Looking for a macroscopic behavior for 2d-lattices.

- Modern understanding: within the “elastic range”, for all BC, the lattice can be replaced by an elastic membrane whose internal energy density is given by the Cauchy-Born density

\[ W_{CB} : F \in \mathbb{M}_{3,2} \mapsto W_{CB}(F) \in \mathbb{R}. \]

**Example:** hexagonal lattices obtained by superposing two simple lattices. Separate nodes in type 1 nodes and type 2 nodes. Write

\[ W_{CB}(F) = \inf_{\tau \in \mathbb{R}^3} W(F, \tau) \]

where \( \tau \) originates from the discrepancy between a node 1 and a node 2 and \( W(F, \tau) \) expresses the base cell energy.

*Can we recover such energies by rigorous methods?*

A. Braides et al., Several papers for two-point interactions. *circa* 2000


Square lattices:

First. Two-point interactions: length changes only.
Introduce a sequence of lattices with mesh size $\varepsilon$.

Internal energy:

$$I^\varepsilon(\psi) = \kappa \sum (|\psi(b_k)| - \varepsilon)^2$$

where

$$\psi(b_k) = \psi(b_k^\varepsilon) = \psi(\varepsilon(i+1,j)) - \psi(\varepsilon(i,j)) \text{ or } \psi(\varepsilon(i,j+1)) - \psi(\varepsilon(i,j))$$

for lattice deformations $\psi : N^\varepsilon(\text{nodes}) \mapsto \mathbb{R}^3$.

$$\min J^\varepsilon = I^\varepsilon - G^\varepsilon$$
over the lattice deformations
**Classical trick:** introduce lattice triangulations, identify $\psi: \mathcal{N}_\varepsilon \mapsto \mathbb{R}^n$ with its piecewise affine interpolate at the nodes.

Then, $I^\varepsilon$ rewrites

$$I^\varepsilon(\psi) = \int_\omega W(\nabla \psi) \, dx, \quad W(F) = k \left((|u| - 1)^2 + (|v| - 1)^2\right) \quad \text{for} \quad \psi \in \mathcal{A}(\varepsilon).$$

(note that the dependence in $\varepsilon$ is in the affine function space $\mathcal{A}(\varepsilon)$).

Set $I^\varepsilon(\psi) = +\infty$ for $\psi \in L^2(\omega) \setminus \mathcal{A}(\varepsilon)$. This does not change the Min.

One easily obtains that $I^\varepsilon$ $\Gamma$-converges in $L^2(\omega)$ to $I$ defined by

$$I(\psi) = \int_\omega QW(\nabla \psi(x)) \, dx$$

that applies to $\psi: \omega \mapsto \mathbb{R}^3$.

Close to Cauchy-Born rule. Indeed,

$$W(F) = k \left((|u| - 1)^2 + (|v| - 1)^2\right), \quad QW(F) = k \left([^u - 1^2]_{+} + [^v - 1^2]_{+}\right)$$
Second. Three-point interactions: Squares with moments, angles.
Correct energies in mechanical network and atomistic lattices modeling should incorporate some resistance to shear. See Stillinger-Weber and Tersoff models.

\[ I^\varepsilon(\psi) = \kappa_1 \sum (|\psi(b_k)| - \varepsilon)^2 + \sum M_{k,l}(\psi) \]

where

\[ M_{k,l}(\psi) = \kappa_2 \varepsilon^2 \left( \frac{\psi(b_k)}{|\psi(b_k)|} \cdot \frac{\psi(b_l)}{|\psi(b_l)|} \right)^2 \]

No way of expressing green and red angles in terms of our piecewise affine functions. Introduce a second triangulation.

