ANALYSIS OF LENNARD-JONES INTERACTIONS IN 2D

Andrea Braides (Roma *Tor Vergata*)

ongoing work with Maria Stella Gelli (Pisa)

Otranto, June 6–8 2012

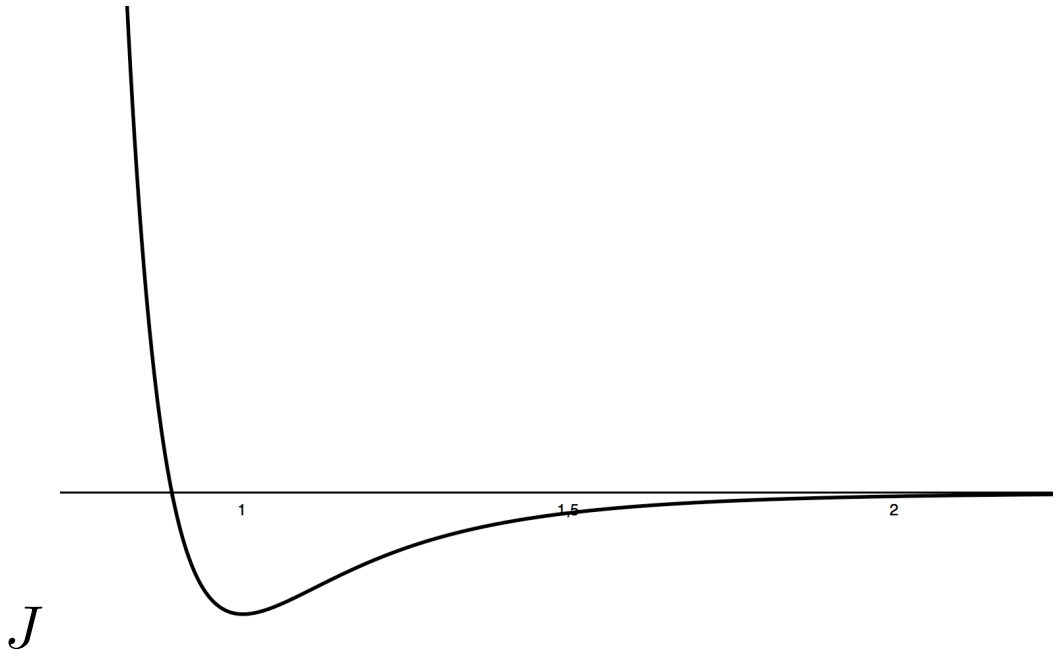
Variational Problems with Multiple Scales

Variational Analysis of Lennard-Jones interactions

Equilibrium configurations linked to the energy

$$\sum_{i \neq j} J(|u_i - u_j|), \qquad \left(e.g.,\ J(z) = \frac{1}{z^{12}} - \frac{2}{z^6} \right)$$

$u_i \in \mathbb{R}^2$; $i = 0, \ldots, N$ as $N \to +\infty$



1D analysis - nearest neighbours

Early works by Truskinovsky ('96), B-Dal Maso-Garroni ('99)

1D parameterization: We can always reparameterize points on $i \in \frac{1}{N}\mathbb{Z} \cap [0,1]$

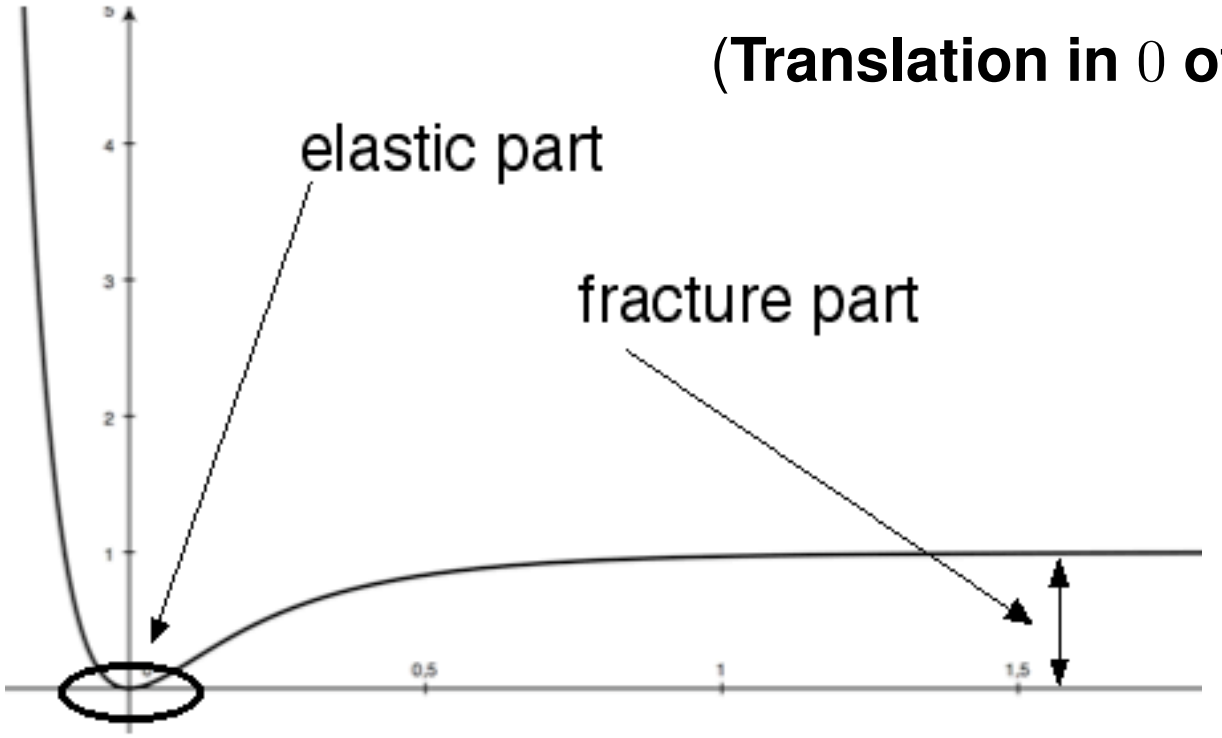
Set $\varepsilon = \frac{1}{N}$ and scale energies

$$\sum_i \varepsilon \, J\left(\frac{u_i - u_{i-1}}{\varepsilon}\right) \qquad \text{with } u_i > u_{i-1}$$

