Analysis of a prototypical multiscale method coupling atomistic and continuum mechanics

Frédéric Legoll

IMA, U of Minnesota (Minneapolis) and ENPC Paris

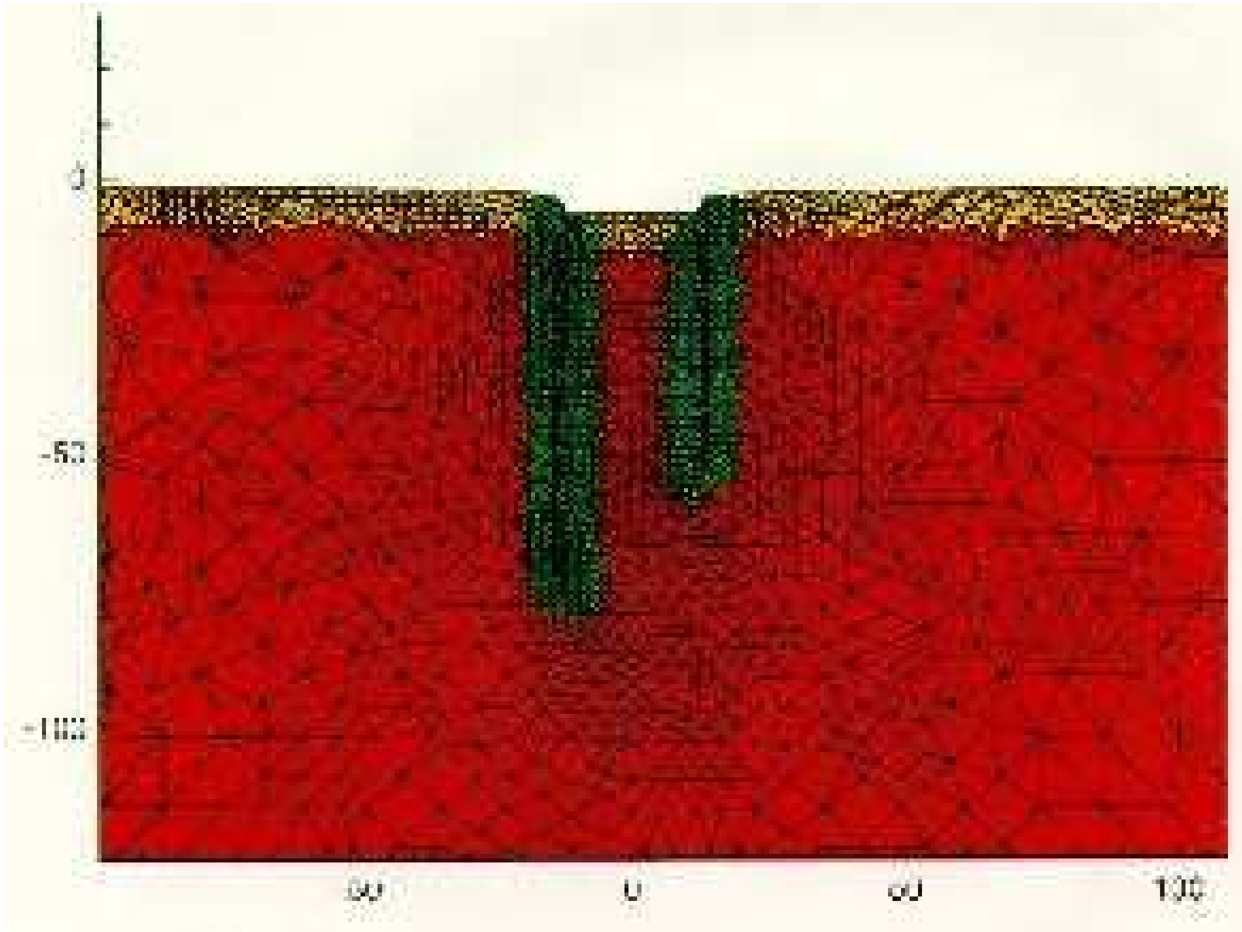
joint work with Xavier Blanc (Université Paris 6) and Claude Le Bris (CERMICS, ENPC).

http://www.ima.umn.edu/~legoll

Outline of the talk

- Some motivations for multiscale methods
- A prototypical 1D multiscale method
- Analysis of the method:
  - case of a convex interatomic potential
  - Lennard-Jones case