and a second piecewise affine mapping: \( \tilde{\psi} \) piecewise affine on the new triangulation that coincides with \( \psi \) at all nodes.
Integral form of the energy:

\[
I^\varepsilon(\psi) = \int_\omega \left( (|\partial_1 \psi| - 1)^2 + (|\partial_2 \psi| - 1)^2 + \left( \frac{\partial_1 \psi}{|\partial_1 \psi|} \cdot \frac{\partial_2 \psi}{|\partial_2 \psi|} \right)^2 \right) dx,
\]

\[
+ (|\partial_1 \tilde{\psi}| - 1)^2 + (|\partial_2 \tilde{\psi}| - 1)^2 + \left( \frac{\partial_1 \tilde{\psi}}{|\partial_1 \tilde{\psi}|} \cdot \frac{\partial_2 \tilde{\psi}}{|\partial_2 \tilde{\psi}|} \right)^2 \right) dx,
\]

\[
I^\varepsilon(\psi) \text{ reads as well}
\]

\[
I^\varepsilon(\psi) = \begin{cases} 
\int_\omega W(\nabla \psi(x)) \, dx + \int_\omega W(\nabla \tilde{\psi}(x)) \, dx, & \psi \in \mathcal{A}_\varepsilon^* \\
+\infty, & \psi \in L^2(\omega) \setminus \mathcal{A}_\varepsilon^*
\end{cases}
\]

Convergence result. \(I^\varepsilon \Gamma\)-converges to \(I\) defined by

\[
I(\psi) = 2 \int_\omega QW(\nabla \psi(x)) \, dx, \quad \psi \in H^1_\Gamma(\omega; \mathbb{R}^n).
\]

Close to Cauchy-Born rule again.

Comments:

- qualitative results on “compressed states” with zero energy, but no explicit formula for \(QW\).
- generalizes to general three-point energies with some (natural) compatibility conditions. Otherwise: homogenization required.
Hexagonal lattices

Complex lattices with type 1 nodes (black), and type 2 nodes (white),

Let us first describe the global hexagonal network in $\mathbb{R}^2$. Let $(e_1, e_2)$ be an orthonormal basis in $\mathbb{R}^2$, and introduce the three vectors $s = \sqrt{3} e_1$, $t = \sqrt{3} e_1 + 3 e_2$, and $p = \frac{1}{3} (s + t)$.

In our description, the network is comprised of two types of nodes: The type 1 nodes that occupy points $i + j t$ with $(i, j) \in \mathbb{Z}^2$, and the type 2 nodes that occupy points $i + j t + p$, again with $(i, j) \in \mathbb{Z}^2$, see Figure 1 below. The hexagonal network is thus a complex lattice, a superposition of two simple Bravais lattices which are translates of each other, shown with different dashed lines below. We are following here the standard description of such complex lattices, see [5].

The hexagonal nature of the sheet is not yet apparent. We now assume that the internal energy of the sheet only derives from chemical bonds that join type 1 nodes to their nearest neighboring type 2 nodes. We model these bonds by bars. There are thus three types of bars: Type 1 bars parallel to $s - p$, type 2 bars parallel to $t - p$, and type 3 bars parallel to $p$, see Figure 2 below. This classification of bars is only for labeling reasons, all bars are physically equivalent.

Unit cell: $T_f$ full triangle, $T_e$ empty triangle.
First: length changes only.

Deformation description: \( \chi : \mathcal{N}^\varepsilon \mapsto \mathbb{R}^3 \).

\[
I^\varepsilon(\chi) = \kappa \sum (|\chi(b_k)| - \varepsilon)^2.
\]

With \( \chi \) we associate
- a piecewise affine function \( \psi \) by \( \psi = \chi \) at nodes 1.
- a piecewise constant function \( \gamma \), deviation between nodes 2 and 1.

On full triangles \( \gamma = \chi(2) - \chi(1) \). On empty triangles, \( \gamma = 0 \).

