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.

- $$\text{S.D. pair}(g, G)$$

  with $f_n \overset{L^\infty}{\longrightarrow} g$, $\nabla f_n \overset{L^\infty}{\rightharpoonup} G$, 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.

Example *Deck of cards*

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

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

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

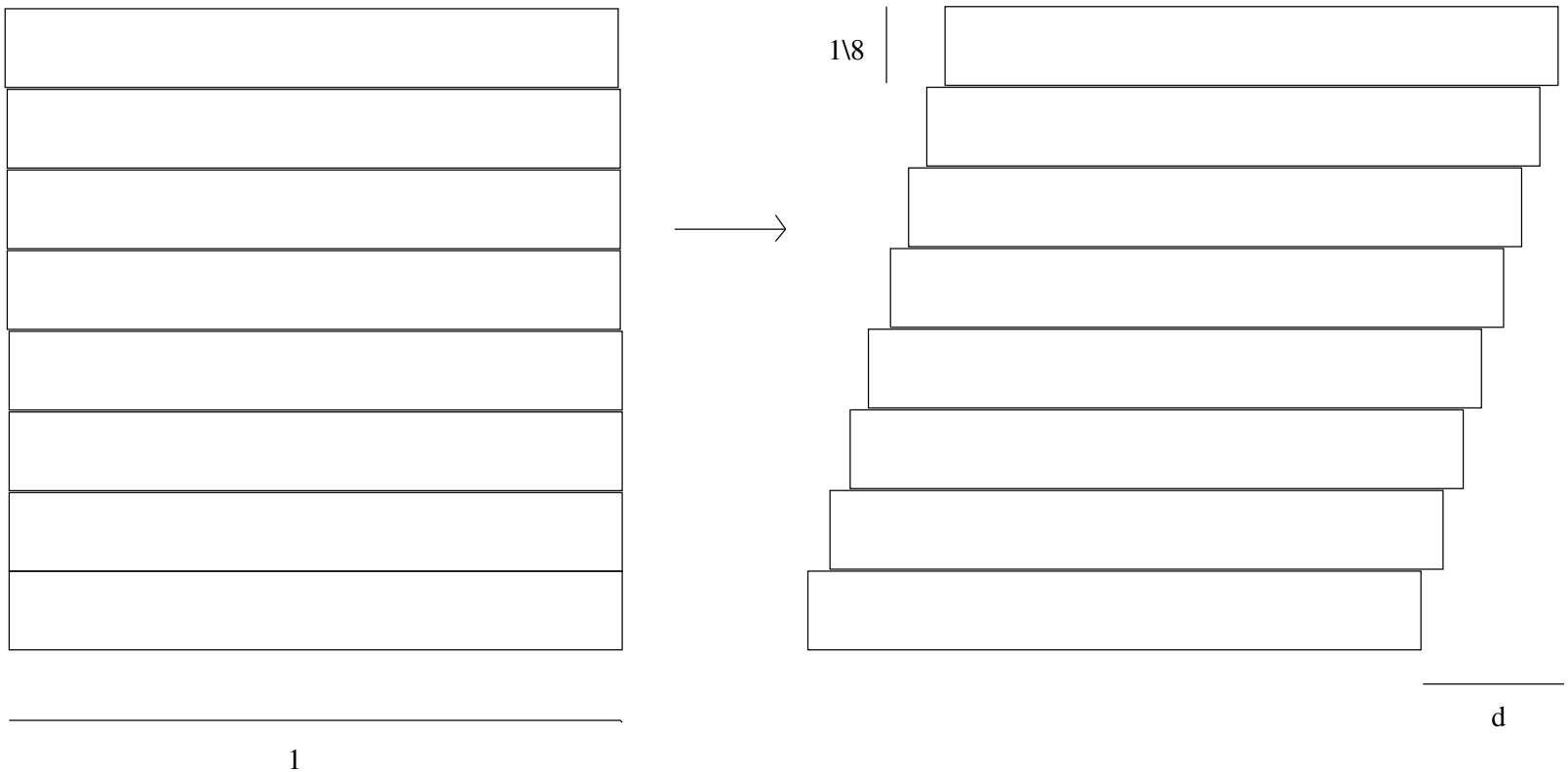
$$f_n \xrightarrow{L^\infty} g,\ \nabla f_n \xrightarrow{L^\infty} G,\ Df_n \rightharpoonup \nabla g = \begin{bmatrix} 1 & 1 \\ 0 & 1 \end{bmatrix}$$

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

Example

Deck of cards

f_8



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:

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

  with H and h defined through appropriate cell formulae.
- The relaxed bulk energy density H depends both on W and ψ.
- In this work we extend the original result in CF, by allowing explicit dependence on the variable x.