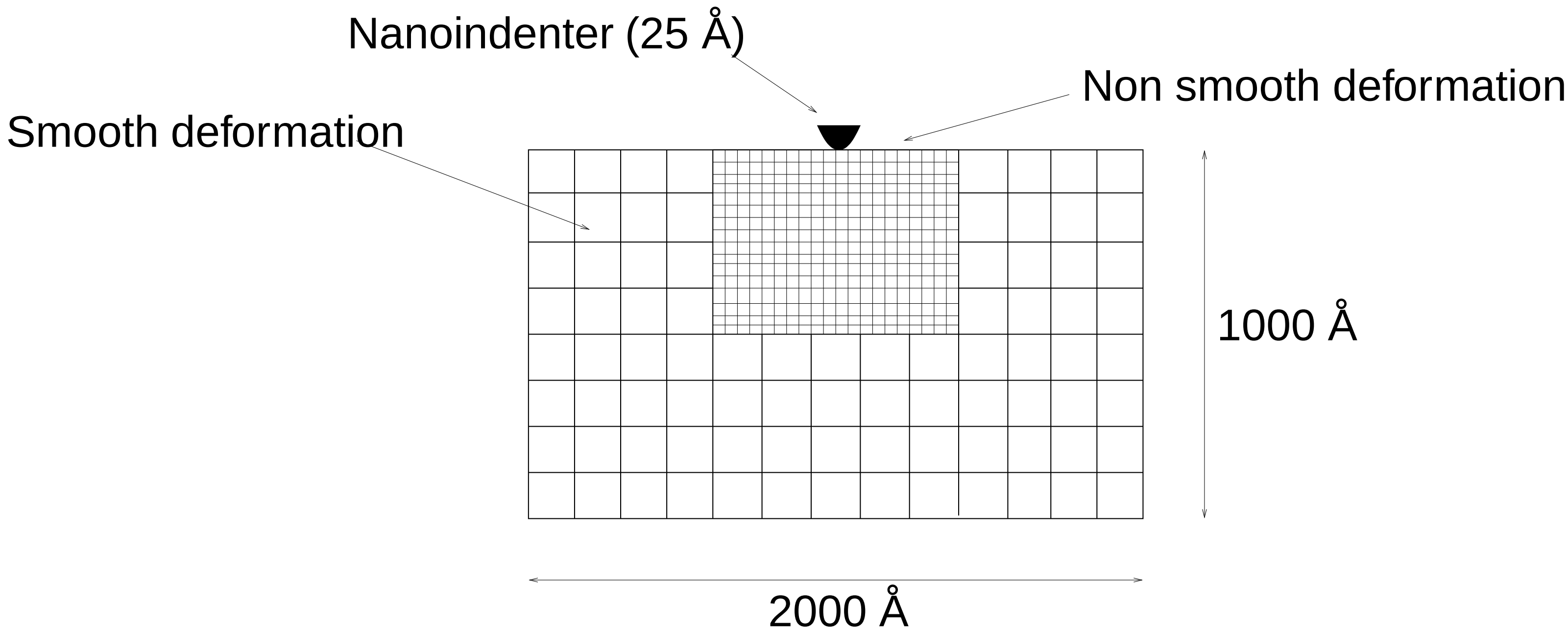
Nanoindentation simulation



Tadmor, Miller, Phillips, Ortiz, J. of Material Research, 1999

(`www.qcmethod.com`)

Paradigm: study nanoscale localized phenomena



- Large computational domain;
- Expected deformation: non-smooth in some small region of the solid.
- Coupling an (accurate) atomistic model with a (cheap) continuum mechanics model.

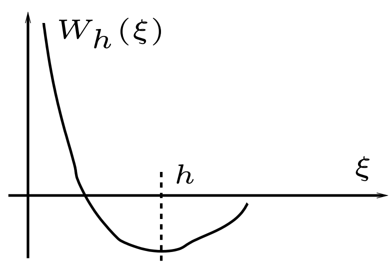
The atomistic model

Reference configuration (1D): $\Omega = (0, L) \subset \mathbb{R}$

Current position of atom i: u^i

Atomic lattice parameter: h, with $Nh = L$

Energy per particle: $E_\mu(u^0, \ldots, u^N) = \frac{1}{2N} \sum_{i \neq j} W_h\left(u^j - u^i\right)$



$$W_h(u^j - u^i) = W\left(\frac{u^j - u^i}{h}\right)$$

Atomistic model (assuming Nearest Neighbour interactions):

$$E_\mu(u^0, \ldots, u^N) = \frac{h}{L} \sum_{i=0}^{N-1} W\left(\frac{u^{i+1} - u^i}{h}\right) - \frac{h}{L} \sum_{i=0}^{N} u^i f(i\,h)$$

$$\inf \left\{ E_\mu(u^0, \ldots, u^N),\ u^0 = 0,\ u^N = a,\ u^{i+1} > u^i \right\} \rightarrow \text{Intractable!}$$

