Finite elements and multi-scale modelling of crystalline materials

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based on work with

- E. Süli, (Oxford) [Atomistic to Continuum passage] *Archive for Rational Mechanics and Analysis, 2013*
- D. Mitsoudis (Athens), P. Rosakis (Crete) [A/C coupling: MultiD] *Applied Mathematics Research Express, 2014, and ongoing work*

Plan of the talk

- Part I : General discussion
  - numerical modeling-sensitivity of schemes
  - model adaptivity
- Part II : Atomistic to continuum passage: Consistency of Cauchy-Born Approximations
- Part III: Atomistic/continuum coupling : design of ghost force free methods

Self adapted methods: smart use of computational resources

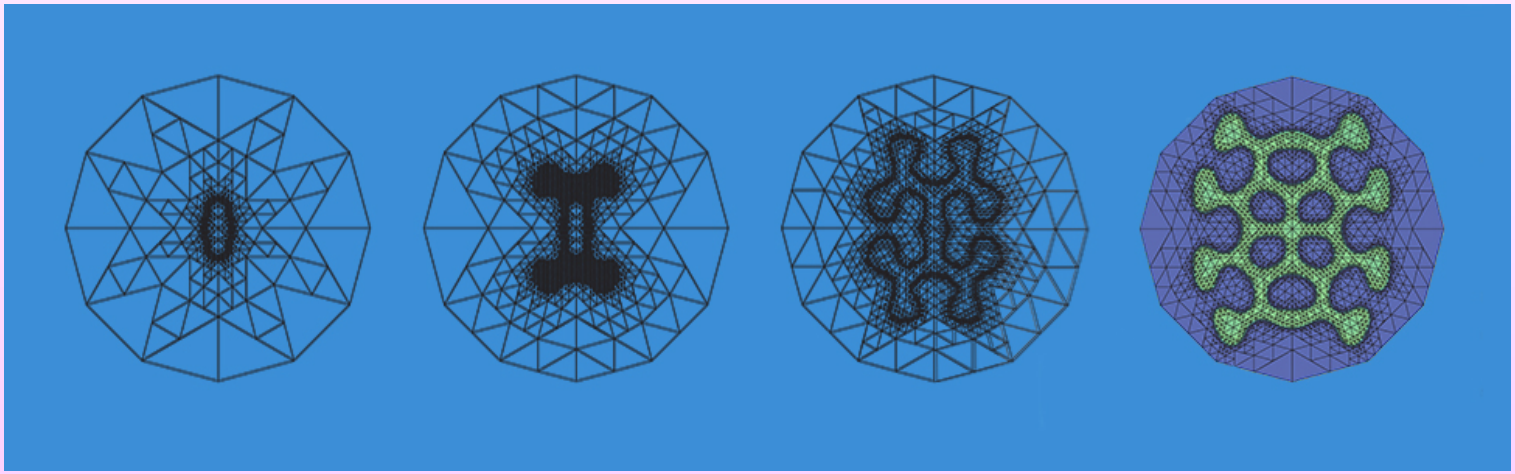
For a given number of degrees of freedom $N*$, we seek approximations $u_{N*}(t)$ such that

- $u_{N*}(t)$ is much better approximation than
- $u_{N*,\text{uniform}}(t)$

Key issues:

- the algorithm should be able to detect the areas of interest of the solution
- Goal: design of intelligent algorithms able to adapt to the "solution" during computation

Self adapted methods: Mesh Adaptation



Self adapted methods: adaptive modeling

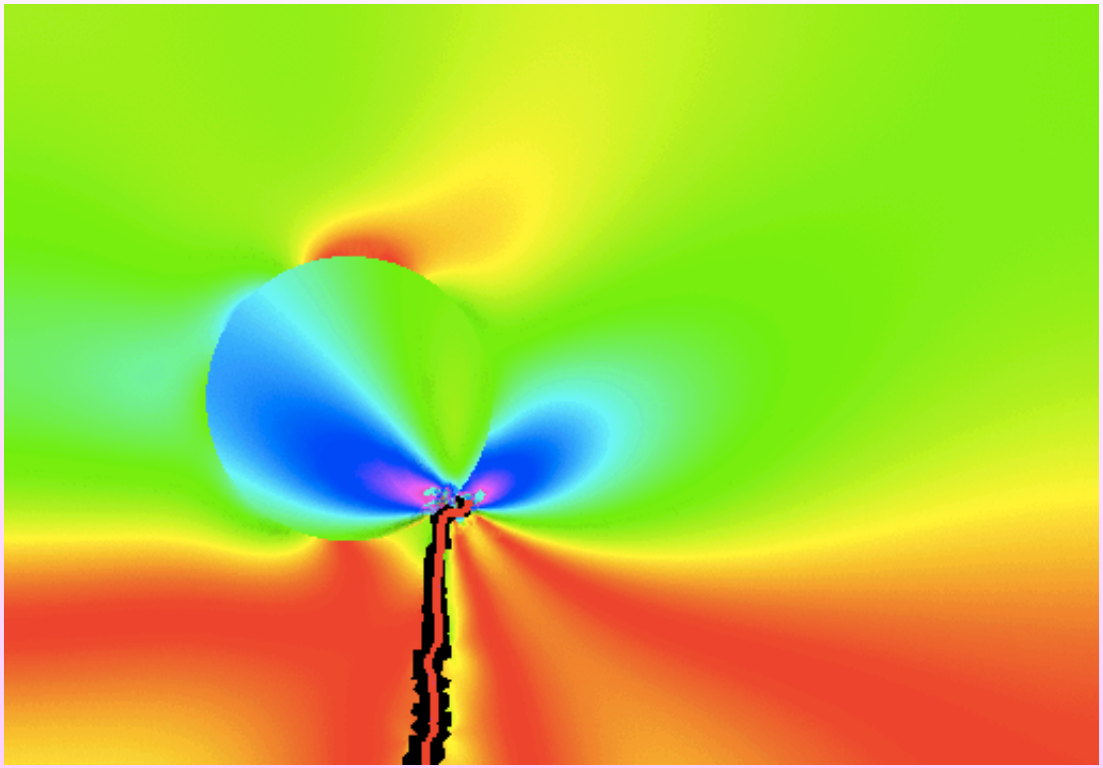
What about if we are not happy with our model?

change the model during the computation: Use different models in different areas of the computational domain / multiscale - complex systems models coupling information at different scales.
WHY?

- reduce the prohibitively high number of degrees of freedom
- not known models at the macroscale

We face new problems for numerical modeling where modelling, analysis, computations should be combined.
We focus on an important such class of problems: atomistic - continuum coupling in crystals.

An example where continuum theory fails to provide satisfactory models: Crack propagation in Crystals



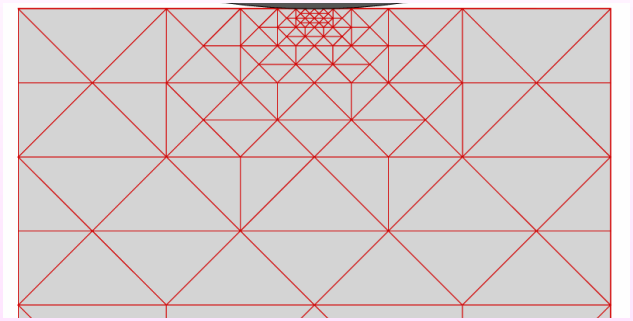
- Valid model only at the microscopic (atomistic) scale.
- There is no (nonlinear) PDE which serves as an acceptable model (at the macro scale) (!)
- Direct atomistic simulations: Extremely high number of unknowns

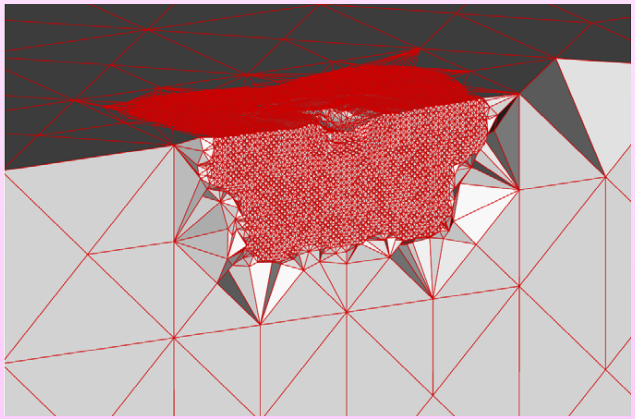
Modeling and adaptivity: coupled atomistic / continuum models

- Aim: design of computational methods, based on hybrid (atomistic-continuous) approximations, for both stationary and evolution problems.