Deformed bar 1 length = \( |(\varepsilon \partial_s \psi - \gamma)(x)| \) for any \( x \) in the associated full triangle. This allows us to rewrite the internal energy as an integral.

\[
I^\varepsilon(\psi, \gamma) = \int_\omega W^\varepsilon(\varepsilon^{-1} x, D\psi(x), \gamma(x)) \, dx
\]

where \( W^\varepsilon : \mathbb{R}^2 \times \mathcal{L}(\mathbb{R}^2; \mathbb{R}^3) \times \mathbb{R}^3 \to \mathbb{R} \) is defined by

\[
W^\varepsilon(y, g, \tau) = 2 \left[ (|g(s) - \varepsilon^{-1} \tau| - 1)^2 + (|g(t) - \varepsilon^{-1} \tau| - 1)^2 + (\varepsilon^{-1} |\tau| - 1)^2 \right],
\]

if \( y \in T_f + \mathbb{L} \), 0 if \( y \in T_e + \mathbb{L} \).

Note that the energy is not homogeneous on a cell.
Obtaining the $\Gamma$-limit

- Define $W_0: \mathbb{R}^2 \times \mathcal{L}(\mathbb{R}^2; \mathbb{R}^3) \to \mathbb{R}$, $W_0(y, g) = \inf_{\tau \in \mathbb{R}^3} W^\varepsilon(y, g, \tau)$.

$W_0$ no longer depends on $\varepsilon$. It is still $\Gamma$-periodic.

Potentially analogous construction in E & Ming, and in Born.

Expliciting $W_0$ leads to (unsolved) innocent looking problems on triangles.

- Finally, for all $\psi \in H^1_\Gamma(\omega; \mathbb{R}^3)$,

$$\Gamma \text{- lim}_{\varepsilon \to 0} I^\varepsilon = \int_\omega W_{\text{hom}}(D\psi(x)) \, dx$$

where

$$W_{\text{hom}}(g) = \inf_{k \in \mathbb{N}} \frac{1}{k^2} \left( \inf_{\theta \in \mathbb{A}(kY)} \int_{kY} W_0(y, g + D\theta(y)) \, dy \right).$$

Comments:
- heuristic Cauchy-Born rule is still visible, because we are looking for it,
- does not resist taking angles into account.

Proof: slicing method by De Giorgi and some arguments by Müller (1997).

Expected properties are there:
- $W_{\text{hom}}$ is frame indifferent (obvious),
- Its material symmetry group contains rotations with angle a multiple of $\pi/3$ (not obvious).
Second: angles and Lennard-Jones (work “at the end” of progress)

Deformation description: $\chi : N^e \mapsto \mathbb{R}^3$.

$$I^e(\chi) = \sum_k B^e_k(\chi) + \sum_k R^e_k(\chi) + \sum_{k,l} M^e_{kl}(\chi)$$  \hspace{1cm} (1)

with

$$B^e_k(\chi) = \kappa_1 \sum (|\chi(b_k)| - \varepsilon)^2 = \varepsilon^2 \kappa_1 \sum (\varepsilon^{-1}|\chi(b_k)| - 1)^2$$

$$R^e_k(\chi) = \varepsilon^2 r(\varepsilon^{-1}|\chi(b_k)|), \text{ Lennard-Jones energy } r(l) \to +\infty, l \to 0$$

$$M_{k,l}(\chi) = \varepsilon^2 \kappa_2 \left( \frac{\chi(b_k)}{|\chi(b_k)|} \cdot \frac{\chi(b_l)}{|\chi(b_l)|} + \frac{1}{2} \right)^2 \text{ rest angles: } \frac{2\pi}{3}$$

Previous approach: cannot be used. Lack of Lipschitz property of the energies with respect to the “deformation gradient”.

Other approach: Braides, Buttazzo, De Giorgi-Letta,… localization
Localization
Requires to define local energies on subsets $U$ of the sheet $\omega$ the lattice lies on as functionals of pairs (function $\psi$, subset $U$). Then, obtain by Buttazzo theorem that the limit energy reads

$$I(\psi, U) = \int_U W(x, \nabla \psi(x)) \, dx = \int_U W(\nabla \psi(x)) \, dx$$

Buttazzo theorem
i) for all $\psi \in H^1(\omega; \mathbb{R}^3)$, the mapping $U \mapsto I(\psi, U)$ is a Borel measure,
ii) there exists a constant $C$ such that for all $\psi \in H^1(\omega; \mathbb{R}^3)$ and all $U \in \partial$, $I(\psi, U) \leq C \int_U (1 + |\nabla \psi|^2) \, dx$,
iii) $I$ is local, i.e., $I(\psi_1, U) = I(\psi_2, U)$ whenever $\psi_1 = \psi_2$ a.e. on $U$,
iv) ....
v) ....