Continuum mechanics model

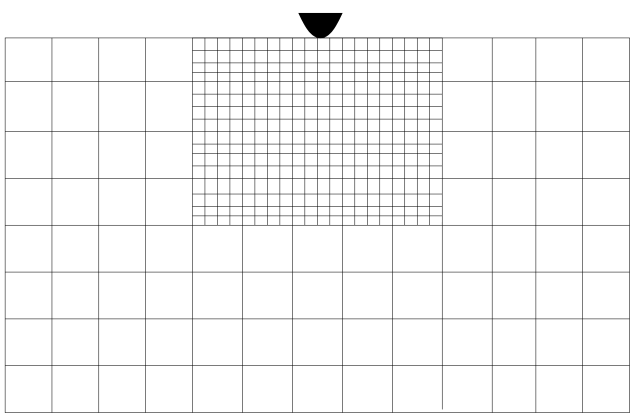
X. Blanc, C. Le Bris, P.-L. Lions (ARMA 2002): if u is smooth enough,

$$\lim_{h\to 0} E_\mu(u(0), u(h), \ldots, u(Nh)) = E_M(u) = \int_\Omega W(u'(x))\,dx - \int_\Omega f(x)\,u(x)\,dx$$

Continuum model (elastic energy density derived from atomistic model).

More generally, $W_{CM}(F) = 1/2 \sum_{k\in\mathbb{Z}^3, k\neq 0} W(F\cdot k)$.

$$\inf\left\{\ E_M(u),\ u\in H^1(\Omega),\ u(0)=0,\ u(L)=a,\ u'>0 \text{ a.e. on } \Omega\right\}$$



What if deformation is not smooth in the whole domain?

Use different models in the different domains.

Coupled model: a first attempt

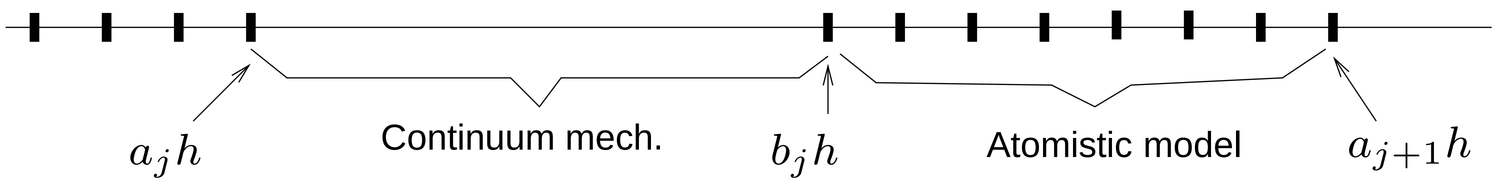
$$E_c(u) := \int_{\Omega_M(u)} W(u'(x)) - f(x)\, u(x)\, dx + h \sum_{i \in \Omega_\mu(u)} W\left(\frac{u^{i+1} - u^i}{h}\right) - u^i f(ih)$$

where $\begin{cases} \Omega_M(u) = \text{subdomain where } u \text{ is smooth,} \\ \Omega_\mu(u) = \text{subdomain where } u \text{ is non-smooth.} \end{cases}$

Highly nonlinear problem $\longrightarrow$
remove the link between u and the partition of Ω

The natural coupled model

For any partition $\Omega = \Omega_M \cup \Omega_\mu$ with $\Omega_M = \cup_j (a_j h, b_j h)$:



$$
\begin{aligned}
E_c(u) \quad &:= \quad \int_{\Omega_M} W(u'(x)) - f(x)\, u(x)\, dx \\
&+ \quad h \sum_{i, [ih, ih+h] \subset \Omega_\mu} W\left(\frac{u^{i+1} - u^i}{h}\right) - h \sum_{i, ih \in \Omega_\mu} u^i f(ih)
\end{aligned}
$$

Balance between numerical efficiency / precision

$$
\inf \left\{ \begin{array}{c} E_c(u), \quad u_{|\Omega_M} \in H^1(\Omega_M), \quad u_{|\Omega_\mu} \equiv (u^i)_{ih \in \Omega_\mu}, \\ u^{a_j} = u\left((a_j h)^+\right), \; u^{b_j} = u\left((b_j h)^-\right), \; u(0) = 0, \; u(L) = a, \; u \uparrow \end{array} \right\}
$$

The coupled problem after discretization

Discretization of the continuum mechanics term on a mesh of size $H \gg h$:

$$E_c^H\left(U, u_{|\Omega_\mu}\right) := \int_{\Omega_M} W\left(\sum_k U_k N_k'(x)\right) dx - \sum_k U_k \int_{\Omega_M} f(x) N_k(x)\, dx$$
$$+ \quad h \sum_{i,[ih,ih+h]\subset\Omega_\mu} W\left(\frac{u^{i+1}-u^i}{h}\right) - h \sum_{i,ih\in\Omega_\mu} u^i f(ih)$$

