

# **Multiscale methods coupling atomistic and continuum mechanics: analysis of a simple case**

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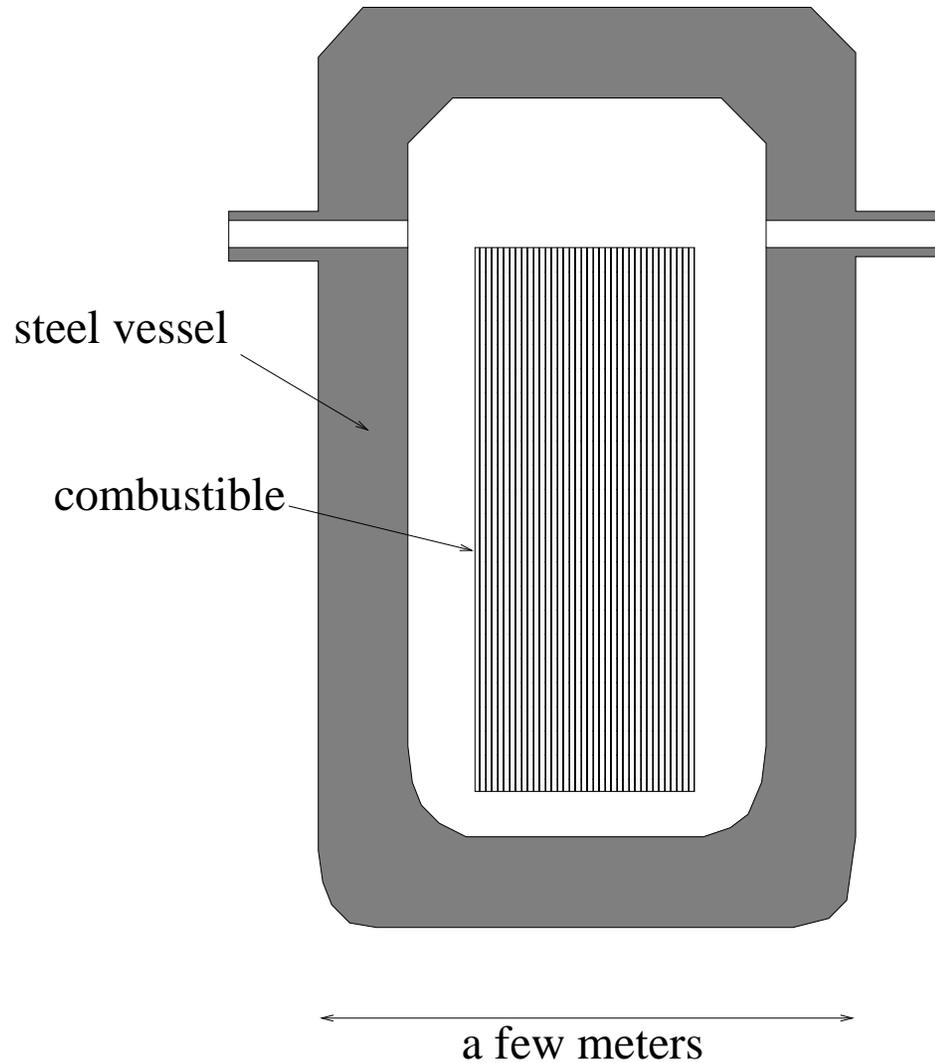
joint work with Xavier Blanc (Université Paris 6) and Claude Le Bris  
(CERMICS, ENPC).

<http://cermics.enpc.fr/~legoll>

# Outline of the talk

- Examples of multiscale problems
- A prototypical 1D multiscale method
- Analysis of the method:
  - case of a convex interatomic potential
  - Lennard-Jones case

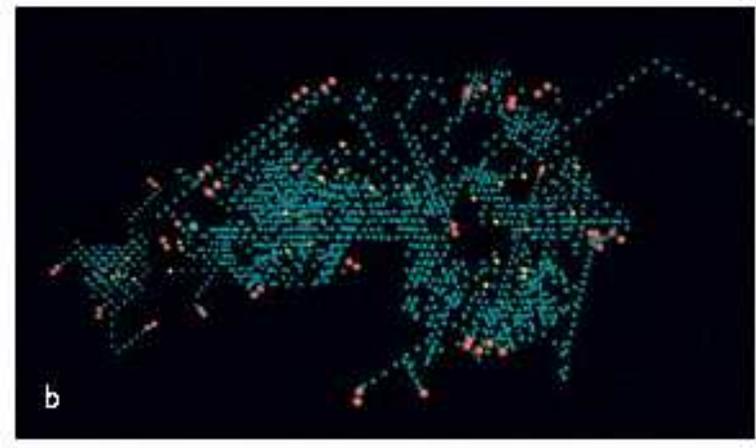
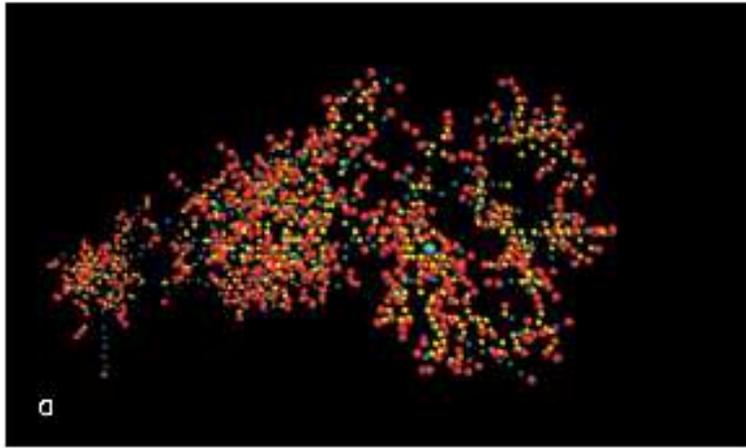
# Materials aging