  Goal: Computation with atomistic accuracy at the cost of continuous computational techniques.

Crystals in Materials





Ortiz et. all. 2003

No continuum models are known to describe the atomistic model when defects are present: The quasi-continuum idea (atomistic/continuum coupling) seems natural *Tadmor, Ortiz & Phillips 1996* compare to the work in multiscale modeling of materials, e.g., *Lu & Kaxiras: Review article 2005.* Several works in the engineering literature.

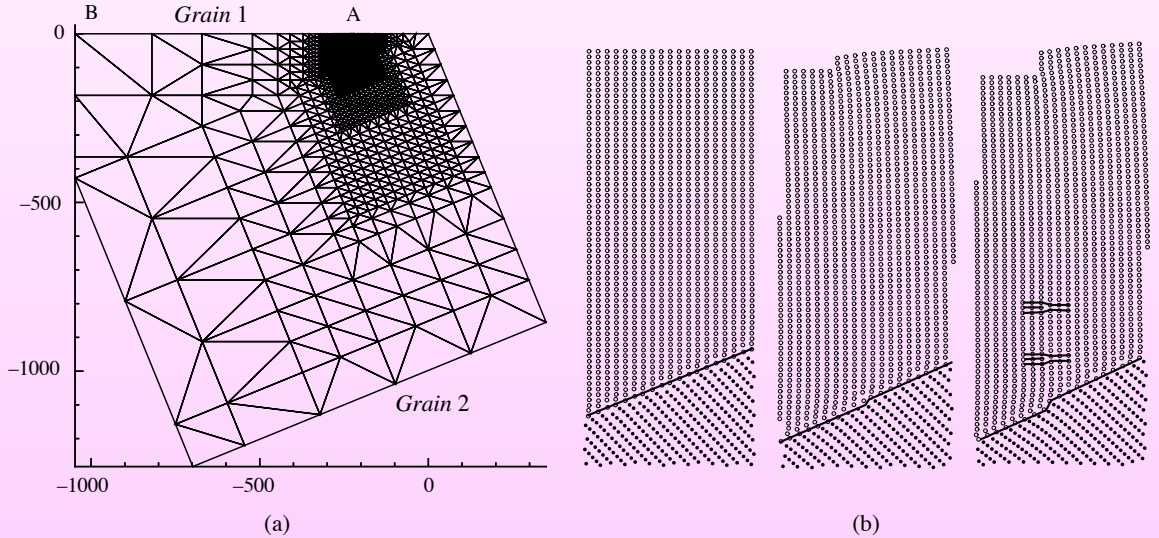


Figure 6. Example of a multiscale simulation using the quasicontinuum method. (a) Finite-element mesh used to model dislocation-grain boundary interaction. The surface marked AB is rigidly indented to generate dislocations at A (distance in Amstroms). (b) Snapshots of atomic positions at different stages in the deformation history. Absorption of the first pair of dislocations at the GB results in a step, while the second pair form a pileup.

Figure: Lu & Kaxiras 2005

Mathematical understanding and method development: Current status and open problems

- The formulation and behavior of such methods has been understood to a satisfactory extend in *one dimension*. *Luskin, et al, Dobson, Luskin & Ortner, Ortner & Süli,*
  Ming & E, Abdulle, Lin & Shapeev, Gunzburger & Zhang, ...
- *Ongoing work by several groups:* The foundation and analysis of methods of quasicontinuum character in two and three dimensions.
- *Time-dependent case:* Models are used for the qualitative study of the propagation of face change interfaces as well as crystal dislocations arising in crystal grids. The evolution problem is of particular interest but it still remains unaccessible even at the engineering level.

  A basic technical issue: The existence of traveling waves of kink type (transition from one well to another) corresponding to moving dislocations under external pressure: Mathematical issues: nonclassical/dispersive shocks, oscillations, dispersive approximations, reflections at the interfaces

Atomistic problems in crystalline materials

- The atoms within a undeformed crystalline structure are assumed to be nodes of an $\mathbb{R}^d$ rectangular lattice.
- The (closest) interatomic distance is denoted by ε (lattice mesh size).
- The energy of a deformed crystal is described through given potentials accounting for interactions between atoms. (a highly nonlinear function involving "discrete derivatives")
- Atomistic problem: *energy minimisation problem* (Euler-Largange equations: "nonlinear difference equation")

Notation

Lattice, discrete domain, continuous domain: We consider a simple two dimensional lattice which is generated by two independent vectors of $\mathbb{R}^2$.
For simplicitywe will assume that the lattice $\mathcal{L}_{\text{entire}}$ is generated by the the unit vectors of $\mathbb{R}^2$, e_1, e_2.
We will consider discrete periodic functions on $\mathcal{L}_{\text{entire}}$ with periodic domain $\mathcal{L}$.
To be specific let

$$\mathcal{L} = \left\{ \ell = (\ell_1\,, \ell_2) \in \mathbb{Z}^2 \cap [-N_1 - 1, N_1] \times [-N_2 - 1, N_2] \right\}.$$

The actual configuration of the atoms is thus a subset of $\mathbb{R}^2$ which we call *discrete domain* and we denote by Ω_{discr}. The corresponding *continuous domain* is denoted by Ω :

$$\Omega_{\text{discr}} = \left\{ x_{\boldsymbol{\ell}} = (x_{\ell_1}\,, x_{\ell_2}) = \varepsilon\, \ell\,, \quad \ell \in \mathcal{L} \right\},$$
$$\Omega = \left\{ x \in [x_{-N_1-1}, x_{N_1}] \times [x_{-N_2-1}, x_{N_2}] \right\}^o,$$

Functions and spaces: We consider atomistic deformations

$$y_\ell = y(x_\ell)\,, \quad \ell \in \mathcal{L} \quad \text{of the form}$$
$$y_\ell = Fx_\ell + v_\ell, \quad \text{with } v_\ell = v(x_\ell) \text{ periodic with respect to } \mathcal{L}\,.$$

The corresponding spaces for y and v are denoted by $\mathcal{X}$ and $\mathcal{V}$:

$$\boldsymbol{\mathcal{X}} = \{y : \mathcal{L} \to \mathbb{R}^2, \quad y_\ell = Fx_\ell + v_\ell, \quad v \in \mathcal{V}\}\,,$$
$$\mathcal{V} = \{u : \mathcal{L} \to \mathbb{R}^2, \quad u_\ell = u(x_\ell) \quad \text{periodic with respect to } \mathcal{L}\}\,.$$

For functions $y, v : \mathcal{L} \to \mathbb{R}^2$ we define the product

$$\langle\, y, v \,\rangle_\varepsilon := \varepsilon^d \sum_{\ell \in \mathcal{L}} y_\ell \, v_\ell\,.$$

Discrete and continuous derivatives:

$$\overline{D}_\eta y_\ell = \frac{y_{\ell+\eta} - y_\ell}{\varepsilon}, \qquad \ell,\ \ell+\eta \in \mathcal{L},$$

$$\partial_{\zeta_i}\phi(\zeta) = \frac{\partial\phi(\zeta_1,\ldots,\zeta_d)}{\partial\zeta_i}\,, \qquad \zeta = (\zeta_1,\ldots,\zeta_d)\,,$$

$$\nabla_\zeta\phi(\zeta) = \left\{\partial_{\zeta_i}\phi(\zeta)\right\}_i\,,$$

$$\partial_i v(x) = \frac{\partial v(x)}{\partial x_i},$$

$$\nabla u(x) = \left\{\frac{\partial u^i(x)}{\partial x_\alpha}\right\}_{i\alpha}.$$

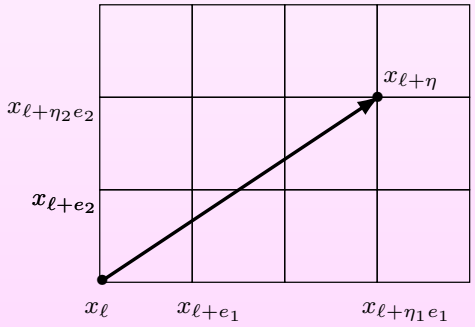
To avoid confusion we distinguish between derivatives with respect to arguments—denoted by ∂_{ζ_i}—which usually appear in composite functions and derivatives with respect to the spatial variable x_i and denoted by ∂_i .