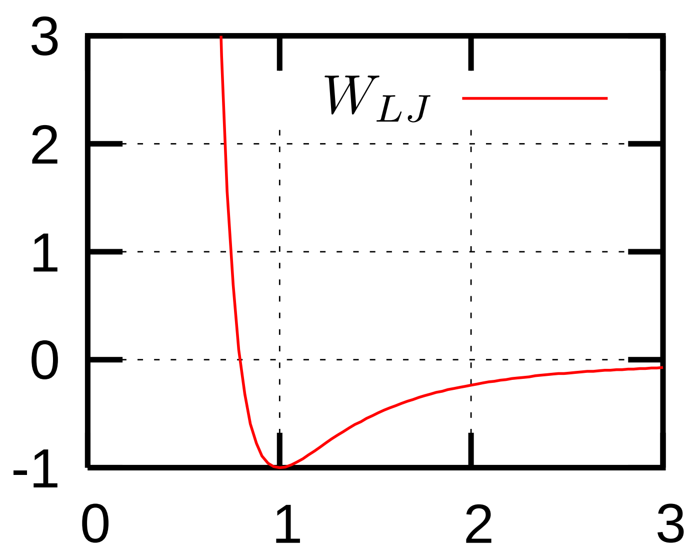
Questions:

- How to choose the partition?
  Idea: the set Ω_M should consist of all the zones of regularity of u_μ
- Is E_c a good definition for the coupled energy?

We will show that $\inf E_c^H$ is not always the discretized version of $\inf E_c$!

Two different cases for the potential

- Convex interatomic potential W;
- The Lennard-Jones case.



Convex case: definition of the partition

$$f \in \mathcal{C}^0(\overline{\Omega}); \quad W \in \mathcal{C}^2(\mathbb{R}) \text{ with } 0 < \alpha \leq W''(z) \text{ and } |W'(z)| \leq \beta\, |z-1|$$

The atomistic, macroscopic and coupled problems are well-posed.

W convex $\Longrightarrow$ elliptic regularity: $\{$singularities of $u\} = \{$singularities of $f\}$

Assume $f \in \mathcal{C}^0(\overline{\Omega})$. The interval $(ih, ih+h)$ is said to be regular if

$$\|f\|_{L^\infty(ih,ih+h)} \leq \kappa_f \quad \text{and} \quad f' \in L^1(ih, ih+h), \; \|f'\|_{L^1(ih,ih+h)} \leq \frac{h\kappa_f}{L}$$

$$\text{Set} \quad \Omega_M := \cup \left\{ (ih, ih+h) \text{ which are regular} \right\} = \cup_j (a_j h, b_j h)$$

Partition just depends on f!

Estimates between u_c and u_μ (convex case)

With previous definition of partition, $\exists \, h_0$ such that, for all $h \leq h_0$,

$$\sup_{i \in \Omega_\mu} \left| \frac{u_c^{i+1} - u_c^i}{h} - \frac{u_\mu^{i+1} - u_\mu^i}{h} \right| \leq C_1 h \kappa_f,$$

$$\| u_c' - (\Pi_c u_\mu)' \|_{L^\infty(\Omega_M)} \leq C_1 h \kappa_f,$$

$$\sup_{i \in \Omega_\mu} \left| u_c^i - u_\mu^i \right| \leq C_2 h \kappa_f, \qquad \| u_c - \Pi_c u_\mu \|_{L^\infty(\Omega_M)} \leq C_2 h \kappa_f,$$