$\{u_i\} \approx$ piecewise-constant or piecewise-affine function

Note: minimum is achieved for u_i the discretization of the identity (up to constants)

Derivation of bulk and surface energies

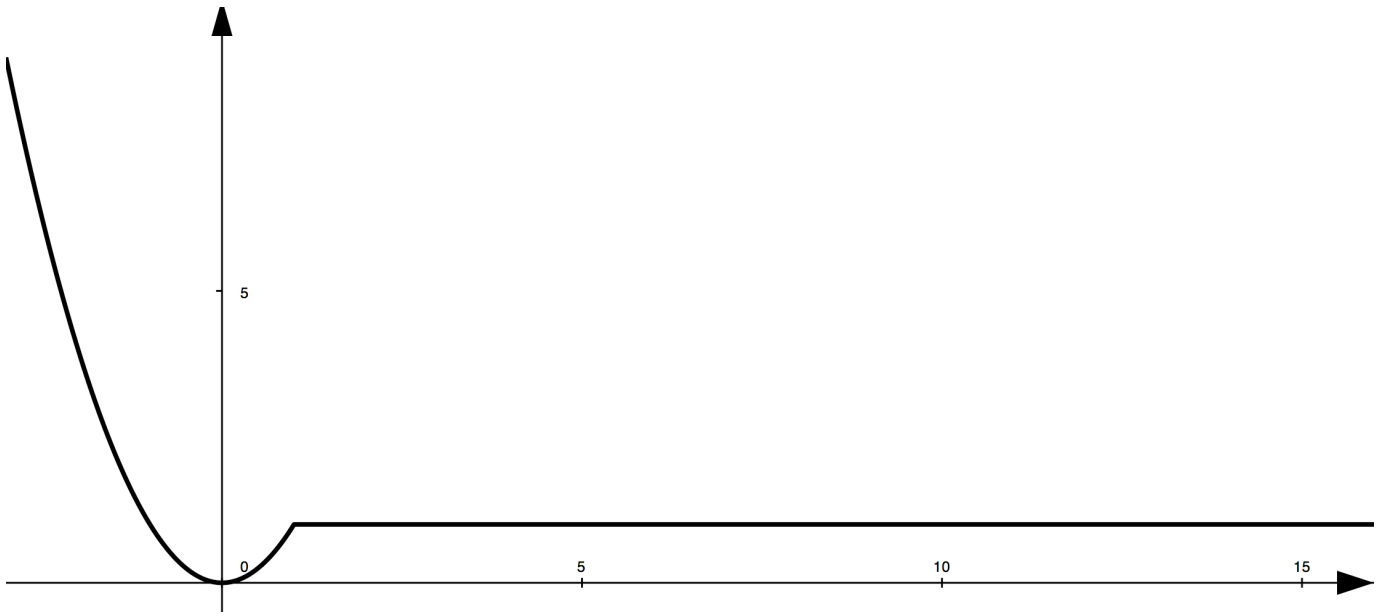


Limit analysis by different scalings
Bulk scaling $(u_{i-1} - u_i << \varepsilon) \Longrightarrow$ elastic approximation
Surface scaling $(u_{i-1} - u_i >> \varepsilon) \Longrightarrow$ (opening) fracture

Note: Bulk energy$= O(1)$, surface energy$= O(\varepsilon) \Longrightarrow$ relaxation

(Asymmetric) Blake-Zisserman weak membrane

$$\Psi_\varepsilon(z) = \begin{cases} \min\left\{z^2, \frac{1}{\varepsilon}\right\} & \text{if } z > 0 \\ z^2 & \text{if } z \leq 0 \end{cases}$$



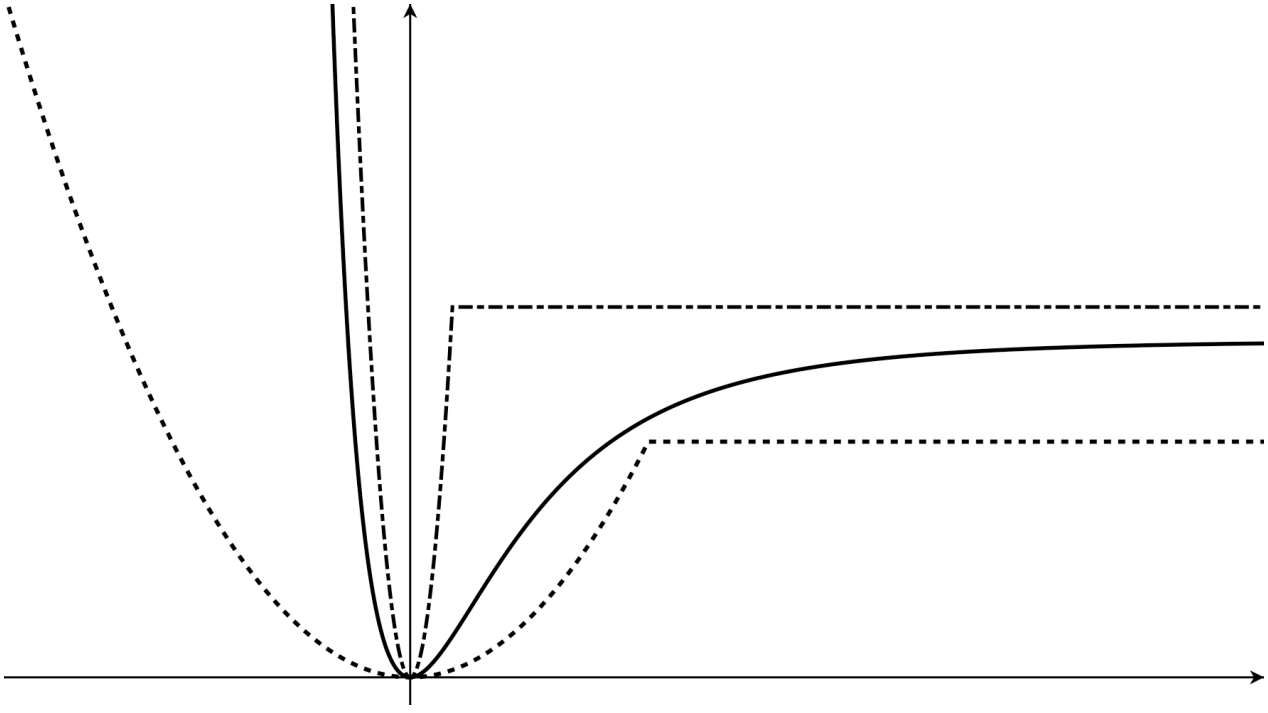
Asymptotic behaviour (Chambolle '92 - Γ-limit)