Nuclear power plants:

Nuclear reaction => emission of neutrons, that interact with the atomistic lattice (billiard).

## Materials aging (CEA pictures)



- **defects** formation (vacancies or interstitials);
- these defects **diffuse** and **react** one with each other;
- at the macroscopic scale, the material properties are modified.

Several space scales ( $10^{-10}$  to 1 m) and time scale ( $10^{-15}$  s to tens of years) are involved.

**Hierarchical** approach: compute parameters of a coarse-grain model with a fine scale model (MD  $\Rightarrow$  kMC  $\Rightarrow$  ...  $\Rightarrow$  Continuum mechanics)

# Multiscale methods: concurrent coupling

## Domain decomposition approach:

- the macroscopic constitutive law (either postulated or computed from a finer scale model) is **valid** only in the subregion  $\Omega_M \subset \Omega$ .
- Idea: model  $\Omega_M$  at the **macroscopic scale** and  $\Omega \setminus \Omega_M$  at the **fine scale**; difficulty: **couple** both models at the interface.

## Approach without any macroscopic constitutive law:

- one does not want / cannot make use of a constitutive law at the macroscopic scale.
- Idea: **numerically compute the macroscopic constitutive law**  
 $\varepsilon_M \rightarrow \sigma_M$  through computations at the microscopic scale.

## The two models that we consider here

- Continuum Mechanics:  $u(x)$  the current position:

$$E_M(u) = \int_{\Omega} W_M(\nabla u(x)) dx$$

→ Minimize  $E_M(u)$ ;

→ Solve the equilibrium equations.

⊕ computational efficiency;

⊖ postulate  $W_M$ ; does not take into account atomistic nature of matter;

- Molecular mechanics (lattice statics):

$$E_{\mu}(u^0, \dots, u^N) = \frac{1}{2} \sum_{i \neq j} W(u^j - u^i)$$

⊕ atomic scale phenomena can be described;

⊖ cost!

# Domain decomposition methods

## Examples:

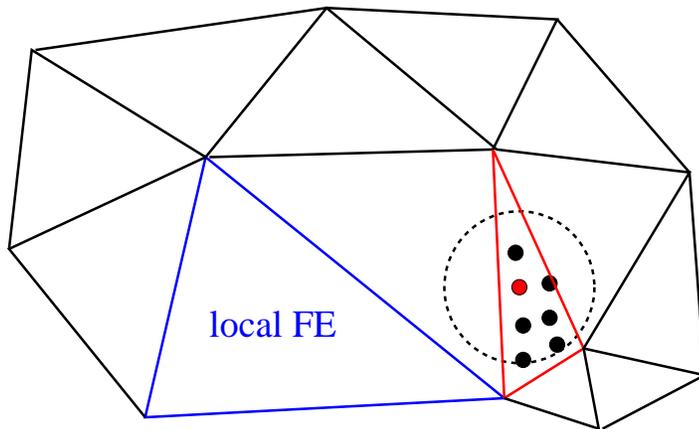
- Quasi Continuum Method:  
Tadmor, Phillips, Ortiz, Langmuir 1996  
Shenoy, Miller, Tadmor, Rodney, Phillips, Ortiz, JMPS 1999  
Dupuy, Tadmor, Miller, Phillips, PRL 2005  
Website: [www.qcmethod.com](http://www.qcmethod.com)
- MAAD method (QM / MD/ FE):  
Rudd and Broughton, Abraham, Bernstein, Kaxiras, Phys. Rev. B 60,  
1999  
  
See also Nakano, Kalia, Vashishta, Lidorikis, Belytschko, ...
- Bridging scale coupling approach: Karpov et al.