$$|I_c - I_\mu| \leq C_3 h \kappa_f.$$

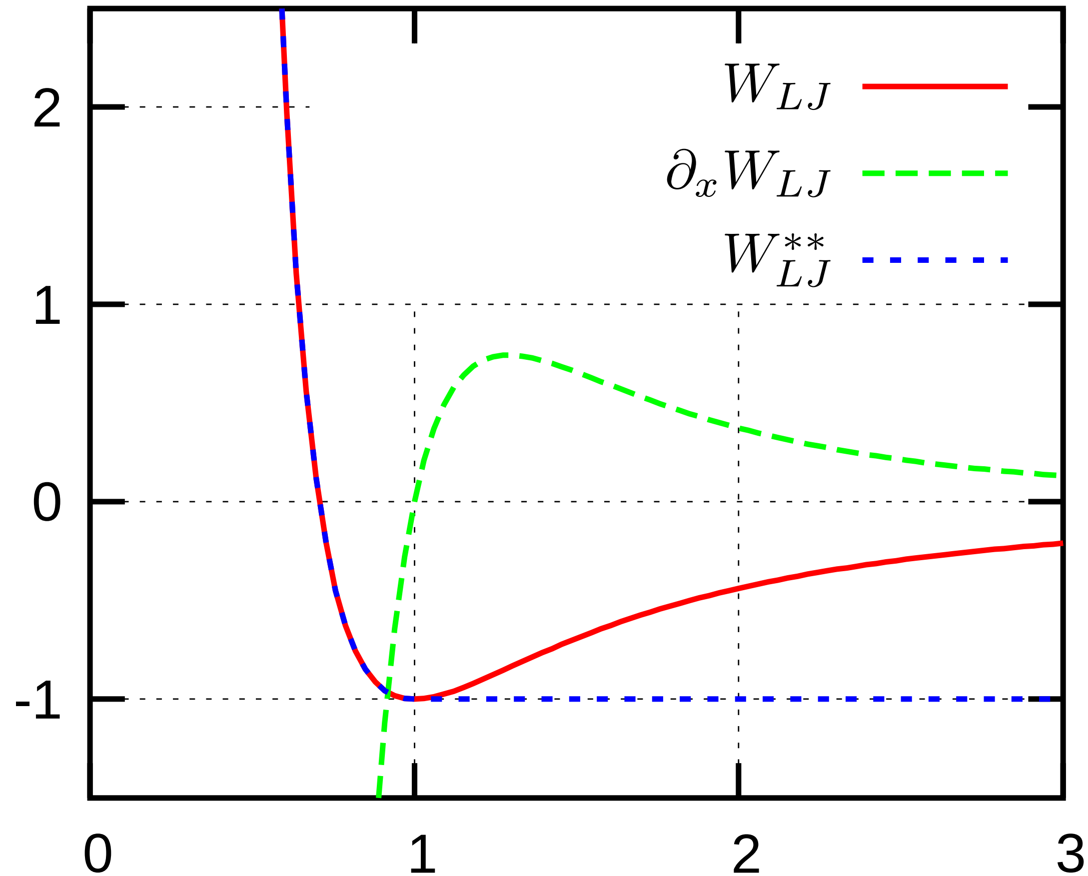
Π_c: affine interpolation operator

The Lennard-Jones case

$$W_{LJ}(z) := \frac{1}{z^{12}} - \frac{2}{z^6}$$

$$W'_{LJ}(1) = 0$$

$$W''_{LJ}(r_c) = 0$$

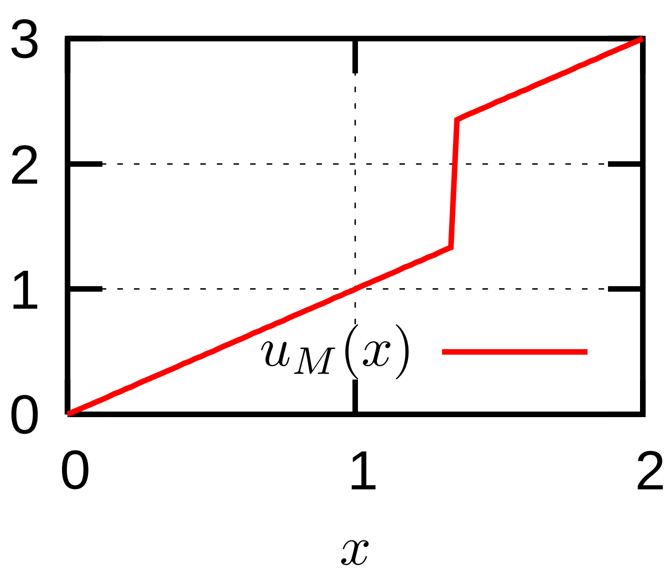


Macroscopic problem ($f \equiv 0$)

Natural variational space:

$$X_M(a) = \left\{ u \in W^{1,1}(\Omega),\ \frac{1}{u'} \in L^{12}(\Omega),\ \ u' > 0 \text{ a.e.},\ \ u(0) = 0,\ u(L) = a \right\}$$

$$E_M(u) = \int_0^L W_{LJ}(u'(x))\, dx : \qquad \inf E_M = L W_{LJ}^{**}\left(\frac{a}{L}\right)$$



If $a > L$:

$\inf \{E_M(u), u \in X_M(a)\} = L W_{LJ}(1)$

Problem has no minimizers in $X_M(a)$.

"Minimizers" u_M are s.t. u_M' has Dirac masses ("crack" nucleation).

Macroscopic problem

$$SBV(\Omega) = \left\{ u \in \mathcal{D}'(\Omega), \ u' = Du + \sum_{i \in \mathbb{N}} v_i \delta_{x_i}, \ Du \in L^1(\Omega), \ x_i \in \Omega \right\}.$$

$$\inf \left\{ E_M(u), \ u \in SBV(\Omega), \frac{1}{Du} \in L^{12}(\Omega), u' > 0 \text{ a.e.}, u(0) = 0, u(L) = a \right\}$$

When $f \equiv 0$:

- If $a \leq L$: $\quad u_M(x) = ax/L$.
- If $a > L$: infinity of solutions, $u_M = x + \sum_i v_i H(x - x_i)$.
  Crack location is not determined (because NN interaction and $f \equiv 0$).

Results can be generalized to the case $f \neq 0$, $f \in L^1(\Omega)$: $\exists\, \theta_M$ s.t.
– if $a \leq \theta_M$, $\exists!$ solution, which is smooth;
– if $a > \theta_M$, "crack".