$$\int_0^1 |u'|^2\, dt + \#(S_u) \qquad u^+ > u^- \text{ on } S_u$$

(*Griffith brittle fracture energy with unilateral constraint*)

‘Universal form’ of the Blake-Zisserman energy

Analysis of the Γ-development by comparison with (scaled, asymmetric) Blake-Zisserman energies:



$$\min\Big\{\alpha' z^2, \beta'\Big\} \leq J(z) \leq \min\Big\{\alpha'' z^2, \beta''\Big\} \qquad (z > 0)$$

NOTE: $\sup \alpha' = \inf \alpha'' = \frac{1}{2} J''(0) =: \alpha$ (Taylor expansion at 0)

$\sup \beta' = \inf \beta'' = J(+\infty) =: \beta$ (depth of the well)

Scaling argument to recover Griffith fracture (B-Lew-Ortiz '06):

$$\min\Big\{\alpha' z^2, \frac{\beta'}{\varepsilon}\Big\} \le \frac{1}{\varepsilon}\, J(\sqrt{\varepsilon} z) \le \min\Big\{\alpha'' z^2, \frac{\beta''}{\varepsilon}\Big\}$$

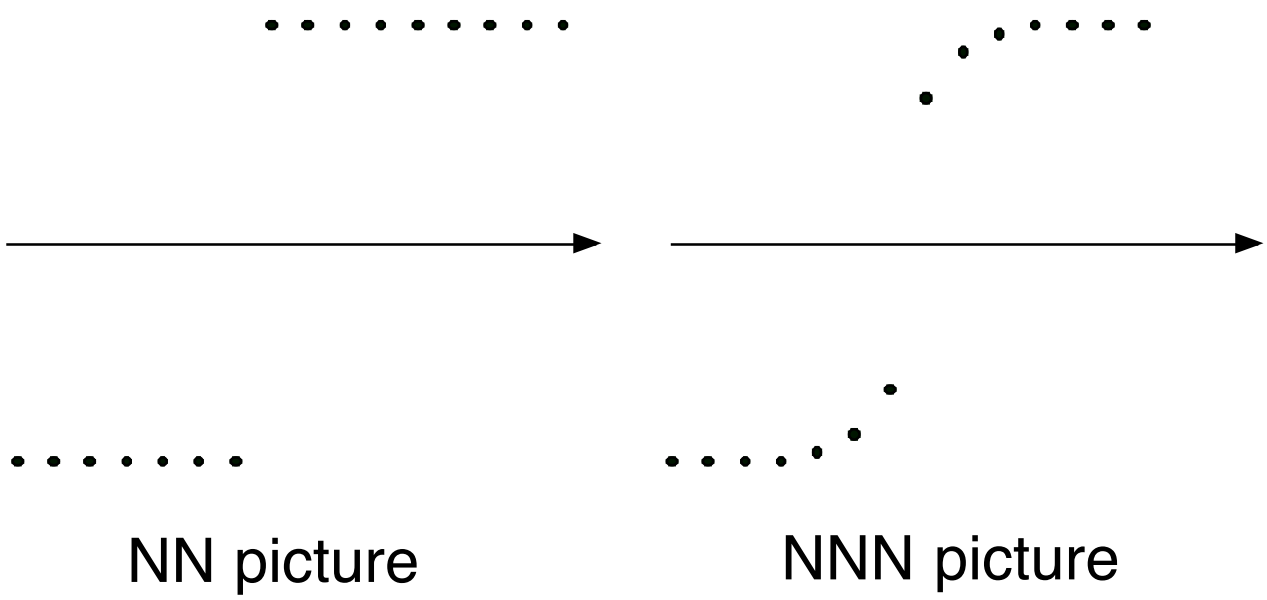
Change of variables ('linearization' around 0) $u = \sqrt{\varepsilon}\, v$

$$\begin{aligned}
E_\varepsilon(u) &= \sum_i \varepsilon J\Big(\frac{u_i - u_{i-1}}{\varepsilon}\Big) = \varepsilon \sum_i \varepsilon \cdot \frac{1}{\varepsilon} J\Big(\sqrt{\varepsilon}\Big(\frac{v_i - v_{i-1}}{\varepsilon}\Big)\Big) \\
&\approx \varepsilon\Big(\alpha \int |v'|^2\, dt + \beta \#(S_v)\Big) \\
&= \varepsilon\Big(\alpha \int \Big|\frac{u'}{\sqrt{\varepsilon}}\Big|^2\, dt + \beta \#(S_u)\Big) \\
&= \alpha \int |u'|^2\, dt + \varepsilon\beta \#(S_u) \qquad \text{(with } u^+ > u^-\text{)}
\end{aligned}$$

(*Griffith energy with an internal parameter*)
(Uniform equivalence by Γ-convergence, B-Truskinovsky '08)

Effects of long-range interaction

1) Surface relaxation: The fracture energy density β is not simply given by a scaling argument (resizing the depth of the well of J), but must take into account *atomic relaxation* on the side(s) of the fracture
(B-Cicalese '07)



NN picture NNN picture

2) Optimization of the reference lattice: (in this case we cannot translate the minimum in 0) ground state are achieved on some discretization of rx with $0 < r < 1$.