# The QuasiContinuum Method (QCM) in its first version

Tadmor, Phillips, Ortiz (Langmuir, 1996):

$$E_\mu = \sum_{j>i} W(u_j - u_i)$$

$$E_\mu \approx E = \underbrace{\sum_{\text{local FE}} |\Omega_e| W_M(\nabla u|_{\Omega_e})}_{\text{local FE}} + \underbrace{\sum_{\text{nonlocal FE}} \sum_{i \in \Omega_e} e_i}_{\text{nonlocal FE}}$$



$$\text{P1 interpolation : } u(x) = \sum_k U_k N_k(x)$$

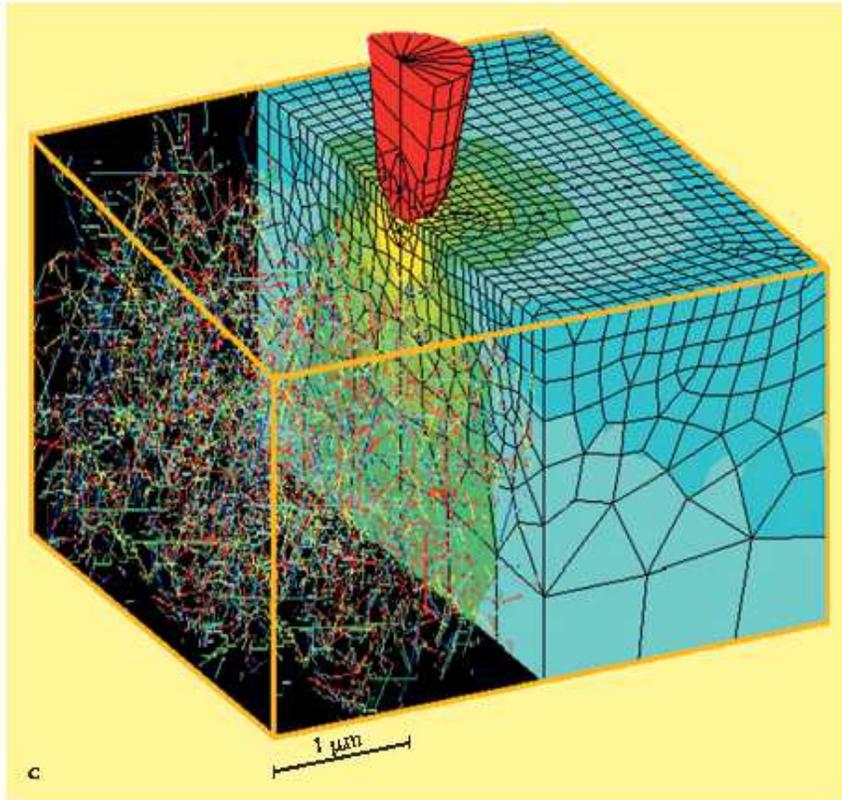
$$e_i = e_i(U) = \sum_{j \neq i} W_\mu(u(jh) - u(ih))$$

$h$  : atomistic lattice parameter

⊕ the micro/macro partition of  $\Omega$  can **evolve** along the simulation (adaptivity);

⊖ global minimum: **equilibrium** at **zero temperature**.

## Nanoindentation simulation (CEA picture)



Dislocations appear: localized core, long range effects.

Other possible applications: fracture simulation, . . .

## Some more recent approaches to QCM

- split the set of atoms (and not the Finite Elements) into local / nonlocal atoms:  
Shenoy, Miller, Tadmor, Rodney, Phillips, Ortiz, JMPS 1999  
Knap and Ortiz, JMPS 2001
- QCM method to evaluate NVT statistical averages computations:  
Dupuy, Tadmor, Miller, Phillips, PRL 2005

In this work, we will look at some error analysis of the QCM. On this subject, see also Ping Lin works (2002, 2005).

# Derivation of a continuum model from an atomistic model

Point wise approaches:  $E_\mu(u) \rightarrow E_M(u)$

- Equilibrium, deterministic case:

Blanc, Le Bris, Lions, Arch Rat Mech Anal 2002 (bulk energy)

$\mu$  model: interatomic potential, or some QM models (eg TFW).

Blanc, Le Bris, CRAS 2005 (surface energy)

Arndt and Griebel, SIAM MMS 2005 (bulk energy)

- Equilibrium, stochastic networks:

Blanc, Le Bris, Lions (bulk energy)

- Dynamical case: discrete dynamics  $\rightarrow$  time-dependent PDE

Berezhnyy and Berlyand, JMPS 2006

$\Gamma$ -limit approach (equilibrium):  $\inf E_\mu \rightarrow \inf E_M$ : Braides et al, Arch Rat Mech Anal 1999



