Asymptotic analysis of atomistic systems

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MECHANICS – NEW CHALLENGES

Passage from discrete to continuum

Atomistic theories with interaction between (many) particles

$$\Downarrow$$

Continuum theories depending on averaged parameters

Main issue: statement of a meaningful question in analytical terms

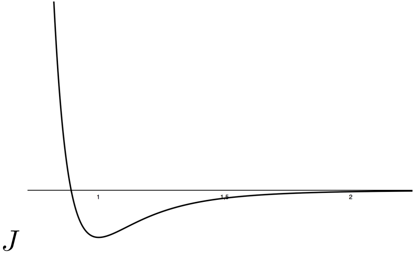
Crystallization

Q: can the crystalline structure of solids be derived from atomistic energetically considerations?

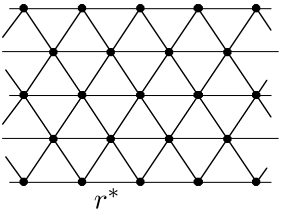
Typical energy (pairwise interactions)

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

$u_i \in \mathbb{R}^d$; $i = 1, \ldots, N$ with N large



2D Ansatz : "ground states can be parameterized as a uniform deformation of the (unit) triangular lattice $\mathbb{T}$"



The lattice spacing r^* is determined by minimization of

$$e(r) = \sum_{i \in \mathbb{T} \setminus \{0\}} J(r|i|)$$

(energy density of the uniformly dilated $r\mathbb{T}$).

Question 1 (Theil): Let u be a compact perturbation of $r^*\mathbb{T}$; then

$$\sum_{i \neq j} \Big(J(|u_i - u_j|) - J(r^*|i-j|) \Big) \geq 0,$$

with equality achieved iff u is a reparameterization of $u_i^* = r^* i$.

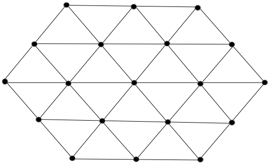
Note: this has been proved for “Lennard-Jones-like” potentials by Theil (earlier work by Radin)

“Challenges”: • prove that this holds for the L-J potential;
• prove the analogue for $d = 3$ (for what lattice?)

Question 2 (Friesecke): Consider the energy

$$E_N(u) = \sum_{i \neq j} J(|u_i - u_j|), \qquad i = 1, \ldots, N$$

Then, up to subsequences, the minimizers u^N tend to arrange on the same $r^*\mathbb{T}$ (up to rotations and translations). Furthermore, the scaled $\overline{u}_N = \frac{1}{\sqrt{N}} u^N$ tend to an hexagonal shape.



Note: this has been proved for very special potentials. The leading role is now played by a *surface energy* (rotationally invariant in the target space)

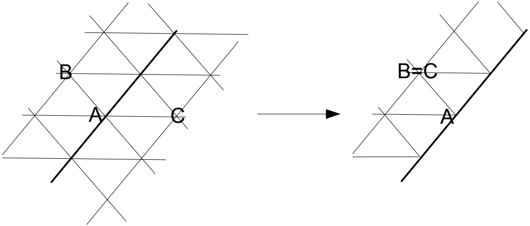
“Challenges”: • prove that this holds for general potentials;
• describe the effective continuum surface energy

Consequence of crystallization: (simplification of the discrete energies) we may restrict to nearest-neighbour (NN) interactions on regular lattices; e.g. to

$$E(u) = \sum_{i,j\ \mathbf{NN}} J(|u_i - u_j|)$$

(upon scaling r^* to 1) with $u : \mathbb{T} \to \mathbb{R}^2$.
Indeed this energy is *pointwise minimized* by (the identity on) $\mathbb{T}$.

Analytical problem: energies as such have *many more ground states*. Beside $\mathbb{T}$ we have "foldings"

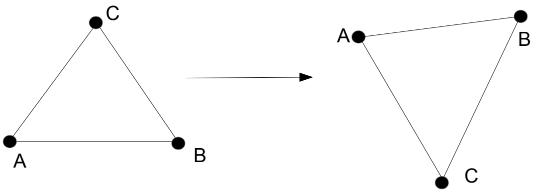


foldings of foldings, etc.

Proposed solution: (Friesecke-Theil) add the geometrical constraint

$$\det \nabla u \geq 0$$

(u extended to a piecewise-affine map).



(forbidden deformation)

Note: this is a three-point interaction (in 2D)

This addition rules out “flipping” and allows to state a first question on the asymptotic analysis of *energies*.

Energies of Continuum Mechanics

Small deformations (B-Solci-Vitali)
Scale the lattice size and localize energies on a bounded domain Ω:

$$E_\varepsilon(u) = \sum_{i,j \ \mathbf{NN}} \varepsilon^2 J\Big(\frac{|u_i - u_j|}{\varepsilon}\Big) \qquad \det \nabla u \geq 0$$

$u : \Omega \cap \varepsilon\mathbb{T} \to \mathbb{R}^2$. Suppose that

$$u_i = i + \delta v_i, \qquad\qquad \delta << \sqrt{\varepsilon}$$

Then E_ε Γ-converge to a linear elastic energy

$$F(u) = \int_\Omega W(\nabla u)\, dx$$

W obtained by Taylor-expanding J.

Main issue: deduce that the domain of F is $H^1(\Omega;\mathbb{R}^2)$ by a *rigidity estimate* (Friesecke-James-Müller); use the validity of the *Cauchy-Born rule* close to the identity to Taylor expand.