1D ANALYSIS

1) Different behaviour in **compression** (no fracture/elasticity) and in **tension** (Griffith fracture)
2) **Opening fracture**
3) Surface energy with possible surface relaxation (that can be characterized by taking the limit of $\frac{1}{\varepsilon}F_\varepsilon$)
4) An approximate **linearized Griffith fracture** description (with parameter ε and an opening constraint)
5) (up to slightly changing potential) can consider only nearest neighbours

The two-dimensional case

Simplified hypotheses

Parameterization on the triangular lattice $\mathbb{T}$: justified by the **validity of the "Cauchy-Born rule" for ground states** (*crystallization*; see Theil '06 in 2D)

Positive-determinant constraint (this replaces the condition $u' > 0$): admissible functions are $\{u_i\}_{i\in\mathbb{T}}$ whose piecewise-affine interpolation u satisfies

$$\det \nabla u > 0$$

(see Friesecke-Theil '02)
(geometrically: vertices of deformed triangles maintain the order)

Nearest-neighbour interactions. This reduces surface relaxation (for that see recent work of Theil)

The scaled energy reads

$$E_\varepsilon(u) = \sum_{NN} \varepsilon^2 J\left(\left|\frac{u_i - u_j}{\varepsilon}\right|\right) \quad (+ \text{ positive-det. constraint})$$

with the sum taken on nearest neighbors of $\Omega \cap \varepsilon\mathbb{T}$
(Ω fixed open subset of $\mathbb{R}^2$).

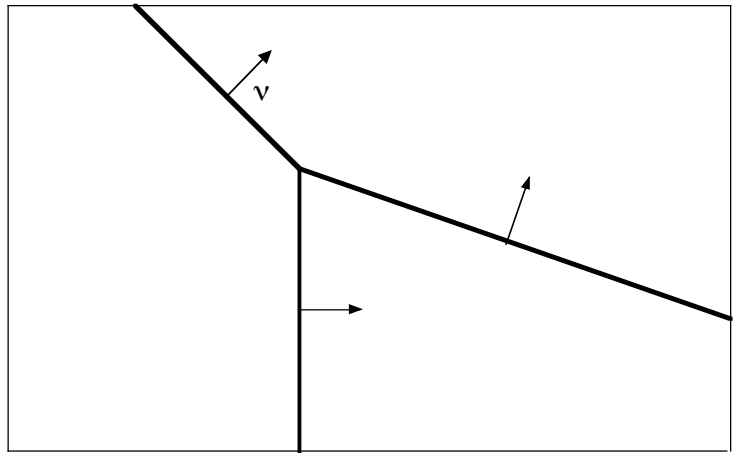
Surface scaling

Consider

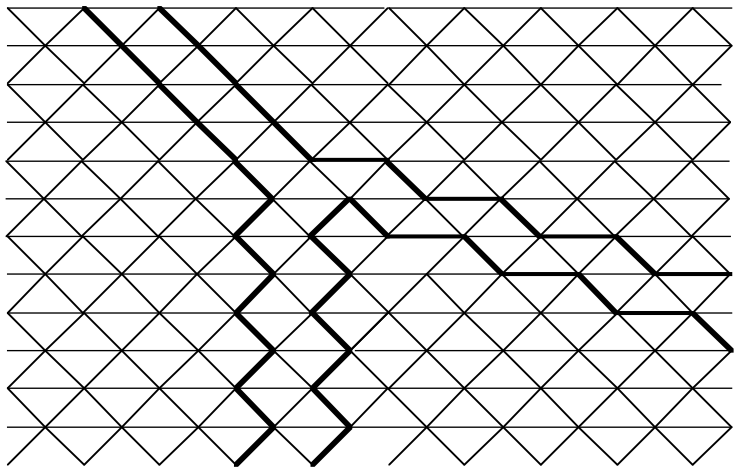
$$\frac{1}{\varepsilon}E_\varepsilon(u) = \sum_{NN} \varepsilon\left(J\left(\left|\frac{u_i - u_j}{\varepsilon}\right|\right) - \min J\right) \quad \text{(+ positive-det. constraint)}$$

and analyse its behaviour through its Γ-limit.
Questions:
- can we derive a **opening-crack condition**?
- can we characterize a surface energy?

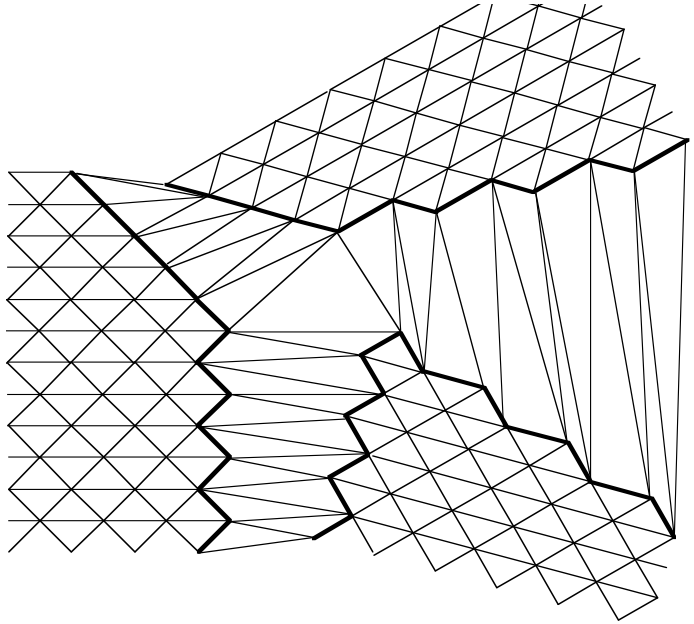
Domain of the limit: the limit is finite only if $u \in SBV$ and $\nabla u \in SO(2)$; $\Longrightarrow \nabla u$ is a **piecewise rotation** (**piecewise rigidity** Chambolle-Giacomini- Ponsiglione '07);