# Alternative approaches to multiple scale coupling

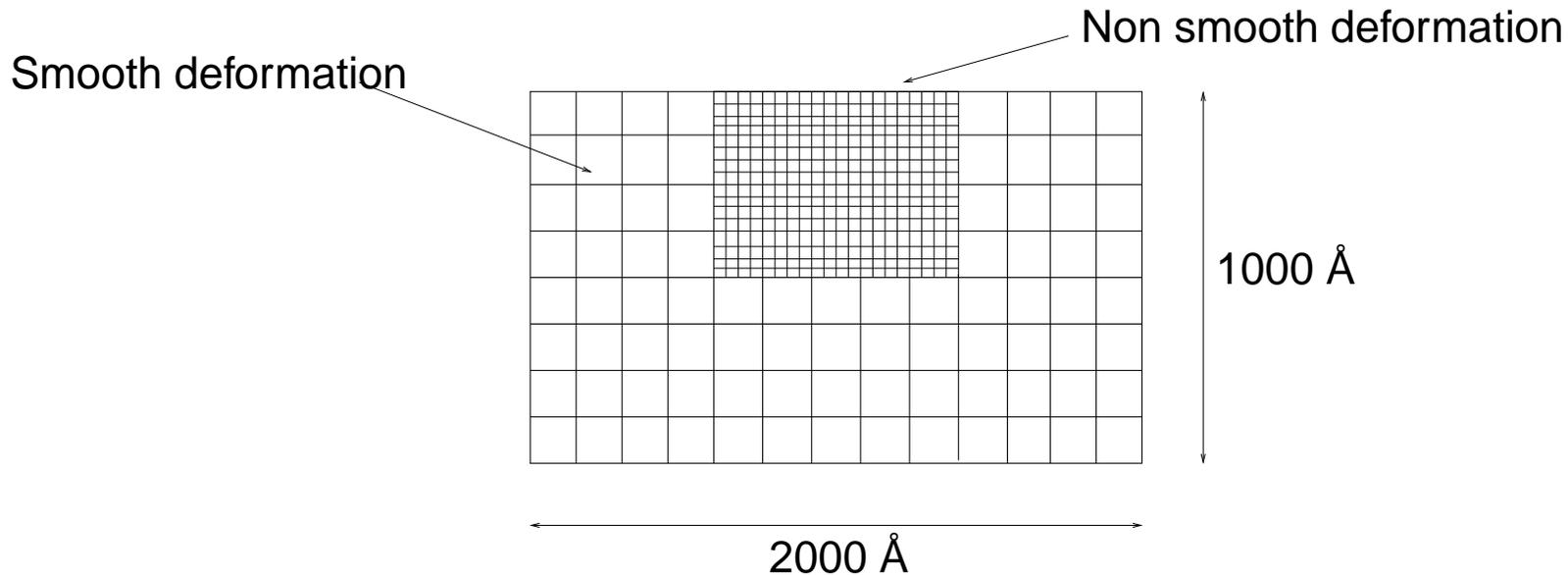
- From the atomistic model, derive a continuum mechanics model with **higher order derivatives**:

$$E_M(u) = \int_{\Omega} W_M(\nabla u(x), \nabla^2 u(x)) dx$$

and minimize / look for critical points (Triantafyllidis, Bardenhagen).

- Approximation of the discrete variational problems through a  **$\Gamma$  limit** homogenization approach (Braides, Dal Maso, Garroni);
- Compare **local** (instead of **global**) minimizers of macro and micro energies (E, Ming).

# Paradigm: coupling atomistic with continuum mechanics



- Large computational domain;
- Expected deformation: non-smooth in some small region of the solid.

Method: variational problem coupling an (accurate) atomistic model with a (cheap) continuum mechanics model (Domain Decomposition idea).

Search for global minima: statics, temperature = 0.

# The atomistic model

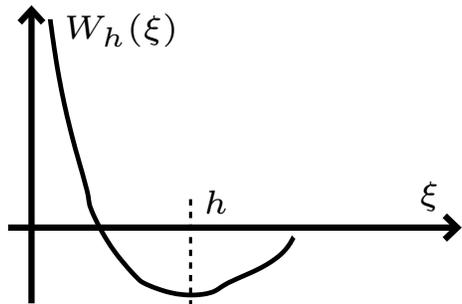
# The atomistic model

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: 
$$E_\mu(u^0, \dots, u^N) = \frac{1}{2N} \sum_{i \neq j} W_h(u^j - u^i)$$



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

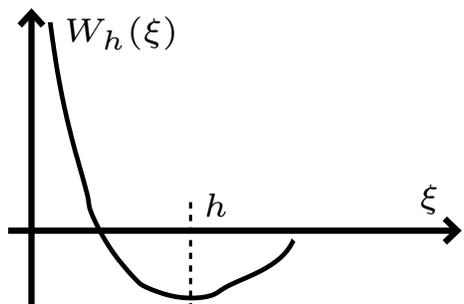
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Energy per particle:  $E_\mu(u^0, \dots, u^N) = \frac{1}{2N} \sum_{i \neq j} W_h(u^j - u^i)$



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

**Atomistic model** (assuming Nearest Neighbor interactions):

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

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

# Derivation of a continuum model from an atomistic model

Blanc, Le Bris, Lions, Arch Rat Mech Anal 2002: Consider a macroscopic **smooth** deformation  $u$ :

$$\begin{aligned} E_\mu(u(0), u(h), \dots, u(Nh)) &= \frac{h}{L} \sum_{i=0}^{N-1} W \left( \frac{u((i+1)h) - u(ih)}{h} \right) \\ &\xrightarrow{h \rightarrow 0} \frac{1}{L} \int_{\Omega} W(u'(x)) dx =: E_M(u) \end{aligned}$$

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

This derivation can be done in 3D, without the nearest neighbor interaction assumption:  $\implies W_{CM}(\nabla u)$  as a function of  $W(\nabla u)$ .

## Toward a coupled problem

If  $u$  is smooth on  $\Omega$ , we associate to

$$\inf \{ E_\mu(u^0, \dots, u^N), u^0 = 0, u^N = a, u^{i+1} > u^i \}$$

the problem

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

What if the deformation is not smooth on the whole domain?

