0$

$$\psi(x, t\lambda, \nu) = t\psi(x, \lambda, \nu);$$

($\psi 3$) (sub-additivity) for all $x \in \Omega$, $\lambda_1, \lambda_2 \in d$, and $\nu \in \mathcal{S}^{N-1}$,

$$\psi(x, \lambda_1 + \lambda_2, \nu) \leq \psi(x, \lambda_1, \nu) + \psi(x, \lambda_2, \nu);$$

($\psi 4$) there exists a continuous function $\omega_\psi : [0, +\infty) \to [0, +\infty)$ with $\omega_\psi(s) \to 0$ as $s \to 0^+$ such that, for every $x, x_0 \in \Omega$, $\lambda \in d$, and $\nu \in \mathcal{S}^{N-1}$,

$$|\psi(x, \lambda, \nu) - \psi(x_0, \lambda, \nu)| \leq \omega_\psi(|x - x_0|)|\lambda|.$$

Integral representation result in CF

We introduce the classes of competitors for the cell formulae for the relaxed bulk and surface energy densities. For $A, B \in \mathbb{R}^{d\times N}$ let

$$\mathcal{C}_p^{bulk}(A,B) = \Big\{ u \in SBV(Q;\mathbb{R}^d) : u|_{\partial Q}(x) = Ax, \int_Q \nabla u \, dx = B, |\nabla u| \in L^p(Q) \Big\} \tag{3}$$

and for $\lambda \in \mathbb{R}^d$ and $\nu \in \mathcal{S}^{N-1}$ let

$$\mathcal{C}_p^{\text{surface}}(\lambda,\nu) = \Big\{ u \in SBV(Q_\nu;\mathbb{R}^d) : u|_{\partial Q_\nu}(x) = u_{\lambda,\nu}(x) \quad \nabla u(x) = 0 \text{ for } \mathcal{L}^N\text{-a.e. } x \in Q_\nu \Big\}$$

where the function $u_{\lambda,\nu}$ is defined by

$$u_{\lambda,\nu}(x) = \begin{cases} \lambda & \text{if } x\cdot\nu \geq 0, \\ 0 & \text{if } x\cdot\nu < 0, \end{cases}$$

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Integral representation result in CF

Let $p > 1$ and let $W\colon \Omega \times \mathbb{R}^{d\times N} \to [0,+\infty)$ and $\psi\colon \Omega \times \mathbb{R}^d \times \mathcal{S}^{N-1} \to [0,+\infty)$ be continuous functions satisfying hypotheses $(W1)_p$, $(W2)$, $(\psi 1)$, $(\psi 2)$, $(\psi 3)$, and $(\psi 4)$; let $(g, G) \in \mathrm{StD}(\Omega)$. Then there exist $H_p\colon \Omega \times \mathbb{R}^{d\times N} \times \mathbb{R}^{d\times N} \to [0,+\infty)$ and $h_p\colon \Omega \times \mathbb{R}^d \times \mathcal{S}^{N-1} \to [0,+\infty)$ such that

$$I_L(g,G) = \int_\Omega H_p(x, \nabla g(x), G(x))dx + \int_{\Omega\cap S_g} h_p(x,[g](x),\nu_g(x))\, d\mathcal{H}^{N-1} \tag{4}$$

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Integral representation result in CF

Furthermore, for all $x_0 \in \Omega$ and $A, B \in \mathbb{R}^{d\times N}$,

$$H_p(x_0, A, B) = \inf \left\{ \int_Q W(x_0, \nabla u(x))\, dx + \int_{Q\cap S_u} \psi(x_0, [u](x), \nu_u(x))\, d\mathcal{H}^{N-1} : u \in \mathcal{C}_p^{\text{bulk}}(A, B) \right\}$$

and for all $x_0 \in \Omega$, $\lambda \in \mathbb{R}^d$, and $\nu \in \mathcal{S}^{N-1}$,

$$h_p(x_0, \lambda, \nu) = \inf \left\{ \int_{Q_\nu\cap S_u} \psi(x_0, [u](x), \nu_u(x))\, d\mathcal{H}^{N-1} : u \in \mathcal{C}_p^{\text{surface}}(\lambda, \nu) \right\}$$