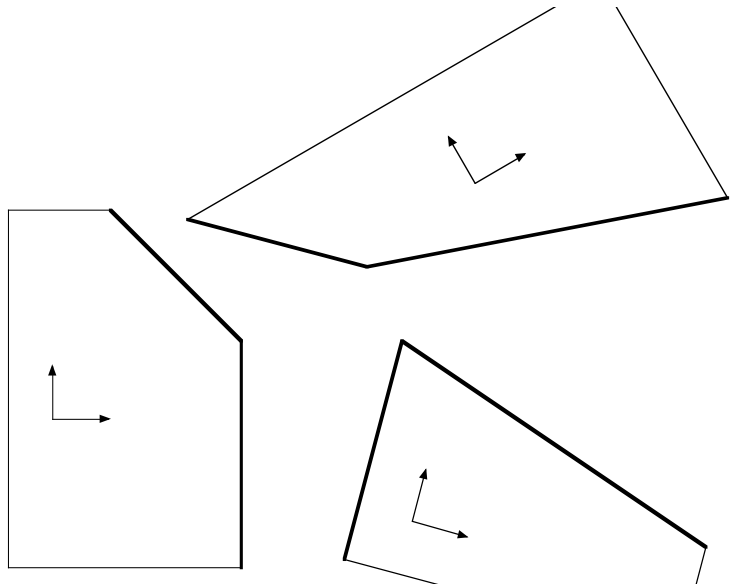
A reference configuration with fracture site and its macroscopic normals



An underlying triangulation at step ε



Deformed configuration at the level of the triangulation



Macroscopic deformed configuration

Constraints on the jump set

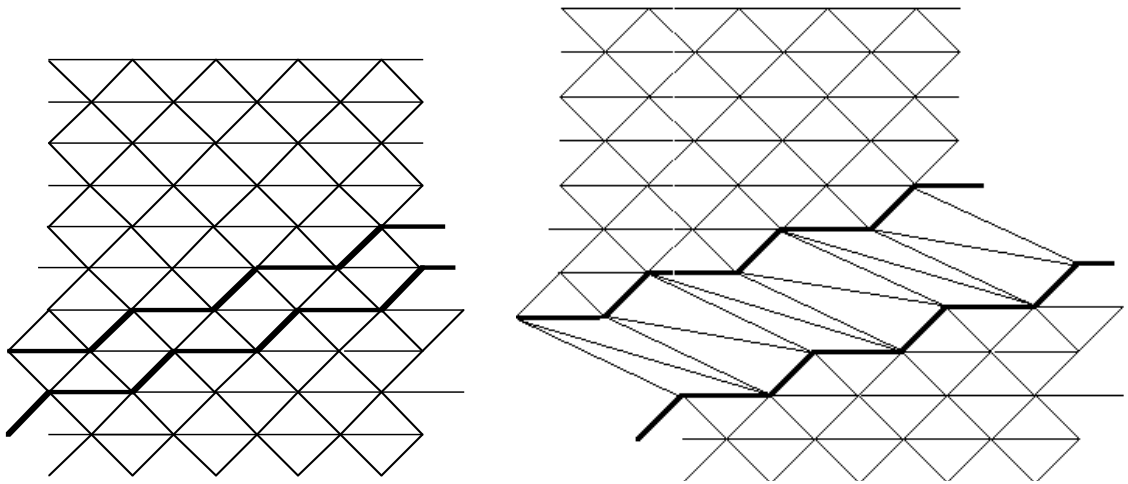
If the limit interface is achieved by only 'breaking a single row of atoms' (rigid otherwise) we obtain a surface term

$$2 \int_{S_u} \varphi(\nu_u) d\mathcal{H}^1$$

(φ with hexagonal Wulff shape), and the positive determinant gives an **opening-angle condition**

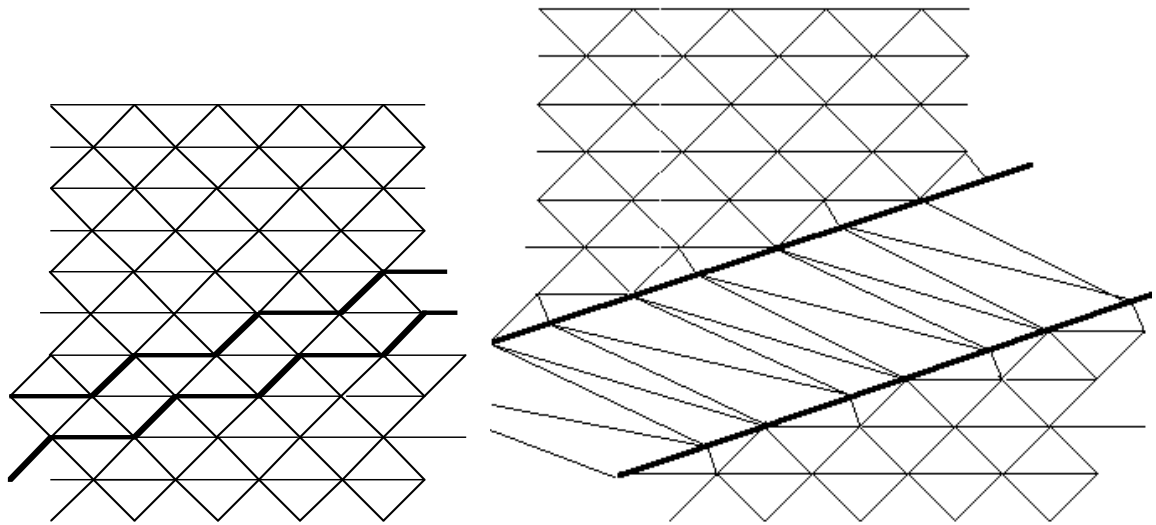
$$\langle u^+(x) - u^-(x), R^{\pm}\nu_i \rangle \geq 0 \qquad i = 1, 2$$

where $u^{\pm}$ are the approximate values, ν_u the macroscopic normal, $R^{\pm}$ are the rotations on both sides of S_u, and $(\nu_i)^{\perp}$ are the directions of $\mathbb{T}$ that 'average' to ν
(if ν is itself orthogonal to the directions of $\mathbb{T}$ then $\nu_i = \nu$)