Atomistic and Cauchy Born potential:

We consider the atomistic potential

$$\Phi^a(y) = \varepsilon^d \sum_{\ell \in \mathcal{L}} \sum_{\eta \in R} \phi_\eta \left(\overline{D}_\eta y_\ell \right),$$

where R is the set of interaction vectors.



For a given field of external forces $f : \mathcal{L} \to \mathbb{R}^2$ the atomistic problem reads:

find a local minimizer y^a in $\mathcal{X}$ of :

$$\Phi^a(y^a) - \langle f, y^a \rangle_\varepsilon .$$

If such a minimizer exists, then

$$\langle D\Phi^a(y^a), v \rangle_\varepsilon = \langle f, v \rangle_\varepsilon , \qquad \text{for all } v \in \mathcal{V} .$$

Here,

$$\langle D\Phi^a(y), v \rangle_\varepsilon = \varepsilon^d \sum_{\ell \in \mathcal{L}} \sum_{\eta \in R} \nabla_\zeta \phi_\eta \left(\overline{D}_\eta y_\ell \right) \cdot \overline{D}_\eta v_\ell .$$

Reverse point of view:

- The atomistic problem is the exact problem (discrete difference scheme)
- Aim: find a continuum approximation (a PDE) to the atomistic model

A continuum model for smooth deformations: Cauchy Born approximation

The corresponding Cauchy-Born stored energy function is

$$W(F) = W_{CB}(F) = \sum_{\eta \in R} \phi_\eta \left(F\,\eta\right),$$

find a local minimizer y^{CB} in X of :

$$\Phi^{CB}(y) - \langle f, y^{CB} \rangle = \int_\Omega W(\nabla y^{CB}) - \langle f, y^{CB} \rangle \,.$$

Here

$$X = \{y : y : \Omega \to \mathbf{R}^d, \quad y(x) = Fx + v(x), \quad v \in V\}\,,$$

$$V = \{u : \Omega \to \mathbf{R}^d, \quad u \in W^{k,p}(\Omega, \mathbf{R}^d) \cap W^{1,p}_{\#}(\Omega, \mathbf{R}^d), \quad \int_\Omega u dx = 0\}\,.$$

If such a minimizer exists, then

$$\langle D\Phi^{CB}(y), v\rangle = \int_\Omega S_{i\alpha}(\nabla y(x))\,\partial_\alpha v^i(x)\,dx = \langle f, v\rangle\,, \qquad v \in V\,.$$

The stress tensor is defined through

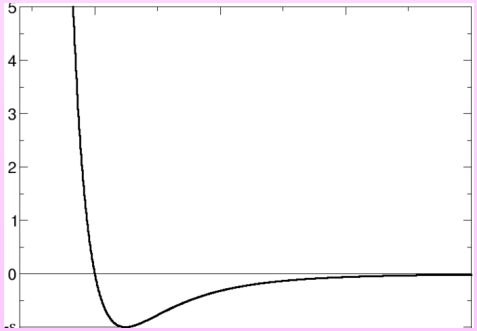
$$S := \left\{\frac{\partial W(F)}{\partial F_{i\alpha}}\right\}_{i\alpha}.$$

A simple calculation yields the relation between the stress tensor and the atomistic potential,

$$\begin{aligned} S_{i\alpha} =& \frac{\partial W(F)}{\partial F_{i\alpha}} = \frac{\partial}{\partial F_{i\alpha}} \sum_{\eta\in R} \phi_\eta\,(F\,\eta) \\ =& \frac{\partial}{\partial F_{i\alpha}} \sum_{\eta\in R} \phi_\eta\,(F_{j\beta}\,\eta_\beta) = \sum_{\eta\in R} \partial_{\zeta_j}\phi_\eta\,(F_{j\beta}\,\eta_\beta)\frac{\partial}{\partial F_{i\alpha}} F_{j\beta}\,\eta_\beta \\ =& \sum_{\eta\in R} \partial_{\zeta_i}\phi_\eta\,(F\,\eta)\,\eta_\alpha\,. \end{aligned}$$

Remarks on the relation between the atomistic and continuum CB models

- The continuum model approximates the atomistic only when deformations are sufficiently smooth. *X. Blanc, C.LeBris & P.L. Lions 2002 and W. E. & P. Ming 2008*
  See also: *G. Friesecke & F. Theil 2002*
- results based on different notions of consistency
- *Key issues:*
  - The interaction potential is non-convex: e.g. $\phi_\eta(r) = V(|r|)$, V the Lennard-Jones-Potential:



  - Long range interactions vs. interactions only of next neighbors (only adjacent atoms interact)

One dimensional example.

- The simplest model:

$$\Phi^a(y) = \varepsilon \sum_{\xi \in \mathcal{L}} \sum_{r=1}^{2} \phi_r \left(\overline{D}_r y_\xi \right) = \varepsilon \sum_{\xi \in \mathcal{L}} \phi_1 \left(\overline{D}_1 y_\xi \right) + \phi_2 \left(\overline{D}_2 y_\xi \right).$$

Then the corresponding Cauchy-Born stored energy function is

$$W(F) = W_{CB}(F) = \sum_{r=1}^{2} \phi_r \left(F\, r \right) = \phi_1 \left(F \right) + \phi_2 \left(2F \right).$$

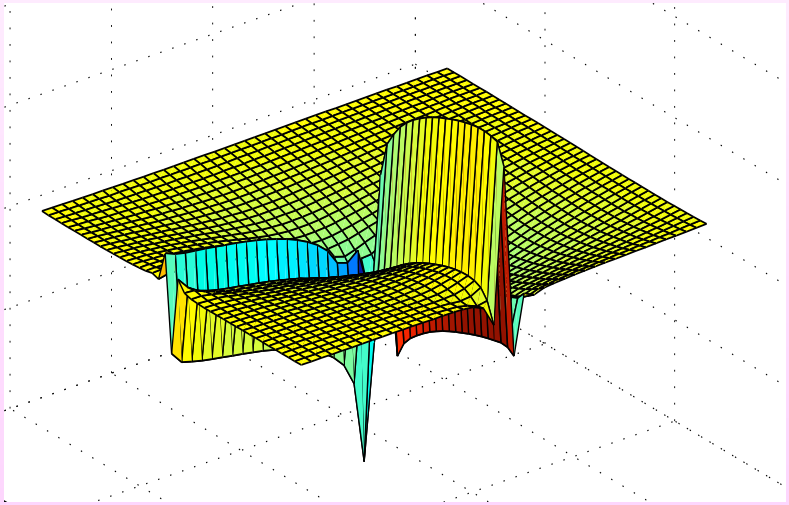
Then the atomistic Cauchy-Born model is defined through the atomistic potential:

$$\Phi^{a,CB}(y) = \varepsilon \sum_{\xi \in \mathcal{L}} W \left(\overline{D}_1 y_\xi \right) = \varepsilon \sum_{\xi \in \mathcal{L}} \phi_1 \left(\overline{D}_1 y_\xi \right) + \phi_2 \left(2\overline{D}_1 y_\xi \right).$$

The continuous potential is defined through

$$\Phi^{CB}(y) = \int_\Omega W(y'(x)) dx\,.$$

- *1D results / Consistency error on potentials (energies)* periodicity + symmetry $\rightarrow \ \mathcal{O}(\varepsilon^2)$
- *Standard coupling (coupling of energies)):* $\mathcal{O}(\varepsilon)$
    - Main Computational Problem: *ad-hoc* coupling $\rightarrow$ Ghost Forces



- *Why?*
- *Other couplings / other consistency notions* Methods with ghost forces are energy consistent
- Can we design Ghost-Force-Free methods?
- Force based coupling *Dobson & Luskin 2008*: Ghost-Force-Free / not energy based.

To understand better we need to go back to the uncoupled problem.