Motivation of our work

The theory of structured deformation in the SBV setting developed by Chocksi & Fonseca only takes into account the linear dependance on jumps along the approximating sequences. Del Piero &Owen proposed a 1-D model toward capturing the non-linear dependence on the jumps. The idea was to modify the initial energy as follows: for each $r \in (0,1)$ let

$$F^r(u) = \int_0^1 W(u'(x))\,dx + \sum_{z \in S_u} \psi([u](z))$$
$$+ \int_0^1 \Psi\left(\sum_{z \in S_u \cap (x-r, x+r)} \frac{[u](z)}{2r} \right) dx,$$

and then undergo a relaxation process in the context of structured deformations followed by taking the limit as $r \to 0^+$.

Framework

The present approach to relaxation of non-local energies rests on two limiting processes:

1. Start from a submacroscopical level where we have a weighted average of disarrangements within neighborhoods of fixed size $r > 0$ and pass to the macrolevel, permitting disarrangements to diffuse through such a neighborhood. This limiting process determines a structured deformation as well as the non-local dependence of the energy density of such a structured deformation.
2. Pass to the limit as $r \to 0$, to obtain purely local bulk and interfacial energy densities for the structured deformation identified in the first step.

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Framework

1. Previous research on relaxation of energies for continuous bodies relies on one or the other, but not on both processes described above. For instance, the approach of CF relies on the first process, while the second process is used for instance in peridynamics.
2. Peridynamics is a new Continuum Mechanics formulation where the governing equations are integro-differential equations that do not contain spatial derivatives. This is an important new tool to address problems with discontinuities such as cracks.

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Framework

1. It is important to point out that the first limiting process, in the context of structured deformations, gives rise to relaxed energy densities that exclude a periodic dependence of the relaxed energy on the disarrangement tensor, which are used to predict yielding (passage from elastic to plastic behavior) and hysterisis (dependence of the state of a system on its history).
2. We consider an explicit dependence on x in both the CF scheme and the bulk part of the relaxed non-local energy Ψ motivated by some explicit applications to crystal plasticity. This is important in order to account for frame-indifference.

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Averaging processes

Let $\Omega \subset \mathbb{R}^N$ a bounded connected open set with Lipschitz boundary $\partial\Omega$ and $u \in SBV(\Omega; \mathbb{R}^d)$. For a continuous function $\Psi : \Omega \times \mathbb{R}^{d\times N} \to [0, +\infty)$ and fixed $r > 0$ we define the non-local contribution by

$$E^{\alpha_r}(u) := \int_{\Omega_r} \Psi\big(x, (D^s u * \alpha_r)(x)\big)\, dx, \tag{5}$$

where $\Omega_r := \{x \in \Omega : \operatorname{dist}(x; \partial\Omega) > r\}$.

Averaging processes

In (??)

$$\alpha_r := \frac{1}{r^N}\alpha\left(\frac{x}{r}\right),$$

where

$$\alpha \in C_c^\infty(B_1)$$

with

$$\int_{B_1} \alpha(x)\,dx = 1, \qquad \alpha \geq 0, \qquad \alpha(-x) = \alpha(x)$$

The symbol $*$ denotes the convolution operation.

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Averaging processes

Given $(g, G) \in \mathrm{StD}(\Omega; \mathbb{R}^d)$, let $\{u_n\} \subset SBV(\Omega; \mathbb{R}^d)$ such that

(a) $u_n \to g$ in L^1, $\quad \nabla u_n \rightharpoonup G$ in L^p ($\overset{*}{\rightharpoonup}$ in L^1),

(b) $D^s u_n \overset{*}{\rightharpoonup} (\nabla g - G)\mathcal{L}^N + D^s g$ in $\mathcal{M}^+(\Omega)$,

We will denote by $Ad(g, G)$ the class of sequences satisfying (a) and (b).