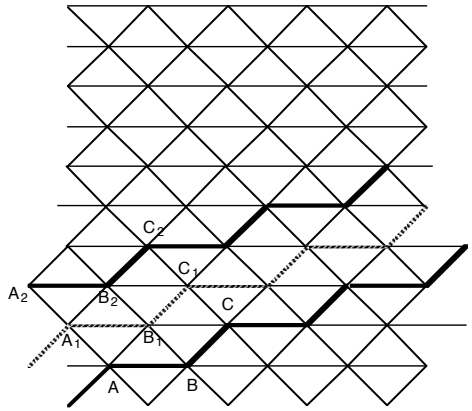


Note: “surface relaxation” allows to have finite (but larger) energy when

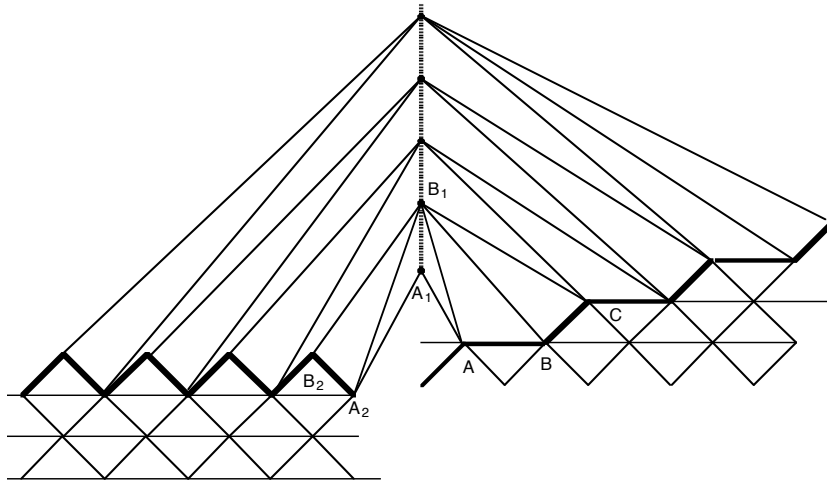
$$\langle u^+(x) - u^-(x), R^{\pm}\nu \rangle \geq 0 \qquad \textbf{(opening constraint)}$$



Loss of the constraint on interfaces

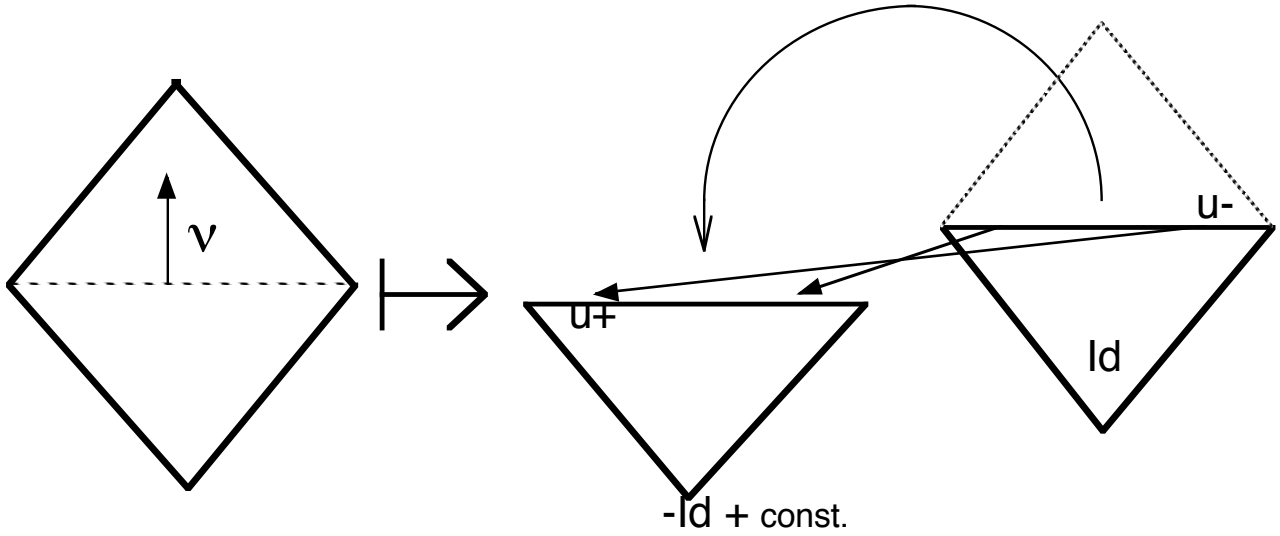


reference triangulation with a double-layer interface

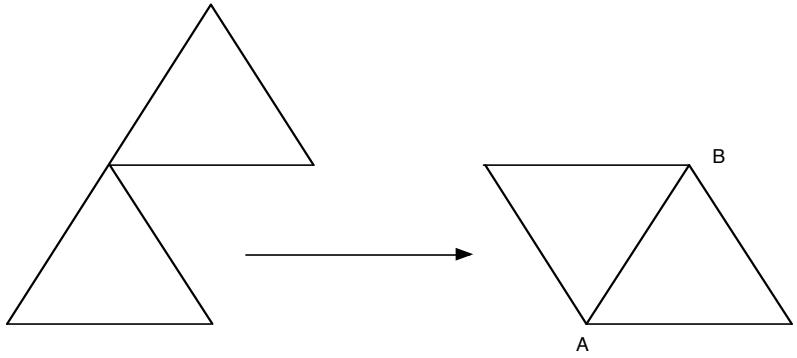


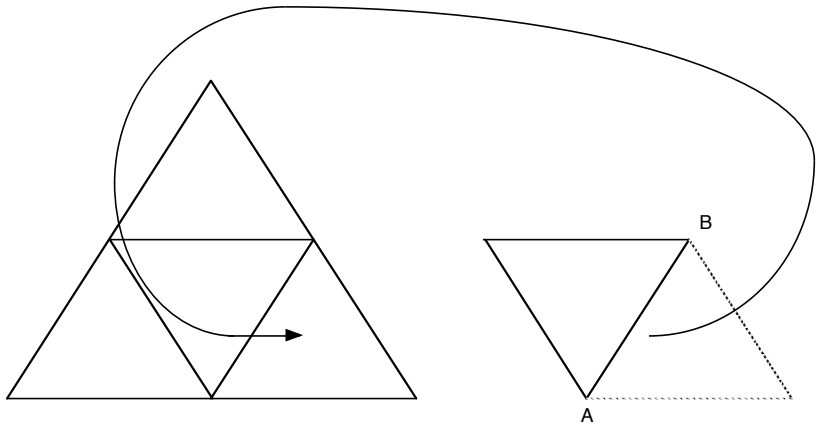
deformed configuration with ‘fictitious’ extra fracture