- We need a sharp analysis on the approximation properties of the continuum model
- Consistency analysis:
  - Variational Consistency:

$$\mathcal{C}_V(y) := \sup \Big\{ \; |\langle D\Phi^a(y), v\rangle_\varepsilon - \langle D\Phi^{CB}(y), v\rangle| \; : \\ v \in \mathcal{V} \quad \text{with } \|v\|_{W^{1,p}(\Omega)} = 1 \Big\},$$

    where in the last relation y is any smooth function. We we shall refer to $\mathcal{C}_V(y)$ as the *variational consistency error*.
  - *Energy Consistency error*

$$\mathcal{C}_\mathcal{E}(y) := |\Phi^a(y) - \Phi^{CB}(y)|.$$

Construction of an atomistic Cauchy-Born model in MultiD

- We provide a link of the continuous model to the atomistic model by introducing an intermediate model which we call *atomistic Cauchy-Born model (A-CB)* .
- To construct this model we start from the continuous model and perform appropriate approximate steps yielding finally the A-CB model. [Key : Link to Finite Elements]
- The final model has variational consistency error of the order $O(\varepsilon^2)$ compared to the continuous Cauchy-Born.
- We show that the A-CB has $O(\varepsilon^2)$ variational consistency error compared to the original atomistic model.

Bilinear Finite Elements on the Lattice: Let $\mathbb{V}_h$ be the space of bilinear periodic functions on the Lattice $\mathcal{L}$. To be specific let

$$\mathcal{T} = \{K \subset \Omega : \quad K = (x_{\ell_1}, x_{\ell_1+1}) \times (x_{\ell_2}, x_{\ell_2+1}), \quad x_{\boldsymbol{\ell}} = (x_{\ell_1}, x_{\ell_2}) \in \Omega_{\text{discr}}\},$$

$$\mathbb{V}_h = \{v : \Omega \to \mathbb{R}^2, \quad v \in C(\Omega),\ v|_K \in \mathbb{Q}_1(K) \text{ and } v_\ell = v(x_\ell) \quad \text{periodic}\},$$

where $\mathbb{Q}_1(K)$ denotes the set of bilinear functions on K :
$v|_K(x) = \alpha_0 + \alpha_1 x_1 + \alpha_2 x_2 + \alpha_3 x_1 x_2$.

The atomistic Cauchy-Born model :

Definition of the model.
We define the average discrete derivatives as follows:

$$\overline{\overline{D}}_{e_1} v_\ell = \frac{1}{2} \left\{ \overline{D}_{e_1} v_\ell + \overline{D}_{e_1} v_{\ell+e_2} \right\},$$
$$\overline{\overline{D}}_{e_2} v_\ell = \frac{1}{2} \left\{ \overline{D}_{e_2} v_\ell + \overline{D}_{e_2} v_{\ell+e_1} \right\}.$$

Thus we can define the discrete gradient matrix as

$$\left\{ \overline{\nabla} v_\ell \right\}_{i\alpha} = \overline{\overline{D}}_{e_\alpha} v_\ell^i \,.$$

We introduce the atomistic potential

$$\Phi^{a,CB}(y) = \varepsilon^d \sum_{\ell \in \mathcal{L}} \sum_{\eta \in R} \phi_\eta \left(\overline{\nabla} y_\ell \, \eta \right)$$
$$= \varepsilon^d \sum_{\ell \in \mathcal{L}} W_{CB}(\overline{\nabla} y_\ell) \,.$$

Now, for a given field of external forces $f : \mathcal{L} \to \mathbb{R}^d$ the *atomistic Cauchy-Born* problem reads:

find a local minimizer $y^{a,CB}$ in $\mathcal{X}$ of :

$$\Phi^{a,CB}(y^{a,CB}) - \langle f, y^a \rangle_\varepsilon \,.$$

If such a minimizer exists, then

$$\langle D\Phi^{a,CB}(y^{a,CB}), v \rangle_\varepsilon = \langle f, v \rangle_\varepsilon \,, \qquad \text{for all } v \in \mathcal{V} \,.$$

Theorem. (ENERGY CONSISTENCY.) Let y be a smooth function. Then the atomistic energy $\Phi^a(y)$ is is a second order approximation of the continuum Cauchy-Born energy $\Phi^{CB}(y)$ in the sense that there exists a constant $M_E = M_E(y)$,

$$\left|\Phi^a(y) - \Phi^{CB}(y)\right| \leq \; M_E\, \varepsilon^2.$$

Sketch of the Proof: We start from the continuum Cauchy-Born energy

$$\begin{aligned}
\Phi^{CB}(y) &= \int_\Omega W_{CB}(\nabla y(x))\, dx = \sum_{K\in\mathcal{T}} \int_K W_{CB}(\nabla y(x))\, dx \\
&= \sum_{K\in\mathcal{T}} |K| W_{CB}(\nabla y(m_K)) + \sum_{K\in\mathcal{T}} \int_K \Big[W_{CB}(\nabla y(x)) - W_{CB}(\nabla y(m_K))\Big]\, dx \\
&=: I_1 + I_2
\end{aligned}$$

where m_K is the barycenter of K. Using Bramble-Hilbert Lemma we get

$$\left|I_2\right| \leq \; C(y)\, \varepsilon^2.$$

We will compare I_1 to the atomistic energy $\Phi^a(y)$.

Since m_K is the barycenter of K the key point here is to rearrange the terms in $\Phi^a(y)$ in order to create symmetries around the cell K. In fact, using the periodicity, we have

$$\begin{aligned}\Phi^a(y) =& \varepsilon^d \sum_{\ell\in\mathcal{L}} \sum_{\eta\in R} \phi_\eta\left(\overline{D}_\eta y_\ell\right)\\ =& \varepsilon^d \sum_{\ell\in\mathcal{L}} \sum_{\eta\in R} \frac{1}{4}\Big[\phi_\eta\left(\overline{D}_\eta y_\ell\right) + \phi_\eta\left(\overline{D}_\eta y_{\ell-(\eta_1-1)e_1}\right) + \phi_\eta\left(\overline{D}_\eta y_{\ell-(\eta_2-1)e_2}\right)\\ &+ \phi_\eta\left(\overline{D}_\eta y_{\ell-(\eta_1-1)e_1-(\eta_2-1)e_2}\right)\Big].\end{aligned}$$

.....

Comparison of atomistic Cauchy-Born and atomistic models:
Atomistic stresses

To compare the atomistic and atomistic Cauchy-Born models we start from the atomistic potential and notice:

$$\begin{aligned}\langle D\Phi^a(y), v\rangle_\varepsilon &= \varepsilon^d \sum_{\ell\in\mathcal{L}} \sum_{\eta\in R} \nabla_\zeta \phi_\eta\left(\overline{D}_\eta y_\ell\right) \cdot \overline{D}_\eta v_\ell \\ &= \varepsilon^d \sum_{\ell\in\mathcal{L}} \sum_{\eta\in R} \nabla_\zeta \phi_\eta\left(\overline{D}_\eta y_\ell\right) \cdot \left\{\frac{1}{2}\overline{D}_{\eta_1 e_1} v_\ell + \frac{1}{2}\overline{D}_{\eta_1 e_1} v_{\ell+\eta_2 e_2}\right\} \\ &\quad + \varepsilon^d \sum_{\ell\in\mathcal{L}} \sum_{\eta\in R} \nabla_\zeta \phi_\eta\left(\overline{D}_\eta y_\ell\right) \cdot \left\{\frac{1}{2}\overline{D}_{\eta_2 e_2} v_\ell + \frac{1}{2}\overline{D}_{\eta_2 e_2} v_{\ell+\eta_1 e_1}\right\}\end{aligned}$$

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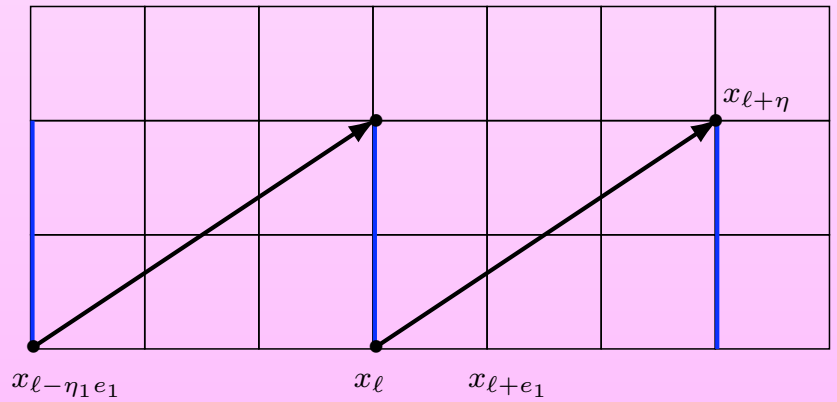