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Averaging processes - the limit in n

We take the limit as $n \to \infty$ of $E^{\alpha_r}(u_n)$, obtaining

$$
\begin{aligned}
I^r_{NL}(g, G) &:= \lim_{n\to\infty} E^{\alpha_r}(u_n) \\
&= \lim_{n\to\infty} \int_{\Omega_r} \Psi\big(x, (D^s u_n * \alpha_r)(x)\big)\, dx \\
&= \int_{\Omega_r} \Psi\Big(x, \big((\nabla g - G)\mathcal{L}^N + D^s g) * \alpha_r\big)\Big)\, dx
\end{aligned}
\tag{6}
$$

Averaging processes

We consider now an extension of (g, G) to $(\tilde{g}, \tilde{G}) \in \mathbb{R}^N \times \mathbb{R}^{d\times N}$ in the following sense:

(e1) $(\tilde{g}, \tilde{G})\lfloor_\Omega = (g, G)$,

(e2) $|D\tilde{g}|(\mathbb{R}^N) \leq C||g||_{BV(\Omega;\mathbb{R}^d)}$,

(e3) $|D\tilde{g}|(\partial\Omega) = 0$.

Averaging processes

For such $(\tilde{g}, \tilde{G})$, we extend $I^r_{NL}(g, G)$ to Ω by defining:

$$\begin{aligned}\widetilde{I}^r_{NL}(\tilde{g}, \tilde{G}) := &\int_{\Omega_r} \Psi\big(x, ((\nabla g - G)\mathcal{L}^N + D^s g) * \alpha_r\big)\, dx \\ &+ \int_{\Omega \setminus \Omega_r} \Psi\big(x, ((\nabla \tilde{g} - \tilde{G})\mathcal{L}^N + D^s \tilde{g}) * \alpha_r\big)\, dx\end{aligned} \tag{7}$$

In any case, independently of the extension considered, we can show that the difference between $I^r_{NL}(g, G)$ and $\widetilde{I}^r_{NL}(\tilde{g}, \tilde{G})$ goes to zero as $r \to 0^+$.

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The limit as $r \to 0^+$

We work with $\widetilde{I}^r_{NL}(\tilde{g}, \tilde{G})$ where Ψ can be of two types:

E) $\Psi \in C(\Omega \times \mathbb{R}^{d\times N})$ and $\Psi^\infty(x,\xi) := \lim_{\substack{x'\to x\\ \xi'\to\xi\\ t\to+\infty}} \frac{\Psi(x',t\xi')}{t}$ exists in $\overline{\Omega} \times \mathbb{R}^{d\times N}$

L) $\Psi \in C(\Omega \times \mathbb{R}^{d\times N})$, Lipschitz continuous in the second variable with Ψ^∞ defined as $\Psi^\infty(x,\xi) := \limsup_{\substack{x'\to x\\ \xi'\to\xi\\ t\to+\infty}} \frac{\Psi(x',t\xi')}{t}$

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The limit as $r \to 0^+$

We have that, for any $(g, G) \in \mathrm{StD}(\Omega; \mathbb{R}^d)$,

$$I_{NL}(g, G) := \lim_{r \to 0^+} \widetilde{I}^{\alpha_r}_{NL}(\overline{g}, \overline{G}) = \int_\Omega \Psi\Big(x, (\nabla g - G)(x)\Big)\, dx + \int_{\Omega \cap S(g)} \Psi^\infty\Big(x, \frac{dD^s g}{d|D^s g|}(x)\Big)\, d|D^s g|$$

Coupling

- $I(g, G) = I_L(g, G) + I_{NL}(g, G)$ where

$$I_L(g, G) = \int_\Omega H(x, \nabla g(x), G(x))\, dx + \int_{S_{(g)} \cap \Omega} h(x, [g](x), \nu_{(g)}(x))\, d\mathcal{H}^{N-1}$$

and

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Example from crystal plasticity

- Crystallographic slip: The discontinuity in deformation arises only across a limited family of slip planes.
- For a single crystal in the reference configuration Ω the data required for the analysis of crystallographic slip consists of pairs of orthogonal unit vectors (s^a, m^a) for $a = 1, \cdots, A$, with A the number of potentially active slip systems.
- The unit vector s^a provides the direction of slip, while the unit vector m^a is a normal to the slip plane for the a^{th} slip-system (s^a, m^a).