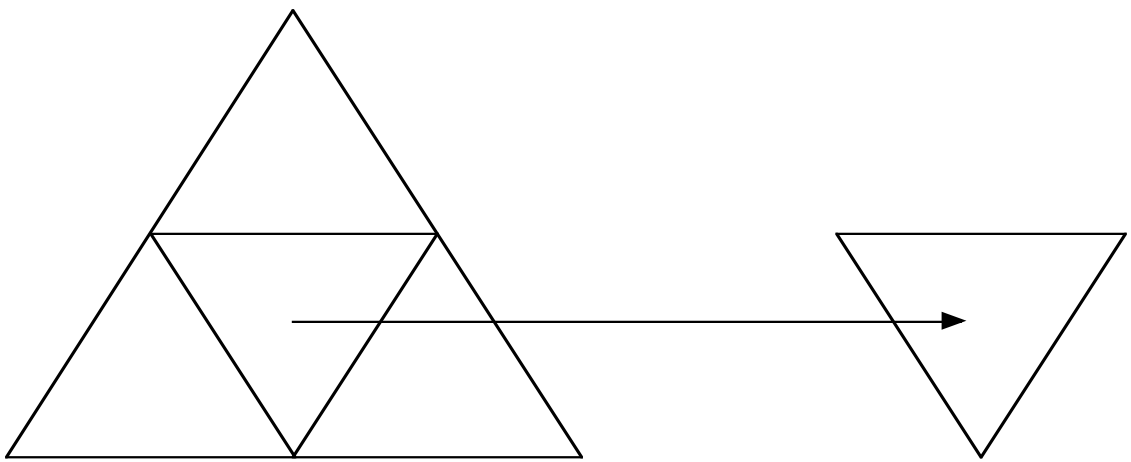
Note: we may easily obtain deformations violating the opening constraint



... or non impenetrability...







By using multiple-layer fracture we can remove all constraints on the interface, but the final energy will have a surface term of the form

$$2N \int_{S_u} \varphi(\nu_u) d\mathcal{H}^1$$

(N the number of layers)

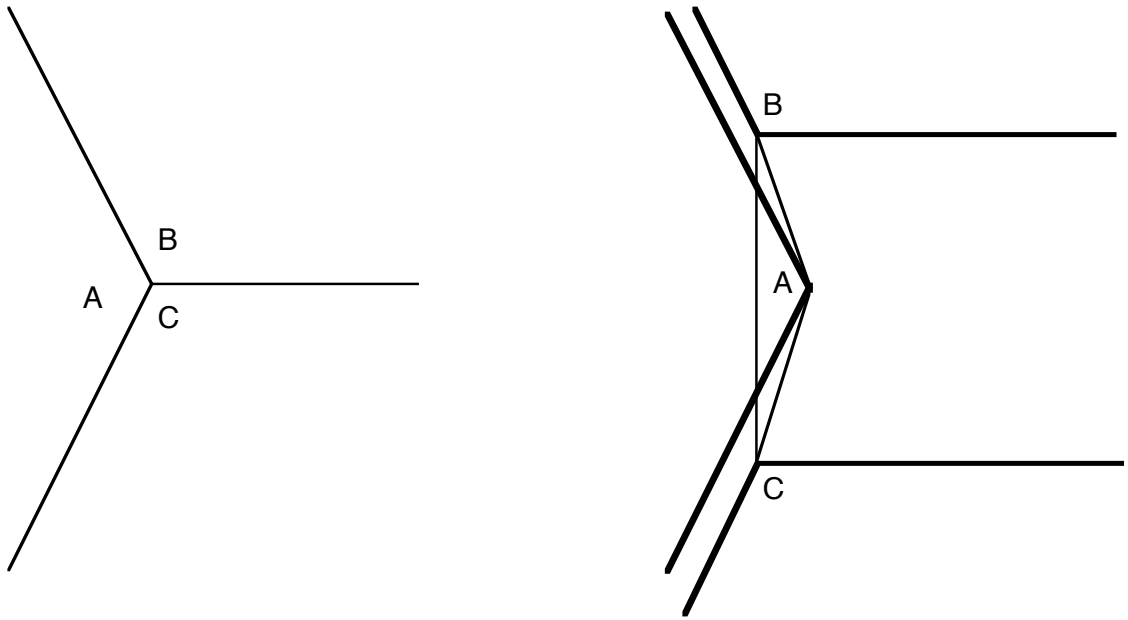
Note: even when the constraint

$$\langle u^+(x) - u^-(x), R^{\pm}\nu \rangle \geq 0$$

is satisfied we may have to optimize between surface relaxation and fictitious interfaces