Make use of **different models** in different domains, and pass to the limit only in some part of  $\Omega$ .

# Coupled model: a first attempt

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

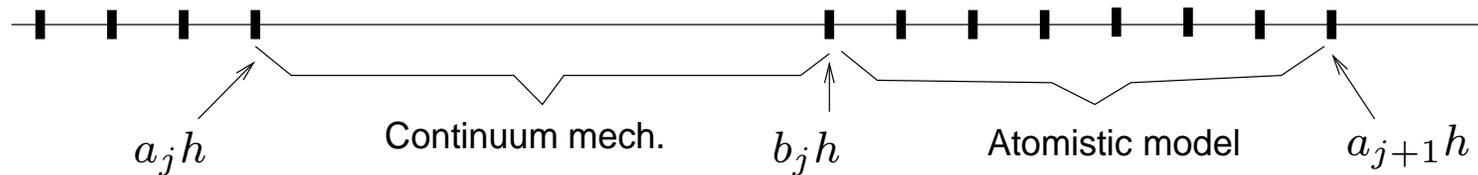
where  $\begin{cases} \Omega_M(u) = \text{subdomain where } u \text{ is smooth,} \\ \Omega_\mu(u) = \text{subdomain where } u \text{ is non-smooth.} \end{cases}$

For instance:  $\Omega_M(u) = \{x \in \Omega; |u''(x)| \leq C\}$ .

Highly nonlinear problem  $\rightarrow$   
remove the link between  $u$  and the partition of  $\Omega$

# The natural coupled model

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



$$E_c(u) := \int_{\Omega_M} W(u'(x)) - f(x) u(x) dx$$

$$+ h \sum_{i, [ih, ih+h] \subset \Omega_\mu} W\left(\frac{u^{i+1} - u^i}{h}\right) - h \sum_{i, ih \in \Omega_\mu} u^i f(ih)$$

Balance between numerical efficiency / precision

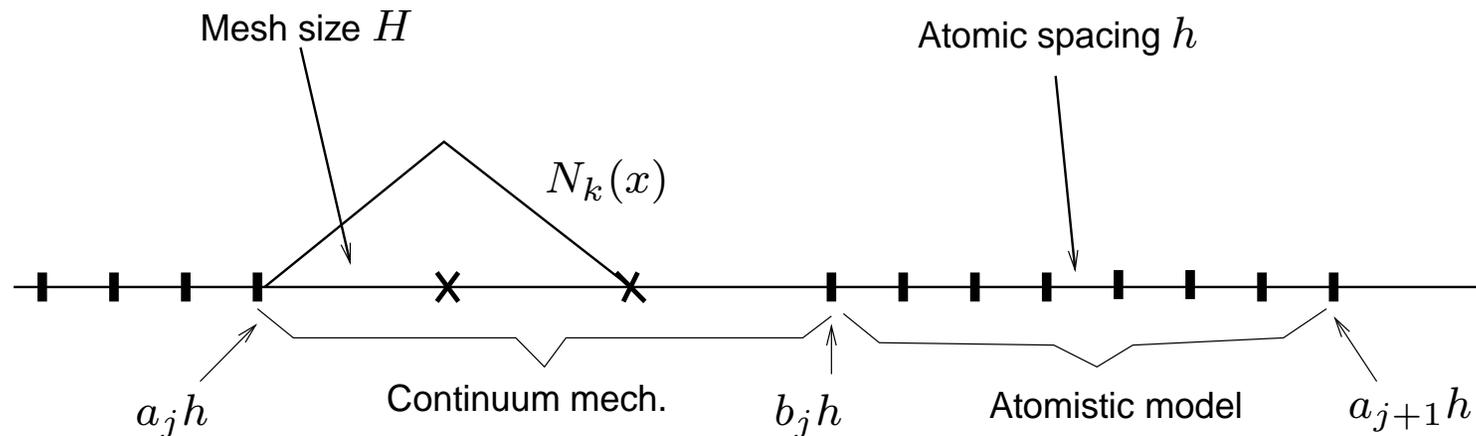
**Consistency:**  $\lim_{h \rightarrow 0} E_c(u) = E_M(u)$ .

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

## The coupled problem after discretization

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

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



This method is the 1D version of the Quasi-Continuum Method (v 1996).

# Questions

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

- How to **choose** the partition?