Due to the periodicity,

$$\begin{aligned}\left\langle D\Phi^a(y), v\right\rangle_\varepsilon &= \varepsilon^d \sum_{\ell\in\mathcal{L}} \sum_{\eta\in R} \nabla_\zeta \phi_\eta\left(\overline{D}_\eta y_\ell\right) \cdot \overline{D}_\eta v_\ell \\ &= \varepsilon^d \sum_{\ell\in\mathcal{L}} \sum_{\eta\in R} \left\{\frac{1}{2}\nabla_\zeta \phi_\eta\left(\overline{D}_\eta y_\ell\right) + \frac{1}{2}\nabla_\zeta \phi_\eta\left(\overline{D}_\eta y_{\ell-\eta_2 e_2}\right)\right\} \cdot \overline{D}_{\eta_1 e_1} v_\ell \\ &\quad + \varepsilon^d \sum_{\ell\in\mathcal{L}} \sum_{\eta\in R} \left\{\frac{1}{2}\nabla_\zeta \phi_\eta\left(\overline{D}_\eta y_\ell\right) + \frac{1}{2}\nabla_\zeta \phi_\eta\left(\overline{D}_\eta y_{\ell-\eta_1 e_1}\right)\right\} \cdot \overline{D}_{\eta_2 e_2} v_\ell\,.\end{aligned}$$

Since,

$$\begin{aligned}\overline{D}_{\eta_1 e_1} v_\ell &= \overline{D}_{e_1} v_\ell + \cdots + \overline{D}_{e_1} v_{\ell+(\eta_1-1)e_1}\,, \\ \overline{D}_{\eta_2 e_2} v_\ell &= \overline{D}_{e_2} v_\ell + \cdots + \overline{D}_{e_2} v_{\ell+(\eta_2-1)e_2}\,,\end{aligned}$$

we conclude

$$\begin{aligned}&\left\langle D\Phi^a(y), v\right\rangle_\varepsilon \\ &= \varepsilon^d \sum_{\ell\in\mathcal{L}} \sum_{\eta\in R} \sum_{k=0}^{\eta_1-1} \left\{\frac{1}{2}\nabla_\zeta \phi_\eta\left(\overline{D}_\eta y_{\ell-k\,e_1}\right) + \frac{1}{2}\nabla_\zeta \phi_\eta\left(\overline{D}_\eta y_{\ell-k\,e_1-\eta_2 e_2}\right)\right\} \cdot \overline{D}_{e_1} v_\ell \\ &\quad + \varepsilon^d \sum_{\ell\in\mathcal{L}} \sum_{\eta\in R} \sum_{k=0}^{\eta_2-1} \left\{\frac{1}{2}\nabla_\zeta \phi_\eta\left(\overline{D}_\eta y_{\ell-k\,e_2}\right) + \frac{1}{2}\nabla_\zeta \phi_\eta\left(\overline{D}_\eta y_{\ell-k\,e_2-\eta_1 e_1}\right)\right\} \cdot \overline{D}_{e_2} v_\ell\,.\end{aligned}$$

we can show

Theorem (VARIATIONAL CONSISTENCY) Let y be a smooth function; then, for any $v \in \mathbb{V}_h$, the continuum Cauchy–Born variation $\langle D\Phi^{CB}(y), v\rangle$ is a second-order approximation to the atomistic variation $\langle D\Phi^{a}(y), v\rangle_{\varepsilon}$ in the sense that there exist a constant $M_V = M_V(y,p)$, $1 \leq p \leq \infty$, independent of v, such that

$$\left|\langle D\Phi^{CB}(y), v\rangle - \langle D\Phi^{a}(y), v\rangle_{\varepsilon}\right| \leq M_V\, \varepsilon^2\, |v|_{W^{1,p}(\Omega)}.$$

In addition, there exists a constant $M'_V = M'_V(y,p)$, $1 \leq p \leq \infty$, independent of v, such that

$$\left|\langle D\Phi^{a,CB}(y), v\rangle_{\varepsilon} - \langle D\Phi^{a}(y), v\rangle_{\varepsilon}\right| \leq M'_V\, \varepsilon^2\, |v|_{W^{1,p}(\Omega)}.$$

...

Remarks

- Comparison with the results of *X. Blanc, C.LeBris & P.L. Lions 2002 and W. E. & P. Ming 2008, and the recent result of Ortner & Theil 2013*
- Definitions of QC methods in 2 and 3D via the atomistic CB model
- Analysis of QC methods in 2 and 3D as well as of models accounting for surface energy, cf. Recent work by Phoebus Rosakis.
- Extensions: a) AC models based on triangular and tetrahedral meshes, b) multibody potentials

Towards the construction of ghost free methods in multi-D

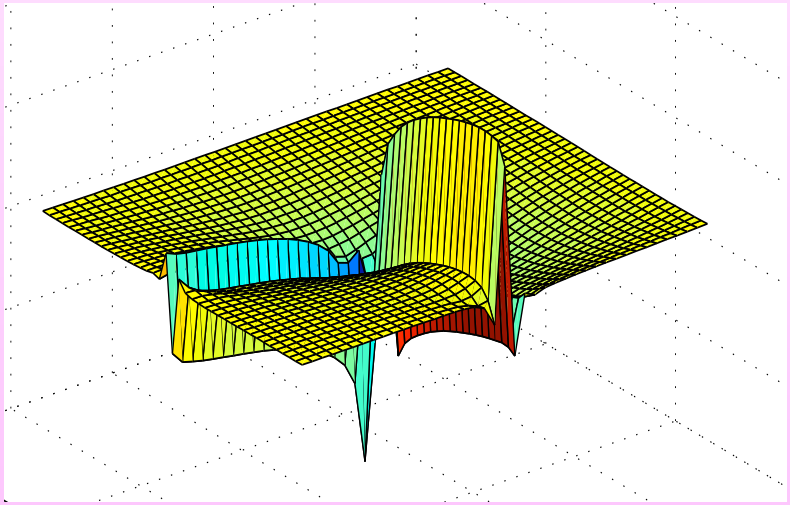
What is a ghost-force free coupling?

- The energy $\mathcal{E}$ is said to be free of ghost forces, if

$$\langle D\mathcal{E}(y_F), v\rangle = 0, \quad y_F(x) = Fx\,,$$

  for all appropriate variations $v\colon \bar{\Omega} \cap L \to \mathbb{R}^2$ such that $v_\ell = 0$ outside a compact set.

- Ad-hoc coupling of energies leads to ghost forces... "energy consistent" coupling may still lead to ghost forces



- Dynamic problem (!!!)

State of the art

1D & 2D : Energy based couplings free of ghost forces have been constructed recently.
3D : Next

- 1D : Li & Luskin 2011 and Shapeev 2011
- 2D : Shapeev 2011
- Other works (mainly special cases) : Belytschko et. al. 2002, Shimokawa et. al. 2004, W. E, J. Lu, & J. Yang 2006, Ortner & Zhang 2011, Shapeev 2011(3D)

Towards the construction of ghost free methods in multi-D: Notation

Let Ω, Ω_a and Ω_* each be the interior of the closure of the union of lattice cells $K \in \mathcal{T}_Q$ and connected, and suppose

$$\bar{\Omega} = \bar{\Omega}_a \cup \bar{\Omega}_*, \quad \Gamma = \bar{\Omega}_a \cap \bar{\Omega}_*.$$

Here Γ is the interface.

- Fix $\eta \in R$ and define the bond $b_\ell = \{x \in \mathbb{R}^2 : x = x_\ell + t\varepsilon\eta,\ 0 < t < 1\}$. The set of all bonds $\mathcal{B}_\eta$ is defined as consists of all $b = b_\ell$ for $\ell \in \mathcal{L}$.

The approach of A. Shapeev

- Work with each bond separately
- Represent long-range differences as line integrals over bonds:

$$\fint_{b_\ell} \nabla y \, \eta = \overline{D}_\eta y_\ell$$

- In two space dimensions was then possible to transform the assembly of line integrals over all possible interactions into an area integral through a counting argument known as *bond density lemma*

  Lemma (Shapeev) Let S be a set consisting of unions of triangles $T \in \mathcal{T}_T$. Then for any fixed $\eta \in R$ the following identity holds:

$$\sum_{b \in \mathcal{B}_\eta} \fint_b \chi_S \, d\tau = |S| \, .$$

- Limitations: Lemma valid only in 2D; the construction works only on piecewise linears over triangles.