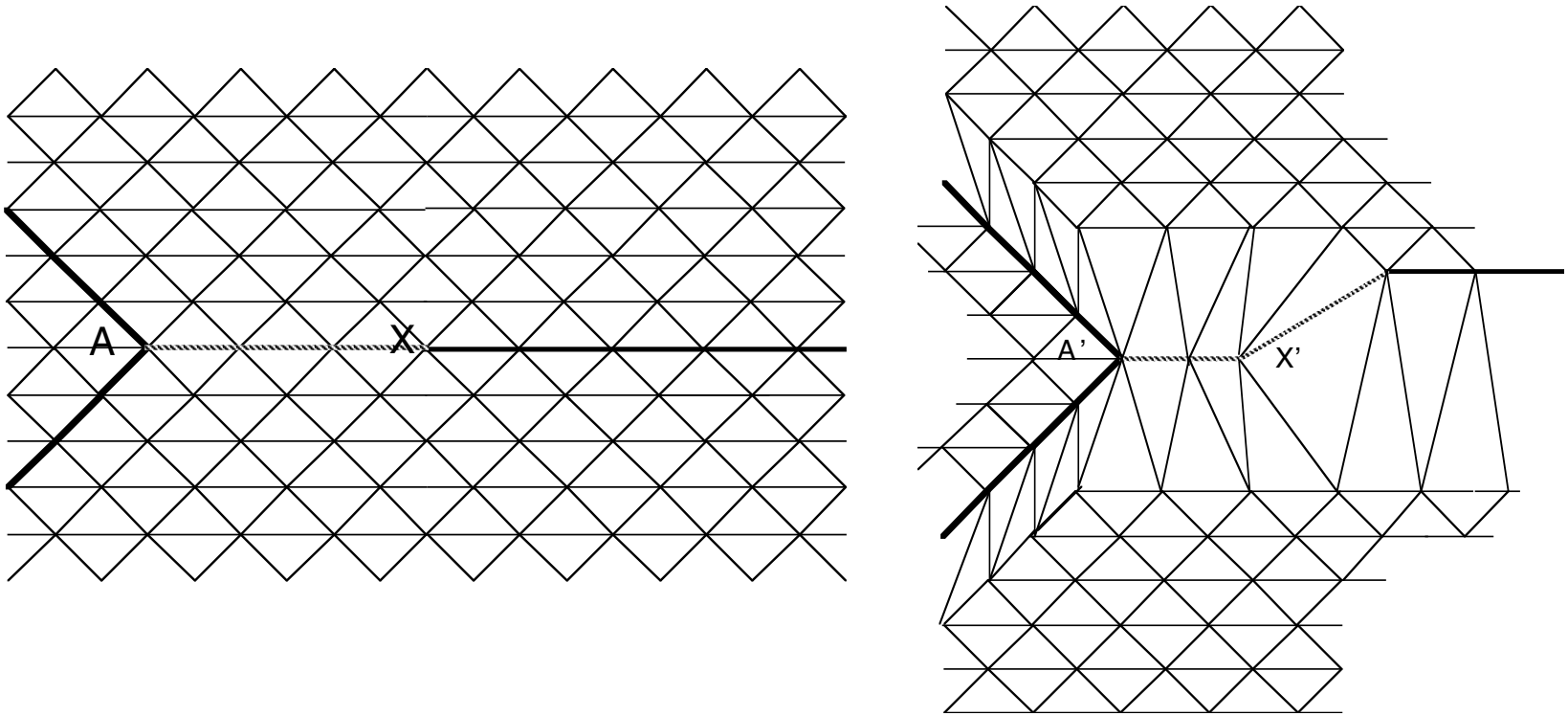
Determinant constraint on triple points

Even if the opening angle condition is verified on all S_u we may have triple points violating the positive determinant constraint



(triple point - reference and deformed configuration)

These can be “accommodated” by introducing extra fractures at level ε (of non-vanishing length)



This gives a strictly positive extra term (depending on the ‘size’ of the deformed ‘negative triangle’)

Limit energy

On a (wide) class of deformations satisfying the *opening angle condition* the Γ-limit is of the form

$$2\int_{S_u}\varphi(\nu_u)d\mathcal{H}^1$$

On the other deformations the computation involves a "relaxation procedure" involving extra layers of highly-deformed triangles at level ε and surface relaxation.

Note: indeed the surface energy density is of the form

$$\varphi=\varphi\left(u^{\pm},\frac{\partial u^{\pm}}{\partial\tau},\nu\right)$$

Such integrands could be defined also if u has 'enough regularity on S_u' (Ambrosio-B-Garroni '97). Any use?

‘Small deformations’

If we suppose that $u = Id + \delta v$ with $\sqrt{\varepsilon} << \delta$ then we still have a compactness theorem with the limit piecewise rigid. The opening constraint reduces to

$$\langle v^+(x) - v^-(x), \nu \rangle \geq 0$$

(‘infinitesimal non-interpenetration condition’). Moreover, the condition on triple points disappears.
This condition is closed (Giaquinta-Giusti, Anzellotti), so that a candidate limit is simply

$$2 \int_{S_v} \varphi(\nu_v) d\mathcal{H}^1$$

(for v satisfying the opening-angle condition)
Question: any density theorem for partitions with this opening condition? (same question in SBV, important for non-interpenetration on the fracture)

Conclusions

In the case of ‘finite deformations’ we have derived
• conditions on the interface that characterize a ‘tensile’ regime
• a characterization via an anisotropic energy density on a (wide) class of deformations
• a complex non-local description for deformations violating the ‘non-impenetrability constraint’

In the case of ‘small deformations’ we have
• a linearized ‘tensile regime’ with a **opening fracture condition**
• a lower-semicontinuous candidate local surface energy

This gives the conjecture that

$$E_\varepsilon(u) \approx \int_\Omega Q(\mathcal{E}u)\,dx + \varepsilon \int_{S_u} \varphi(\nu_u) d\mathcal{H}^1$$

(+ opening-angle condition) in **G**SBD(Ω) in the tensile regime (this amounts to compute the 'critical' linearization $\delta = \sqrt{\varepsilon}$ à la B-Lew-Ortiz))
Q quadratic form derived by computing the linearization around Id on $H^1(\Omega)$ (if $\delta << \sqrt{\varepsilon}$ – B-Solci-Vitali '07)
(without the positive-determinant constraint related results by Alicandro-Focardi-Gelli '99, Friedrich-Schmidt '11)

Final conclusion: probably the positive-determinant constraint is too strict in some cases; the simplifications seem to be 'acceptable' for small deformations (or for problems ensuring the positive-determinat condition on the recovery sequences).