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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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

$$E^{\alpha_r}(u) := \int_{\Omega_r} \Psi\big(x, (D^s u * \alpha_r)(x)\big)\, dx, \tag{3}$$

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

Averaging processes

In (3)

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

where

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

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

The symbol $*$ denotes the convolution operation.

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Averaging processes

Given $(g, G) \in SD(\Omega; \mathbb{R}^d)$, 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

$$
\begin{aligned}
I^r_{NL}(g, G) &:= \lim_{n\to\infty} E^{\alpha_r}(u_n) \\
&= \lim_{n\to\infty} \int_{\Omega_r} \Psi\big(x, (D^s u_n * \alpha_r)(x)\big)\, dx \\
&= \int_{\Omega_r} \Psi\Big(x, \big((\nabla g - G)\mathcal{L}^N + D^s g) * \alpha_r\big)\Big)\, dx
\end{aligned}
\tag{4}
$$

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:

$$\begin{aligned}\widetilde{I}^r_{NL}(\tilde{g}, \tilde{G}) := &\int_{\Omega_r} \Psi\big(x, ((\nabla g - G)\mathcal{L}^N + D^s g) * \alpha_r\big)\, dx \\ &+ \int_{\Omega \setminus \Omega_r} \Psi\big(x, ((\nabla \tilde{g} - \tilde{G})\mathcal{L}^N + D^s \tilde{g}) * \alpha_r\big)\, dx\end{aligned} \tag{5}$$

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 $\Psi^\infty(x,\xi) := \limsup_{\substack{x'\to x\\ \xi'\to\xi\\ t\to+\infty}} \frac{\Psi(x',t\xi')}{t}$

We address the dependance in x with some modulus of continuity assumption on the first variable.The proof relies in Reshetnyak continuity (upper semicontinuity) theorems.

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The limit as $r \to 0^+$

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

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

Coupling

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

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

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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

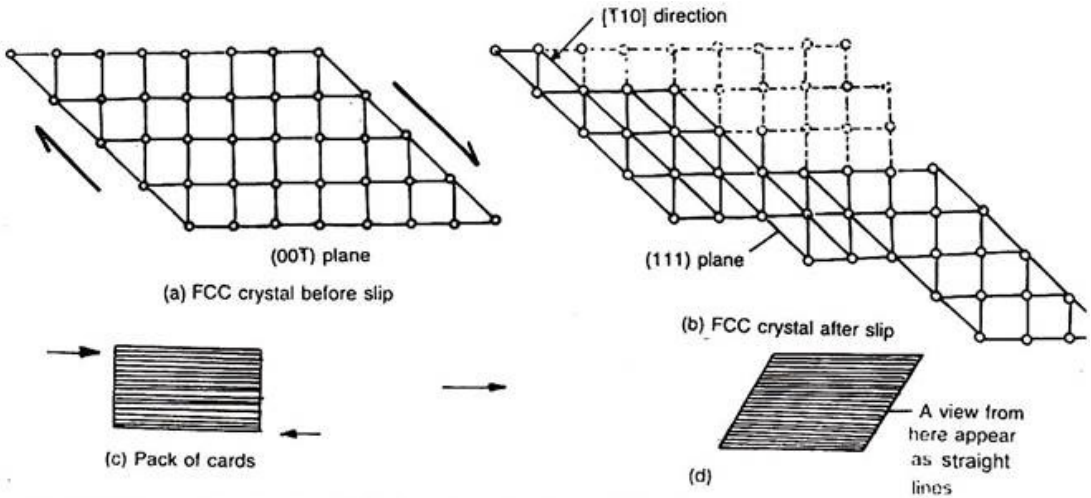

Fig. 6.15. Slip resembles distortion of deck of playing cards when pushed as shown (c & d). (*a*) FCC Crystal before slip, (*b*) FCC crystal after slip, (*c*) Pack of cards, (*d*) Pack of cards after slip.

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

$$\mu - \gamma = mp^a \quad \text{with } m \in \mathbb{Z} \tag{6}$$

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

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.

Thank you for your attention!