Then there exists a Carathéodory function $W: \omega \times M_{3,2} \to \mathbb{R}^+$ such that

$$I(\psi, U) = \int_U W(x, \nabla \psi(x)) \, dx$$

(2)

for all $\psi \in H^1(\omega; \mathbb{R}^3)$ and $U \in \partial$.
vi) If, for all affine $\psi$, $I(\psi, B) = I(\psi, B')$ where $B$ and $B'$ are balls of the same radius included in $\omega$, then $W$ does not depend on $x$. 
To do so.
- with \( \chi \) we associate its piecewise affine function \( \psi \) on a Delaunay triangulation: functional space \( \mathcal{A}(\varepsilon) \),

- we define the local energy: for \( \psi \in \mathcal{A}(\varepsilon) \),

\[
I^{\varepsilon}(\psi, U) = \sum_{b_k \subset t \in T_m(U)} (B_k^\varepsilon(\psi) + R_k^\varepsilon(\psi)) + \sum_{t_{kl} \in T_m(U) \cup T_a(U)} M_{kl}^\varepsilon(\psi)
\]

Otherwise, \( I^{\varepsilon}(\psi, U) = +\infty \).
Tools:
- reduce Lennard-Jones: Let $\psi^\varepsilon \in \mathcal{A}(\varepsilon)$, $\psi^\varepsilon \to \psi$ in $L^2(\omega)$. There exists $\bar{\psi}^\varepsilon \in \mathcal{A}(\varepsilon)$, $\bar{\psi}^\varepsilon \to \psi$ in $L^2(\omega)$, the deformed lengths of all bars “not small’ and

$$I^\varepsilon(\bar{\psi}^\varepsilon, U) \leq I^\varepsilon(\psi^\varepsilon, U).$$

Then,

$$\Gamma - \lim \sup I^\varepsilon(\psi, U) \leq C(\|\nabla \psi\|^2_{L^2(U)} + |U|).$$

- inner regularity, superadditivity, subadditivity: be precise on triangles that are included in subsets. Quite intricated, but user’s friendly theorems in Braides-De Franceschi.

Then, conclude that $I^\varepsilon \Gamma$-converge to $I$ of the form

$$I(\psi) = \int_\omega W(\nabla \psi(x)) \, dx$$

Identify $W$.
- first, introduce boundary conditions.

$$I^\varepsilon_{bc}(\psi) = \begin{cases} 
I^\varepsilon(\psi) & \text{if } \psi - \Pi^\varepsilon \varphi_0 \in H^1_0(\omega; \mathbb{R}^3), \\
+\infty & \text{otherwise},
\end{cases}$$
There holds $\Gamma$-convergence to

$$I_{bc}(\psi) = \begin{cases} \int_{\omega} W(\nabla \psi) \, dx & \text{if } \psi - \varphi_0 \in H^1_0(\omega; \mathbb{R}^3), \\ +\infty & \text{otherwise.} \end{cases} \tag{3}$$

The limit energy is not modified by conditions of place.

- second,

$$W(g) = \frac{1}{|Y|} \min \{ \int_Y W(\nabla \psi) \, dx ; \psi - gx \in H^1_0(Y; \mathbb{R}^3) \} \quad \text{(quasiconvexity)}$$

$$= \frac{1}{|Y|} \min \{ I_{bc}(\psi, Y) ; \psi - gx \in H^1_0(Y; \mathbb{R}^3) \} \quad \text{(def)}$$

$$W(g) = W_{\text{hom}}(g) := \inf_{k \in \mathbb{N}^*} \left\{ \frac{1}{k^2} \inf_{\psi \in \mathcal{A}(kY)} \min_{\psi = gx \text{ on } \partial kY} I^1(\psi, kY) \right\}.$$