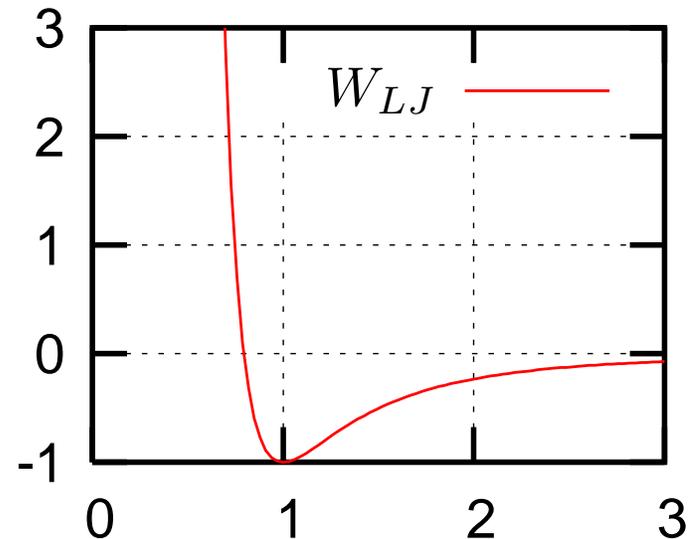
Idea: the set  $\Omega_M$  should consist of all the zones of regularity of  $u_\mu$

- Is  $E_c$  a good definition for the **coupled energy**?

- **Bounds** on the error?

- Convex interatomic potential  $W$ ;

- The Lennard-Jones case.



## Convex case

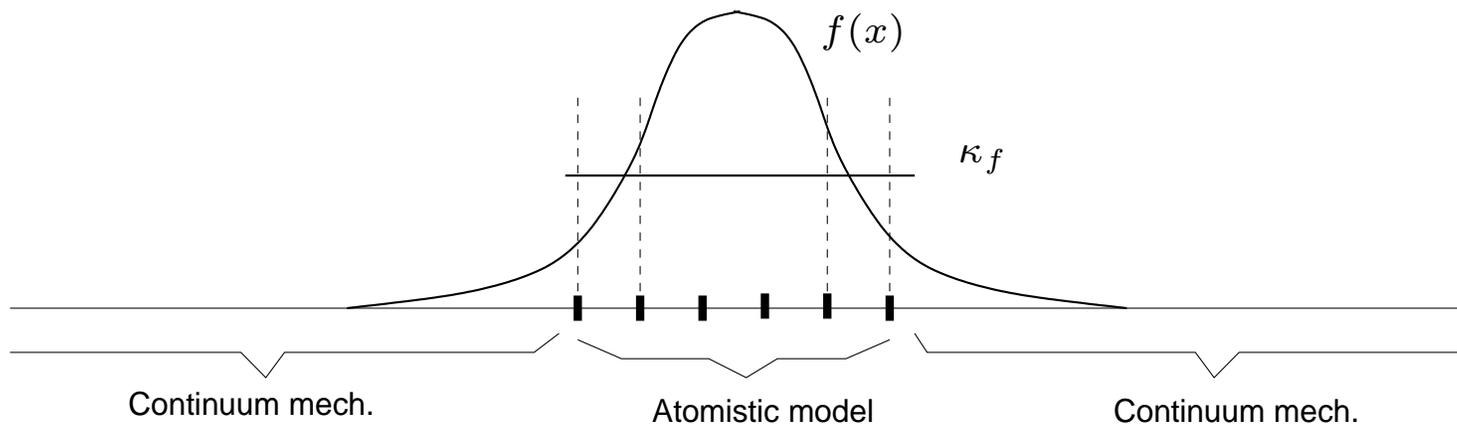
$$f \in \mathcal{C}^0(\bar{\Omega}); \quad W \in \mathcal{C}^2(\mathbb{R}) \text{ with } 0 < \alpha \leq W''(z) \text{ and } |W'(z)| \leq \beta |z - 1|$$

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

The interval  $(ih, ih + h)$  is said to be **regular** if

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

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



Partition just depends on  $f$ !

## Estimates between $u_c$ and $u_\mu$ (convex case)

Let  $u_\mu$  be the minimizer of  $E_\mu$ , and  $u_c$  the minimizer of  $E_c$ .

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

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

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

$$\sup_{i \in \Omega_\mu} |u_c^i - u_\mu^i| \leq Ch\kappa_f, \quad \|u_c - \Pi_c u_\mu\|_{L^\infty(\Omega_M)} \leq Ch\kappa_f,$$