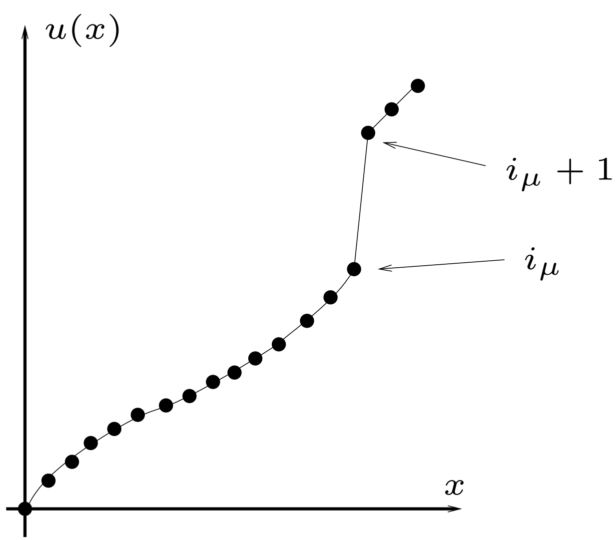
The atomistic problem ($f \in \mathcal{C}^0(\overline{\Omega})$)

$$\inf \left\{ E_\mu(u) = h \sum_{i=0}^{N-1} W_{LJ} \left(\frac{u^{i+1} - u^i}{h} \right) - h \sum_{i=0}^{N} u^i \, f(i\,h), \ u^0 = 0, u^N = a, u \uparrow \right\}$$

There exists a threshold θ_μ such that:

– if $a \leq \theta_\mu$, unique minimizer;

– if $a > \theta_\mu$ and h small enough: one or many minimizers, smooth everywhere except on a single bond $(i_\mu, i_\mu + 1)$:



$$\frac{u_\mu^{i_\mu+1} - u_\mu^{i_\mu}}{h} \sim_{h \to 0} \frac{C}{h} \quad \text{(“crack”)}$$

$$\forall i \neq i_\mu, \ \left(u_\mu^{i+1} - u_\mu^i \right) \to_{h \to 0} 0$$

See L. Truskinovsky, 1996.

Natural micro-macro approach

Suppose $f \equiv 0$, $a > L$ (crack case):

For any partition $\Omega = \Omega_M \cup \Omega_\mu$,

$$E_c(u) = \int_{\Omega_M} W_{LJ}(u'(x))\,dx + h \sum_{i,[ih,ih+h]\subset\Omega_\mu} W_{LJ}\left(\frac{u^{i+1}-u^i}{h}\right)$$

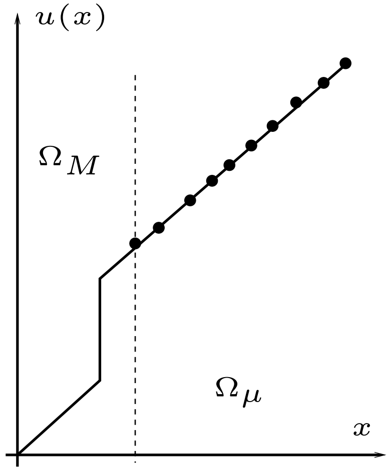
$$\inf \left\{ \begin{array}{c} E_c(u),\ u_{|\Omega_M} \in SBV(\Omega_M),\ u_{|\Omega_\mu} = (u^i)_{ih\in\Omega_\mu}, \\ u^{a_j} = u\left((a_j h)^+\right),\ u^{b_j} = u\left((b_j h)^-\right),\ u(0)=0,\ u(L)=a,\ u\uparrow \end{array} \right\}$$

There exist minimizers u_c.

u_c' has Dirac masses in Ω_M!

Energy cost of crack (case $f \equiv 0$)

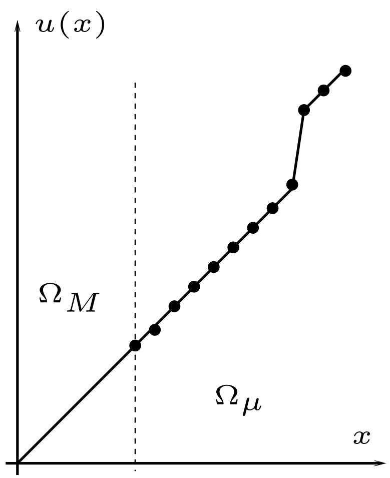
$$E_c(u) = \int_{\Omega_M} W_{LJ}(u'(x)) + h \sum_{\Omega_\mu} W_{LJ}\left(\frac{u^{i+1} - u^i}{h}\right)$$