Towards the construction of ghost free methods in multi-D:

A bond volume approach

- Represent long-range differences as *volume* integrals over bond volumes
- Construction of an underlined globally continuous function representing the coupled modeling method
- Work in two phases: first use in the continuum region appropriate atomistic Cauchy-Born models
- Subsequently: Use in the continuum region finite elements of arbitrary high order
- Possibility of using discontinuous finite elements
- Work in both 2 and 3D.

Finite elements for elliptic problems: methods without ghost forces: consistent discretisations

For a finite element function with support in the interior of the domain Ω (ignore boundary effects)

$$(?)0 = \langle \nabla y_F, \nabla v \rangle = F \int_\Omega \nabla v dx, \qquad y_F(x) = Fx\,.$$

Relation to *"patch test consistency"* / nonconforming methods.

Energy free of ghost forces: what we want to prove

For a fixed η we have

$$(?)0 = \langle D\mathcal{E}_\eta(y_F), v\rangle = \phi_\eta'(F\,\eta)\cdot\Big\{\varepsilon^2 \sum_{\substack{\ell\in\mathcal{L}\\ \overline{B}_{\ell,\,\eta}\subset\Omega_a}} \overline{D}_\eta v_\ell + \int_{\Omega_*} \overline{\nabla} v(x)\eta\,dx$$

$$+ \sum_{\substack{\ell\in\mathcal{L}\\ B_{\ell,\,\eta}\in B_\Gamma}} \frac{1}{|\eta_1\eta_2|}\int_{B_{\ell,\,\eta}} \chi_{\Omega_a}\,\nabla v^{\ell,\eta}\eta\,dx\Big\}$$

$$= \phi_\eta'(F\,\eta)\cdot\int_\Omega \nabla W(x)\eta\,dx(?)$$

2D: bond volumes and long range differences

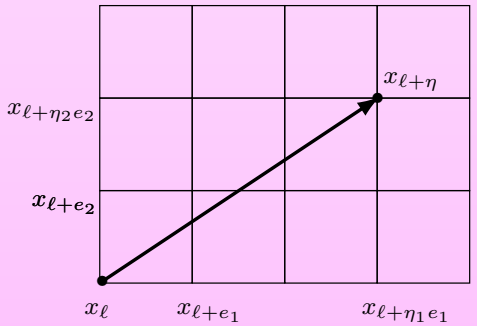
We construct methods based on *bond volumes* instead of bonds. For fixed $\eta \in R$ *bond volume* $B_{\ell,\,\eta}$ is the interior of a parallelogram with diagonal b_ℓ, i.e.,

$B_{\ell,\,\eta}$ is the open quadrilateral with vertices $x_\ell, x_{\ell+\eta_1 e_1}, x_{\ell+\eta_2 e_2}, x_{\ell+\eta}$.

Lemma

Let $v \in \mathbb{Q}_1(B_{\ell,\,\eta})$. *Then*

$$\varepsilon^2 \, \overline{D}_\eta v_\ell = \frac{1}{|\eta_1 \, \eta_2|} \int_{B_{\ell,\,\eta}} \nabla v(x) \eta \, dx \, .$$



2D: bond volumes and energies

The method is designed with respect to bond volumes $B_{\ell,\,\eta}$. In particular, we consider three cases determined by the location of each bond volume $B_{\ell,\,\eta}$

a. The closure of the bond volume is contained in the atomistic region: $\overline{B}_{\ell,\,\eta} \subset \Omega_a$
b. The bond volume is contained in the region Ω_* : $B_{\ell,\,\eta} \subset \Omega_*$
c. We denote by B_Γ the set of bond volumes which do not satisfy a) or b). In fact $B_{\ell,\,\eta} \in B_\Gamma$ if the bond volume intersects the interface: $B_{\ell,\,\eta} \cap \Gamma \neq \emptyset$ or if $B_{\ell,\,\eta} \subset \Omega_a$ and $\overline{B}_{\ell,\,\eta} \cap \Gamma \neq \emptyset$

For a fixed η, the contribution to the energy corresponding to a) is:

$$E^a_{\Omega_a,\eta}\{y\} = \varepsilon^2 \sum_{\substack{\ell\in\mathcal{L} \\ \overline{B}_{\ell,\,\eta}\subset\Omega_a}} \phi_\eta(\overline{D}_\eta y_\ell)\,.$$

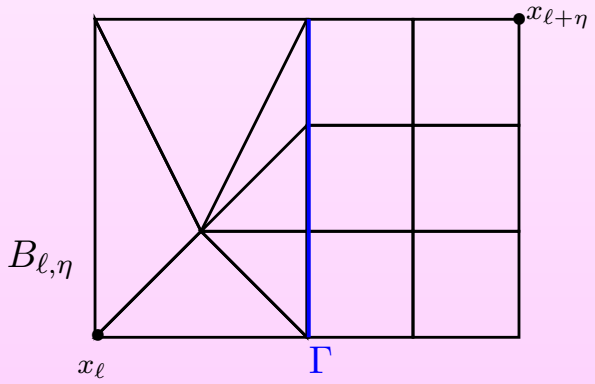
The contribution to the energy from the atomistic CB region will be

$$E^{a,cb}_{\Omega_*,\eta}\{y\} = \int_{\Omega_*} \phi_\eta(\overline{\nabla} y(x)\eta)dx\,.$$

2D: energies on the interface

For each bond volume intersecting the interface we denote by $y^{\ell,\eta}$ a *continuous* piecewise polynomial function on an appropriate decomposition $\mathcal{T}(B_{\ell,\eta})$ of $B_{\ell,\eta}$. satisfying

- (•) only requirement: conforming glue of $\mathcal{T}(B_{\ell,\eta})$ with the neighbor bond volumes.



Corresponding energy:

$$E_{\Gamma,\eta}\{y\} = \sum_{\substack{\ell\in\mathcal{L}\\ B_{\ell,\eta}\in B_\Gamma}} \frac{1}{|\eta_1\eta_2|}\int_{B_{\ell,\eta}} \chi_{\Omega_a}\,\phi_\eta(\nabla y^{\ell,\eta}\eta)\,dx\,.$$

Total energy

the total energy is defined through

$$\mathcal{E}_{bv}\{y\} = \sum_{\eta \in R} \mathcal{E}_{\eta}\{y\}$$

where

$$\mathcal{E}_{\eta}\{y\} = E^{a}_{\Omega_a,\eta}\{y\} + E^{a,cb}_{\Omega_*,\eta}\{y\} + E_{\Gamma,\eta}\{y\}\,.$$

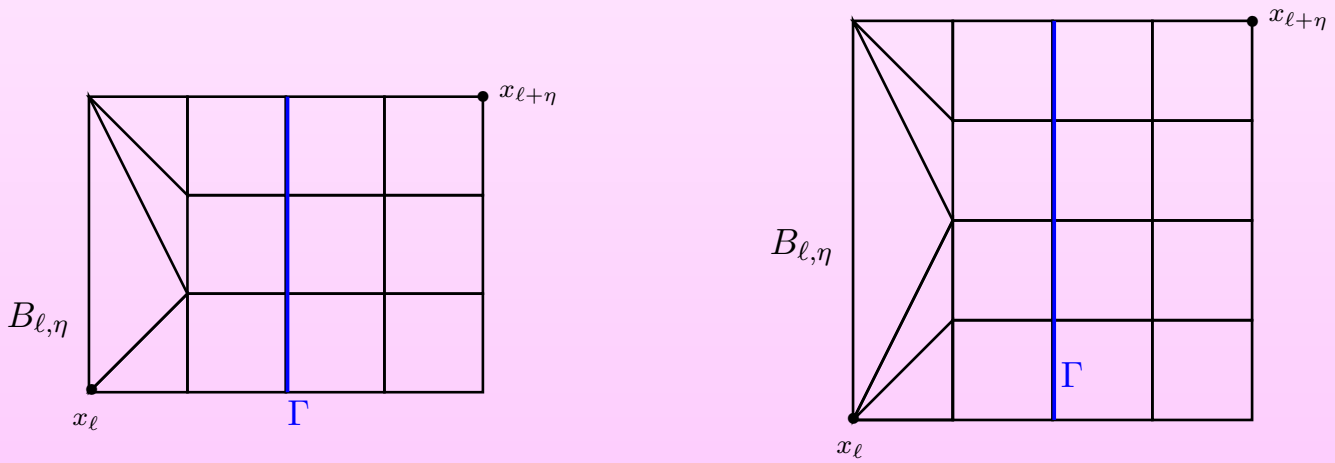


Figure : Alternative decompositions $\mathcal{T}(B_{\ell,\,\eta})$ of $B_{\ell,\,\eta}$ for two different bonds.