$$|I_c - I_\mu| \leq Ch\kappa_f.$$

$\Pi_c$ : affine interpolation operator

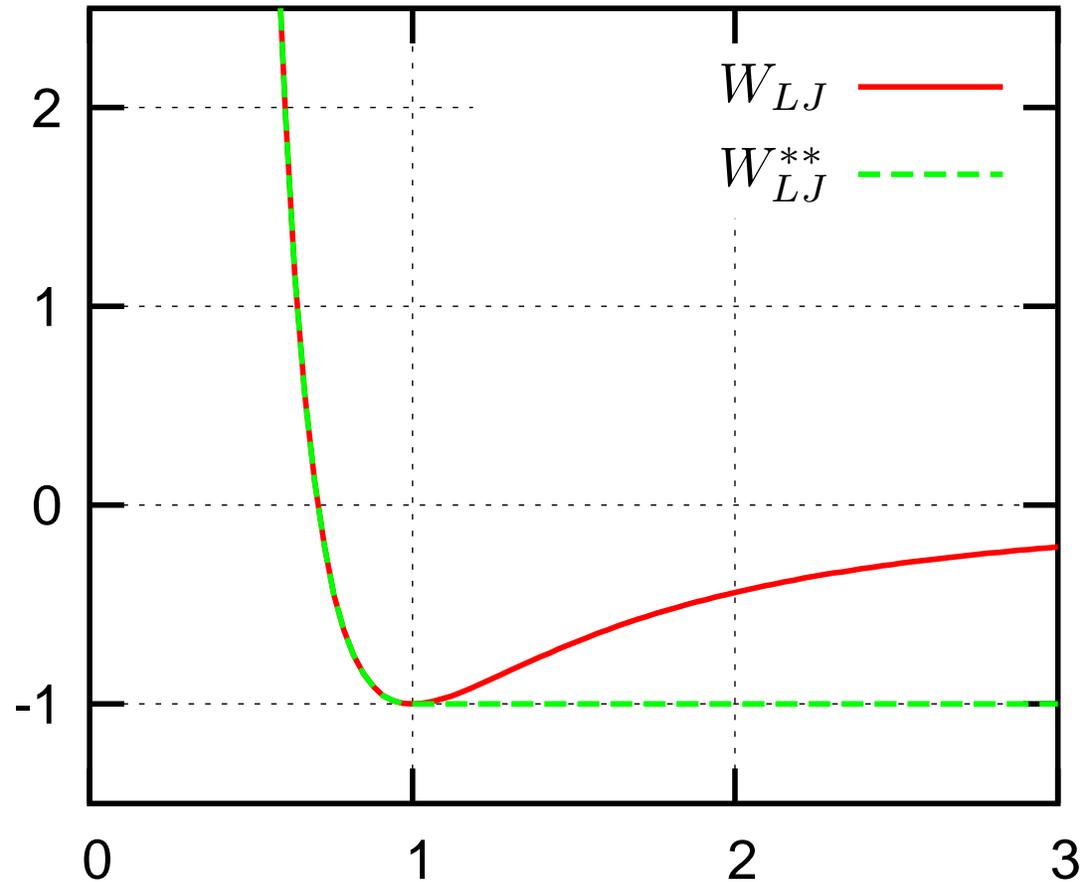
# The Lennard-Jones case

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

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

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

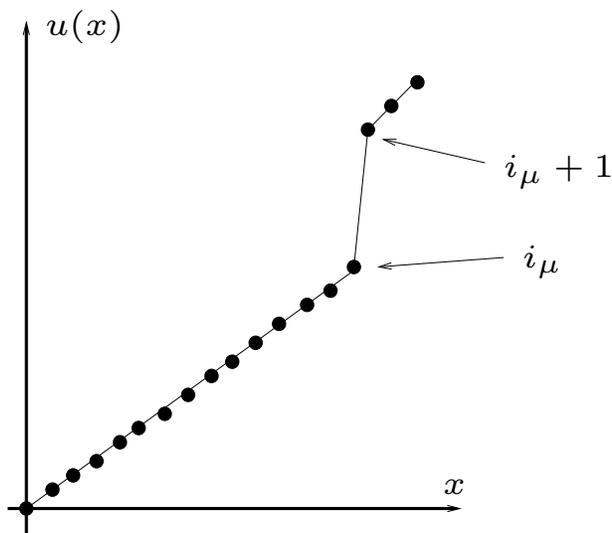
$$r_c = (13/7)^{1/6}$$



## The atomistic problem ( $f = 0$ )

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

- if  $a \leq L$  (compression): **unique minimizer**, smooth (homog. strain).
- if  $a > L$  (tension): **many minimizers**, “smooth” everywhere except on a single bond:



$$\frac{u_\mu^{i_\mu+1} - u_\mu^{i_\mu}}{h} \underset{h \rightarrow 0}{\sim} \frac{a - L}{h} \quad (\text{“crack”})$$

$$\forall i \neq i_\mu, \frac{u_\mu^{i+1} - u_\mu^i}{h} \approx 1$$

L. Truskinovsky, 1996.

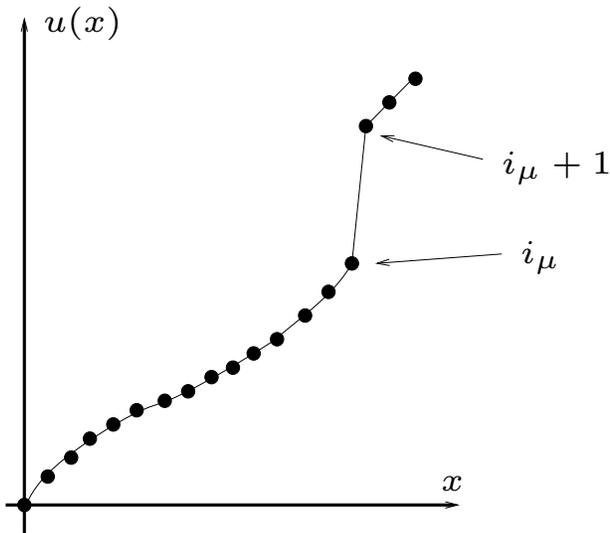
Because NN interaction and  $f = 0$ , crack location can be **anywhere** (same energy).