If crack localized in Ω_M:

$$u'(x) = 1+(a-L)\delta_{x_0}, \quad \forall i, \ \frac{u^{i+1} - u^i}{h} = 1$$

$$E_c(u) \ = \ |\Omega_M| \, W_{LJ}(1) + |\Omega_\mu| \, W_{LJ}(1) \ = \ L \, W_{LJ}(1)$$



If crack in Ω_μ: $u'(x) = 1, \ \frac{u^{i+1} - u^i}{h} = 1 \ (i \neq i_\mu)$

$$\begin{aligned} E_c(u) &= |\Omega_M| \, W_{LJ}(1) \\ &+ (|\Omega_\mu| - h) \, W_{LJ}(1) + h W_{LJ}(\text{broken bond}) \\ &\approx (L-h) \, W_{LJ}(1) \qquad (\text{surface energy}) \end{aligned}$$

So $\quad E_c(F \in \Omega_M) < E_c(F \in \Omega_\mu)$.

The natural algorithm leads to issues

Consider the following algorithm: initialize $\Omega_M = \Omega$,

- solve the coupled problem $\inf_u E_c(u)$ with Ω_M fixed;
- look for the zones where the minimizer u_c is not smooth (e.g. has a large derivative), enlarge Ω_μ correspondingly and go back to step 1.

Then, at the end,

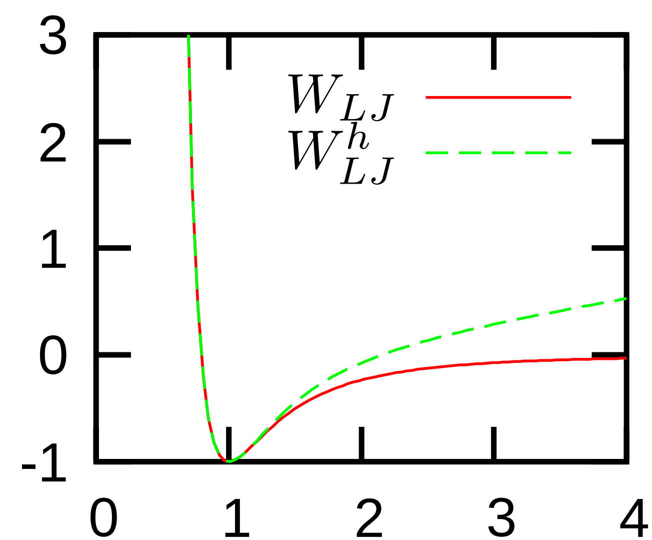
$$\Omega_\mu = \Omega$$

A modified micro-macro approach

Idea: give an energy cost (surface energy) to a crack in Ω_M.

$$E_{\text{mod}}(u) = \int_{\Omega_M} W_{LJ}^h(u'(x)) - f(x)\,u(x)\,dx + h \sum_{i,[ih,ih+h]\subset\Omega_\mu} W_{LJ}\left(\frac{u^{i+1}-u^i}{h}\right) - h \sum_{i,ih\in\Omega_\mu} u^i f(ih)$$

$W_{LJ}^h(r) := W_{LJ}(r) + \sqrt{h}\ (r-r_0)_+$ and $r_0 \in (1, r_c)$.



$\lim_{h\to 0} E_{\text{mod}}(u) = E_M(u)$ (consistency).

For $f \equiv 0$:

- fracture in Ω_μ: $E_{\text{mod}}(F\in\Omega_\mu) = E_c(F\in\Omega_\mu) = L\,W_{LJ}(1) + h$.
- fracture in Ω_M: $E_{\text{mod}}(F\in\Omega_M) = L\,W_{LJ}(1) + O\left(\sqrt{h}\right)$.

Partition Construction (Lennard-Jones case)

(1) Compute a solution u_M for the macro problem

$$\inf \left\{ E_M(u),\ u \in SBV(\Omega),\ \frac{1}{u'} \in L^{12}(\Omega),\ u' > 0,\ u(0) = 0,\ u(L) = a \right\}.$$

(2) Define $\Omega_M := \cup_i (ih, ih+h)$ with $(ih, ih+h)$ s.t.

$$\|f\|_{L^\infty(ih,ih+h)} \leq \kappa_f,\ f' \in L^1(ih, ih+h),\ \|f'\|_{L^1(ih,ih+h)} \leq h \frac{\kappa_f}{L},$$

and u_M is continuous on $(ih, ih+h)$.