Crystallographic structured deformation

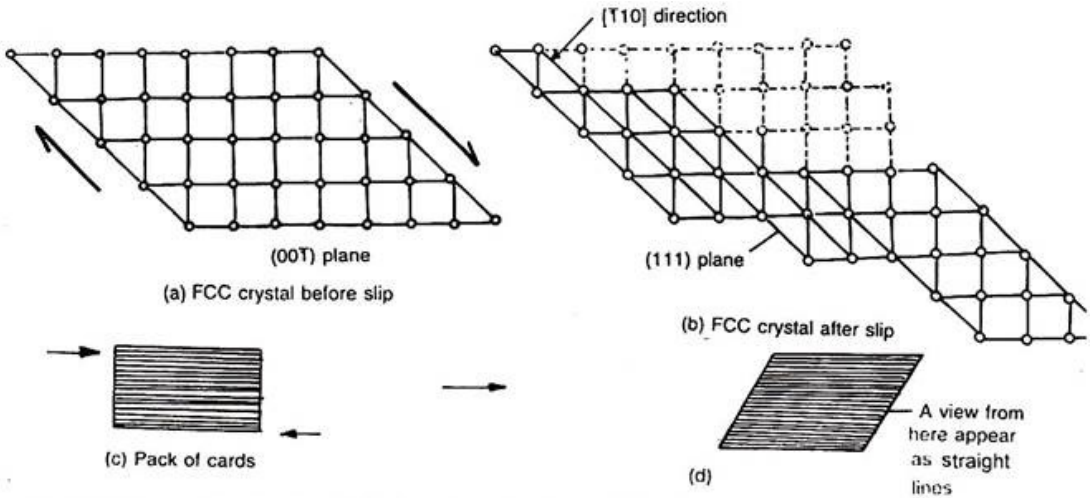

Fig. 6.15. Slip resembles distortion of deck of playing cards when pushed as shown (c & d). (*a*) FCC Crystal before slip, (*b*) FCC crystal after slip, (*c*) Pack of cards, (*d*) Pack of cards after slip.

Slip-neutral two level shears

Crystallographic slip is physically activated within very thin bands, (slip-bands) with thickness typically of the order 10^2 atomic units, while the separation of active slip-bands is typically of order 10^4 atomic units. Following [CDPFO1999], for each $a = 1, \cdots, A$, there is a number $p^a > 0$ such that a two-level shear (g^a_{μ,x_o}, G^a_ν) for which the shear due to slip $\mu - \gamma$ satisfies

$$\mu - \gamma = mp^a \quad \text{with } m \in \mathbb{Z} \tag{8}$$

and gives rise to submacroscopic slips equal to an integer number of atomic units in the direction of slip s^a.

Special properties for Ψ, under crystallografic slip

- Let $x_o \in \Omega$, $a \in A$, $\mu = mp^a$ with $m \in \mathbb{Z}$, and a crystallographic structured deformation (g, G) be given. The lattice on which (g, G) acts, when following the completely neutral two-level shear (g^a_{μ,x_o}, I), differs from that on which (g, G) acts, when not following (g^a_{μ,x_o}, I), only by the undetectable translations of the lattice between active slip-planes for system a.
- Consequently, the submacroscopic kinematical states of the crystal lattice attained by means of the two purely submacroscopic structured deformations $(i, K_{(g,G)\diamond(g^a_{\mu,x_o},I)})$ and $(i, K_{(g,G)})$ are indistinguishable.

Special properties for Ψ, under crystallografic splip

- This leads to the conclusion that, the non-local relaxed bulk density, in the context of crystal plasticity, can have periodicity properties, provided that it is restricted to each member of a family of two-dimensional affine subspaces of $\mathbb{R}^{3x3}$, with (vector) period depending on the corresponding subspace.
- The periodicity stems from the fact that special families of two-level shears associated with the slip systems of the crystal are geometrically undetectable.

Prediction of yielding and hysterisis

- An additive decomposition for the relaxed bulk energy density of the form

$$H(G) + \Psi(M)$$

  is used to predict yielding and hysterisis [CDPFO1999], [Del Piero 2018])
- It was shown ([Larsen2000]) that such a decomposition doesn't always hold in the CF setting.
- Our double limiting process points in that direction. For each crystallographic structured deformation, departing from Ψ satisfying the periodicity properties compatible with completely neutral crystallographic slips and from the CF scheme with $p > 1$ growth on W and with $\psi = 0$ we attain such a decomposition.

Thank you for your attention!