Energy free of ghost forces

Energy free of ghost forces: Idea of the proof

First we fix η and we consider decompositions consisting of bond volumes which cover $\mathbb{R}^2$:

$$\mathcal{S}^m_{B_\eta} := \left\{ B_{\ell,\,\eta} : \text{ (i) } B_{\ell,\,\eta} \cap B_{j,\,\eta} = \emptyset, \text{ if } \ell \neq j, \quad \text{(ii) } \mathbb{R}^2 = \overline{\cup B_{\ell,\,\eta}} \right\},$$

$m = 1, \ldots, |\eta_1 \eta_2|$. The number of different such coverings is $|\eta_1 \eta_2|$, hence the numbering $m, m = 1, \ldots, |\eta_1 \eta_2|$. Notice that bond volumes corresponding to different m may overlap, but within a single $\mathcal{S}^m_{B_\eta}$ its elements consist a decomposition of non-overlapping bond volumes.

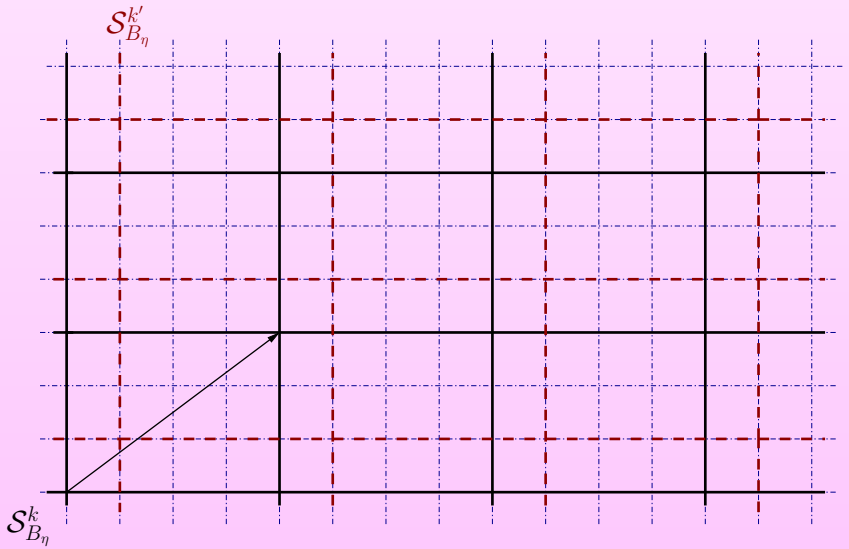


Figure : Two different coverings $\mathcal{S}^k_{B_\eta}$ and $\mathcal{S}^{k'}_{B_\eta}$

Energy free of ghost forces: Idea of the proof II

For a fixed η we have

$$(?)0 = \langle D\mathcal{E}_\eta(y_F), v\rangle = \phi'_\eta(F\,\eta)\cdot\Big\{\varepsilon^2 \sum_{\substack{\ell\in\mathcal{L}\\ \overline{B}_{\ell,\,\eta}\subset\Omega_a}} \overline{D}_\eta v_\ell + \int_{\Omega_*} \overline{\nabla} v(x)\eta\,dx + \sum_{\substack{\ell\in\mathcal{L}\\ B_{\ell,\,\eta}\in B_\Gamma}} \frac{1}{|\eta_1\eta_2|}\int_{B_{\ell,\,\eta}} \chi_{\Omega_a}\,\nabla v^{\ell,\eta}\eta\,dx\Big\}$$

The main idea of the proof is to write the above sum as

$$\varepsilon^2 \sum_{\substack{\ell\in\mathcal{L}\\ \overline{B}_{\ell,\,\eta}\subset\Omega_a}} \overline{D}_\eta v_\ell + \int_{\Omega_*} \overline{\nabla} v(x)\eta\,dx + \sum_{\substack{\ell\in\mathcal{L}\\ B_{\ell,\,\eta}\in B_\Gamma}} \frac{1}{|\eta_1\eta_2|}\int_{B_{\ell,\,\eta}} \chi_{\Omega_a}\,\nabla v^{\ell,\eta}\eta\,dx$$

$$= \frac{1}{|\eta_1\eta_2|}\sum_{m=1}^{|\eta_1\eta_2|}\int_\Omega \nabla v^{[m]}(x)\eta\,dx$$

where $v^{[m]}$, $m = 1,\ldots,\eta_1\eta_2$ are appropriate conforming functions (in $H^1(\Omega)$) each one associated to a different covering $\mathcal{S}^m_{B_\eta}$ consisting of bond volumes.

Energy free of ghost forces: Idea of the proof II

For a fixed η we have

$$(?)0 = \langle D\mathcal{E}_\eta(y_F), v\rangle = \phi'_\eta(F\,\eta)\cdot\Big\{\varepsilon^2 \sum_{\substack{\ell\in\mathcal{L}\\ \overline{B}_{\ell,\,\eta}\subset\Omega_a}} \overline{D}_\eta v_\ell + \int_{\Omega_*} \overline{\nabla} v(x)\eta\,dx + \sum_{\substack{\ell\in\mathcal{L}\\ B_{\ell,\,\eta}\in B_\Gamma}} \frac{1}{|\eta_1\eta_2|}\int_{B_{\ell,\,\eta}} \chi_{\Omega_a}\,\nabla v^{\ell,\eta}\eta\,dx\Big\}$$

The main idea of the proof is to write the above sum as

$$\varepsilon^2 \sum_{\substack{\ell\in\mathcal{L}\\ \overline{B}_{\ell,\,\eta}\subset\Omega_a}} \frac{1}{|\eta_1\eta_2|}\int_{B_{\ell,\,\eta}} \nabla v(x)\eta\,dx + \int_{\Omega_*} \overline{\nabla} v(x)\eta\,dx + \sum_{\substack{\ell\in\mathcal{L}\\ B_{\ell,\,\eta}\in B_\Gamma}} \frac{1}{|\eta_1\eta_2|}\int_{B_{\ell,\,\eta}} \chi_{\Omega_a}\,\nabla v^{\ell,\eta}\eta\,dx$$

$$= \frac{1}{|\eta_1\eta_2|}\sum_{m=1}^{|\eta_1\eta_2|}\int_\Omega \nabla v^{[m]}(x)\eta\,dx$$

where $v^{[m]}$, $m = 1,\ldots,|\eta_1\eta_2|$ are appropriate conforming functions (in $H^1(\Omega)$) each one associated to a different covering $\mathcal{S}^m_{B_\eta}$ consisting of bond volumes.

Construction in 3 D: We need to work with tetrahedra

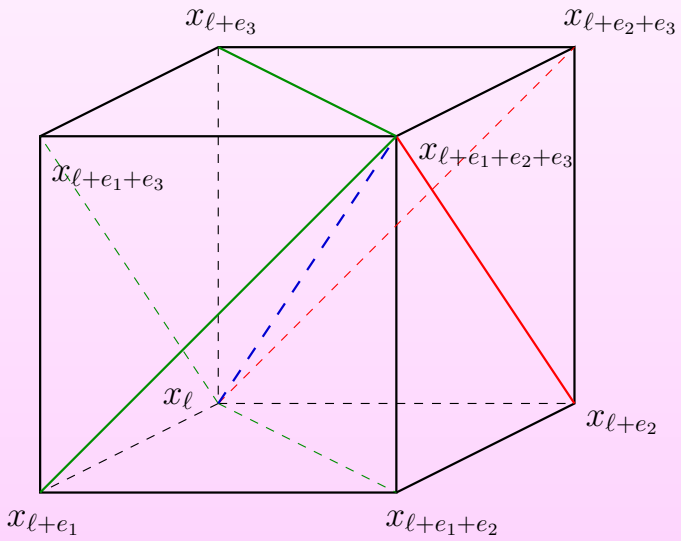


Figure : A *type A decomposition* of the cell K_ℓ into six tetrahedra.