(3) On this partition, consider the modified coupled problem

$$\inf \left\{ \begin{array}{c} E_{\text{mod}}(u),\ u_{|\Omega_M} \in W^{1,\infty}(\Omega_M),\ u_{|\Omega_\mu} \equiv (u^i)_{ih \in \Omega_\mu}, \\ u^{a_j} = u\left((a_j h)^+\right),\ u^{b_j} = u\left((b_j h)^-\right),\ u(0) = 0,\ u(L) = a,\ u \uparrow \end{array} \right\}$$

Modified coupled problem: error estimates

- if $a \leq \theta_M$ (no crack case): $\exists !$ solution u_{mod}, estimates similar to the convex case ones;
- If $a > \theta_M$: There are one or many minimizer(s).
  - For any minimizer u_{mod}, a "crack" nucleates in Ω_μ at some bond i_{mod}. There is no crack in Ω_M.
  - Let u_μ be a minimizer of the atomistic model with "crack" in i_μ.

$$\sup_{i \in \Omega_\mu, \neq i_\mu, i_{\text{mod}}} \left| \frac{u_{\text{mod}}^{i+1} - u_{\text{mod}}^i}{h} - \frac{u_\mu^{i+1} - u_\mu^i}{h} \right| \leq Ch \text{ (and same in } \Omega_M\text{)},$$

$$u_{\text{mod}}^{i_{\text{mod}}+1} - u_{\text{mod}}^{i_{\text{mod}}} \sim_{h \to 0} a - \theta_M, \qquad u_\mu^{i_\mu+1} - u_\mu^{i_\mu} \sim_{h \to 0} a - \theta_M,$$

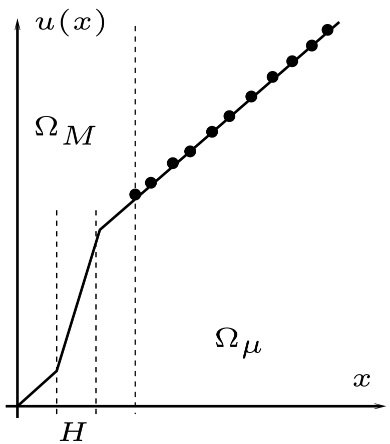
$$\left| (u_{\text{mod}}^{i_{\text{mod}}+1} - u_{\text{mod}}^{i_{\text{mod}}}) - (u_\mu^{i_\mu+1} - u_\mu^{i_\mu}) \right| \leq Ch, \qquad |I_{\text{mod}} - I_\mu| \leq Ch$$

In practice . . .

$$E_c^H\left(U, u_{|\Omega_\mu}\right) = \int_{\Omega_M} W\left(\sum_k U_k N_k'(x)\right)\, dx + h \sum_{i,[ih,ih+h]\subset\Omega_\mu} W\left(\frac{u^{i+1}-u^i}{h}\right)$$

In practice …

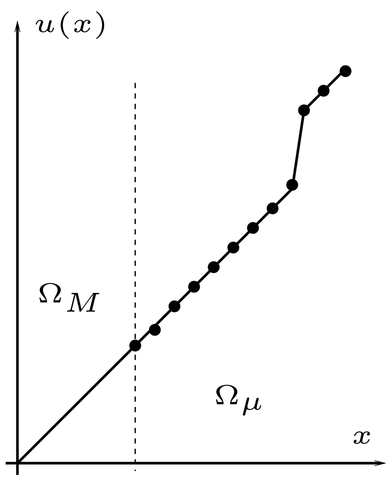
$$E_c^H\left(U, u_{|\Omega_\mu}\right) = \int_{\Omega_M} W\left(\sum_k U_k N_k'(x)\right)\, dx + h \sum_{i,[ih,ih+h]\subset\Omega_\mu} W\left(\frac{u^{i+1}-u^i}{h}\right)$$



If crack localized in Ω_M:

$$\sum U_k N_k'(x) = 1, O(1/H), 1; \quad \forall i,\ \frac{u^{i+1}-u^i}{h} = 1$$

$$E_c^H = (|\Omega_M| - H)\, W_{LJ}(1) + H W_{LJ}\left(\frac{c}{H}\right) + |\Omega_\mu|\, W_{LJ}(1)$$
$$\approx (L-H)\, W_{LJ}(1)$$



If crack in Ω_μ: $\sum U_k N_k'(x) = 1; \quad \frac{u^{i+1}-u^i}{h} = 1\,(i \neq i_\mu)$

$$E_c^H(u) \approx (L-h)\, W_{LJ}(1)$$

When $h \ll H \ll 1$: $E_c^H(F \in \Omega_M) > E_c^H(F \in \Omega_\mu)$.

Conclusions

- in a code, people work with the discretized natural coupled energy E_c^H, which leads to good results, even in the LJ case.
- if $H \to 0$, $E_c^H(u) \to E_c(u)$, the natural coupled energy. However,

  $\inf E_c$ and $\inf E_c^H$ have qualitatively different behaviours.
- the modified coupled energy E_{mod} has a correct behaviour.
- $\inf E_c^H$ is not the discretized version of $\inf E_c$, but of $\inf E_{\text{mod}}$.

X. Blanc, C. Le Bris, F. Legoll, *Analysis of a prototypical multiscale method coupling atomistic and continuum mechanics*, Mathematical Modelling and Numerical Analysis, in press, 2005.