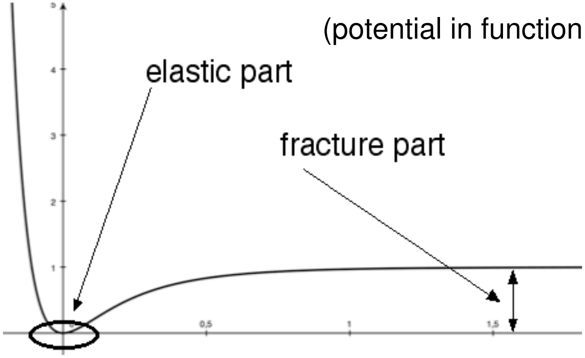
Note: the validity of the Cauchy-Born rule is a major computational issue (see Blanc, Le Bris and Lions, Weinan E *et al.*). It depends both on the lattice and the potentials.

Large deformations

... here it is not clear what the right question is!

1D case (B-Dal Maso-Garroni, Truskinovsky, B-Lew-Ortiz)
Relevant scaling: $\delta = \sqrt{\varepsilon}$. At this scaling we have the possibility of **fracture.**

(potential in function of v)



Γ-limit energy:

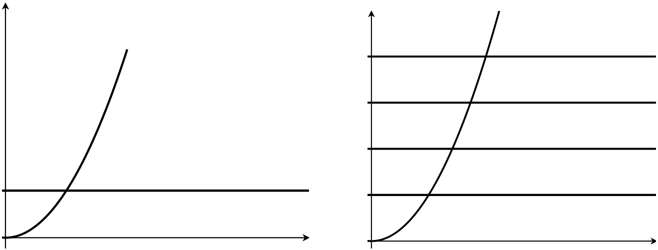
$$F_\varepsilon(v) = \alpha \int_\Omega |v'|^2\,dx + \beta\#(\text{ jump points of } v)$$

(one-dimensional *Griffith fracture energy*)
with the constraint that $v^+ > v^-$ at jump points
(*opening crack condition*)

Note: the scaling $\delta = \sqrt{\varepsilon}$ is justified by Γ*-expansion theory* (B-Truskinovsky). This also allows for a wider choice of the limit energy following additional criteria.

Possible additional criterion: accurate description of *local minimizers*

The pattern of the local minimizers for E_ε and F (in terms of the total displacement) are qualitatively different



Equivalent energies on the continuum:

$$F_\varepsilon(v) = \alpha \int_\Omega |v'|^2\,dx + \beta \sum_{\text{jump points of v}} g\Big(\frac{|v^+ - v^-|}{\varepsilon}\Big)$$

(*Barenblatt fracture energy with internal parameter*)
These energies have the same pattern of local minimizers as E_ε.

2D analysis (B- Gelli).

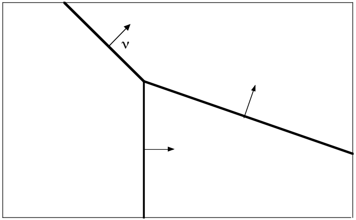
First issue: for large deformations there is no analytical technique to deal with the positive-determinant constraint.

We may consider the **surface scaling**:

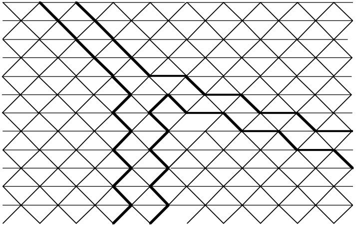
$$\frac{1}{\varepsilon}E_\varepsilon(u) = \sum_{NN} \varepsilon\Big(J\Big(\Big|\frac{u_i - u_j}{\varepsilon}\Big|\Big) - \min J\Big) \quad \text{(+ positive-det. constraint)}$$

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

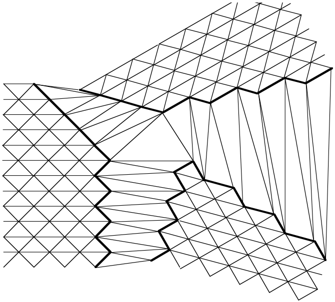
Domain of the limit: the limit is finite iff ∇u is a **piecewise rotation** (**piecewise rigidity** Chambolle-Giacomini-Ponsiglione);



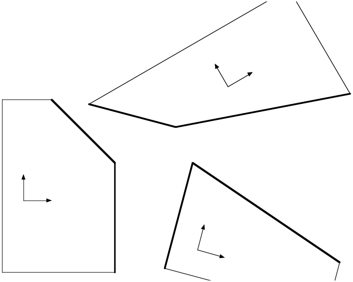
A reference configuration with fracture site and its macroscopic normals



An underlying triangulation at step ε



Deformed configuration at the level of the triangulation



Macroscopic deformed configuration

Very complex behaviour of the limit surface energy, accounting for

- possibility of appearance of layers of cracks at interfaces
- surface relaxation (rearrangement of boundary atoms)
- concentration of energy at triple points
- non-local effects

Note: there is no theory for such types of energies, which seem to arise naturally when dealing with many-points interactions.

Even bigger "challenges"

The static picture can give an idea of some type of dynamics ("gradient-flow type")

- for "fast motions" we have a "gradient flow" of the static limit
- for "slow motions" the system may be trapped by local minimizers (pinning).
- the relevant motion is obtained at one (or more) intermediate time-scale.

Note: for interfacial energies the relevant motion is a "discontinuous" mean-curvature flow depending on the microstructure of interactions (B-Gelli-Novaga, B-Scilla).

Note: for motion of fracture even the gradient flow of the static limit (Grittith energy) is not known.