Construction in 3 D: Atomistic CB model in tetrahedra

$$\mathcal{T}_T = \{T \subset \Omega : \quad T \text{ is a tetrahedron whose vertices are lattice vertices of } K_\ell\,, \quad x_{\boldsymbol{\ell}} \in \Omega_{\text{discr}}\},$$

$$V_{\varepsilon,T} := \{v : \Omega \to \mathbb{R}^2, \quad v \in C(\Omega)\,,\ v|_T \in \mathbb{P}_1(T) \text{ and } v_\ell = v(x_\ell) \quad \text{periodic with respect to } \mathcal{L}\},$$

$$\tilde{\Phi}^{a,CB}(y) := \frac{\varepsilon^3}{6} \sum_{\ell \in \mathcal{L}} \sum_{T \in K_\ell(T)} \sum_{\eta \in R} \phi_\eta\,(\widetilde{\nabla} y\,\eta) = \frac{\varepsilon^3}{6} \sum_{\ell \in \mathcal{L}} \sum_{T \in K_\ell(T)} W_{CB}(\widetilde{\nabla} y).$$

Construction in 3 D: A key result

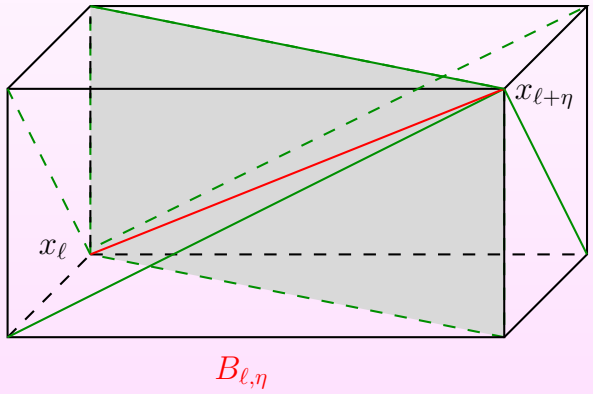


Figure : A *bond volume* $B_{\ell,\,\eta}$ and its *type A decomposition* into six tetrahedra.

Lemma

Let v be a piecewise linear and continuous function on a type A decomposition of the bond volume $B_{\ell,\,\eta}$ into tetrahedra. Then

$$\varepsilon^3\,\overline{D}_\eta v_\ell = \frac{1}{|\eta_1\,\eta_2\,\eta_3|}\int_{B_{\ell,\,\eta}} \nabla v(x)\eta\,dx\,.$$

Construction in 3 D: Proof

We have,

$$\frac{1}{\eta_1\,\eta_2\,\eta_3}\int_{B_{\ell,\,\eta}}\nabla v(x)\eta\,dx=\frac{1}{\eta_1\,\eta_2\,\eta_3}\int_{\partial B_{\ell,\,\eta}}v\,\nu\cdot\eta\,ds$$

$$=\frac{1}{\eta_1\,\eta_2\,\eta_3}\sum_{i=1}^{3}\Big\{\int_{\partial B_{\ell,\,\eta}(-e_i)}(-\eta_i)v\,ds+\int_{\partial B_{\ell,\,\eta}(e_i)}\eta_i\,v\,ds\Big\},$$

where $\partial B_{\ell,\,\eta}(e_i)$ is the face of $B_{\ell,\,\eta}$ with outward unit normal e_i. Therefore, if τ is a triangle on a face:

$$\int_{\tau}\eta_i\,v\,ds=\frac{|\tau|}{3}\sum_{j=1}^{3}\eta_i\,v(z_j),$$

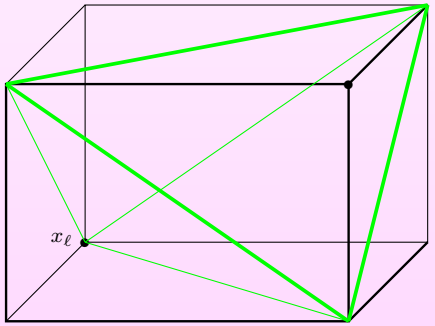
where z_i are the vertices of τ. Since τ is one of the two triangles of $\partial B_{\ell,\,\eta}(\eta_i)$, $|\tau|\,\eta_i=\frac{\varepsilon^2}{2}\,\eta_1\,\eta_2\,\eta_3$. Hence,

$$\frac{1}{\eta_1\,\eta_2\,\eta_3}\int_{\partial B_{\ell,\,\eta}(e_i)}\eta_i\,v\,ds=\frac{\varepsilon^2}{6}\sum_{j=1}^{2}\Big\{v(z_j)+2\,v(\tilde{z}_j)\Big\}.$$

We notice that $x_{\ell+\eta}$ is a shared vertex at each $\partial B_{\ell,\,\eta}(e_i)$, while x_ℓ is a shared vertex at each $\partial B_{\ell,\,-\eta}(-e_i)$, for all $i=1,2,3$.

$$\frac{1}{\eta_1\,\eta_2\,\eta_3}\int_{B_{\ell,\,\eta}}\nabla v(x)\cdot\eta\,dx=\varepsilon^2\Big(v_{\ell+\eta}-v_\ell\Big),$$

Construction in 3 D: Sensitivity on the type of decomposition



Decomposition into 5 tetrahedra, one of them without faces on the boundary

The result is sensitive to the particular decomposition of the bond volume $B_{\ell,\,\eta}$ into tetrahedra.

Construction in 3 D: Energy on interface

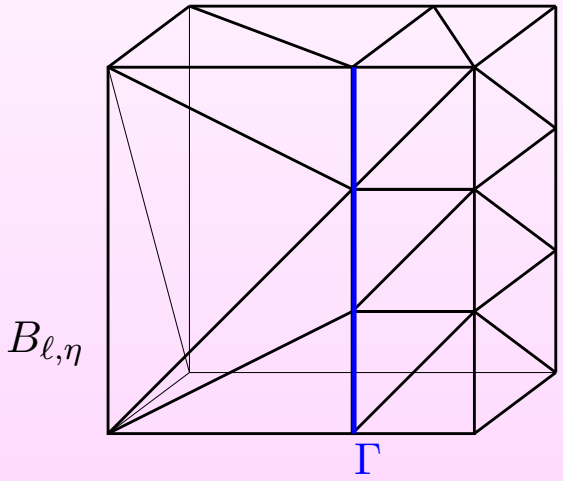


Figure : A possible decomposition $\mathcal{T}(B_{\ell,\,\eta})$ of $B_{\ell,\,\eta}$.

$$E_{\Gamma,\eta}\{y\} = \sum_{\substack{\ell\in\mathcal{L}\\ B_{\ell,\,\eta}\in B_\Gamma}} \frac{1}{\eta_1\eta_2\eta_3}\int_{B_{\ell,\,\eta}} \chi_{\Omega_a}\,\phi_\eta(\nabla y^{\ell,\eta}\eta)\,dx\,.$$

Construction in 3 D: The method is consistent

The energy is free of ghost forces, in the sense that

$$\langle D\mathcal{E}_{bv}(y_F), v\rangle = 0, \quad y_F(x) = Fx\,,$$

Construction in 3 D: Alternative construction: discontinuous on Γ

$$E^D_{\Gamma,\eta}\{y\} = \sum_{\substack{\ell\in\mathcal{L}\\ B_{\ell,\,\eta}\in B_\Gamma}} \frac{1}{\eta_1\eta_2\eta_3}\Big[\int_{B_{\ell,\,\eta}} \chi_{\Omega_a}\,\phi_\eta(\nabla y^{\ell,\eta}\eta)\,dx - \int_{B_{\ell,\,\eta}\cap\Gamma} \phi'_\eta(\{\!\{\nabla y^{\ell,\eta}\eta\}\!\})\,[\![y^{\ell,\eta}\eta]\!]\,dS\Big].$$

Remarks

- The first systematic approach in the literature that leads to ghost force free couplings in dimensions 1, 2 and 3 and for all interatomic potentials of finite range. In particular:
  - The method allows to replace atomistic CB models by any high-order finite element discretization of the continuum energy. The new method is still consistent.
  - The discontinuous method is very flexible:
    - It allows the introduction of penalty-type stabilisation terms,
    - It allows DG finite element discretisations of the continuum energy.
  - There are several alternative ways to treat the interface and its discretisation.

Remarks II

- Finite elements, and modern numerical analysis in general, provide a very valuable toolbox to address subtle modelling issues.
- Several exciting open problems related to physical phenomena are described by discrete models at micro scales.

thank you !