## The atomistic problem ( $f \in C^0(\bar{\Omega})$ )

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

There exists a **threshold**  $\theta_\mu$  such that:

- if  $a \leq \theta_\mu$ , **unique minimizer**;
- if  $a > \theta_\mu$ : **one or many minimizers**, smooth everywhere except on a single bond  $(i_\mu, i_\mu + 1)$ :



$$\frac{u_\mu^{i_\mu+1} - u_\mu^{i_\mu}}{h} \underset{h \rightarrow 0}{\sim} \frac{C}{h}$$

$$\forall i \neq i_\mu, (u_\mu^{i+1} - u_\mu^i) \underset{h \rightarrow 0}{\rightarrow} 0$$

Crack location can be characterized:

$$F_\mu^i := h \sum_{j=1}^i f(jh) : F_\mu^{i_\mu} = \inf_i F_\mu^i$$

## 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  $a \leq L$ :  $u_M(x) = ax/L$ .
- If  $a > L$ : **infinity** of solutions,  $u_M = x + \sum_i v_i H(x - x_i)$ .  
Crack location is **not determined**.

Results can be generalized to the case  $f \neq 0$ :  $\exists \theta_M$  s.t.

- if  $a \leq \theta_M$ ,  $\exists!$  solution, which is smooth;
- if  $a > \theta_M$ , crack whose location can be characterized.

## Natural micro-macro approach

Suppose  $f \equiv 0$ : interesting case is  $a > L$ :

**Atomistic problem:** a unique crack appears, no specific location.

**Aim:** use a coupled model s.t.

- the atomistic zone contains the crack,
- any minimizer of coupled problem is close to a minimizer of the atomistic model.

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

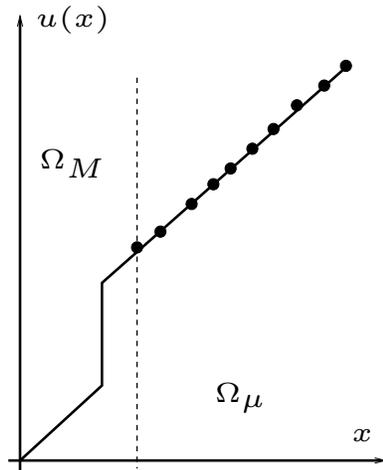
$$E_c(u) = \int_{\Omega_M} W_{LJ}(u'(x)) dx + h \sum_{i, [ih, ih+h] \subset \Omega_\mu} W_{LJ} \left( \frac{u^{i+1} - u^i}{h} \right)$$

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

Where the crack is going to appear?

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

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



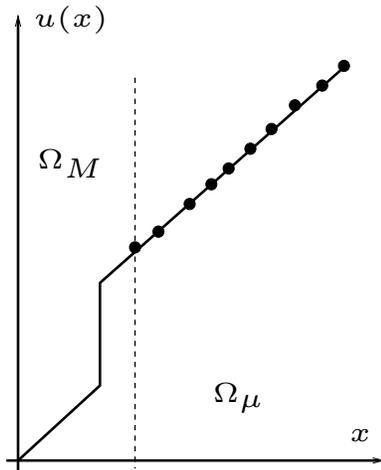
If crack localized in  $\Omega_M$ :

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

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

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

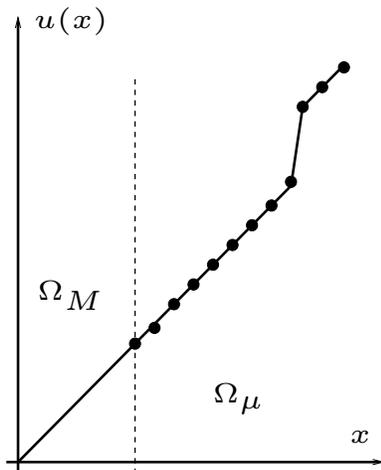
$$E_c(u) = \int_{\Omega_M} W_{LJ}(u'(x)) dx + h \sum_{\Omega_\mu} W_{LJ} \left( \frac{u^{i+1} - u^i}{h} \right)$$



If crack localized in  $\Omega_M$ :

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

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



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

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

$$W_{LJ}(1) < 0: \quad E_c(F \in \Omega_M) < E_c(F \in \Omega_\mu).$$

## The natural algorithm leads to issues

First algorithm (refine): initialize  $\Omega_M = \Omega$ ,

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

Then, at the end,  $\Omega_\mu = \Omega$ .

## The natural algorithm leads to issues

First algorithm (refine): initialize  $\Omega_M = \Omega$ ,

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Then, at the end,  $\Omega_\mu = \Omega$ .

Another algorithm (refine/unrefine): initialize  $\Omega_M = \Omega$ ,

- solve the coupled problem  $\inf_u E_c(u)$  with  $\Omega_M$  fixed;
- look for the zones where the minimizer  $u_c$  is smooth (resp. not smooth), enlarge  $\Omega_M$  (resp.  $\Omega_\mu$ ) correspondingly and go back to step 1.

Then the algorithm **does not converge**.

## A modified micro-macro approach

Idea: give an energy cost (surface energy) to a crack in  $\Omega_M$ .

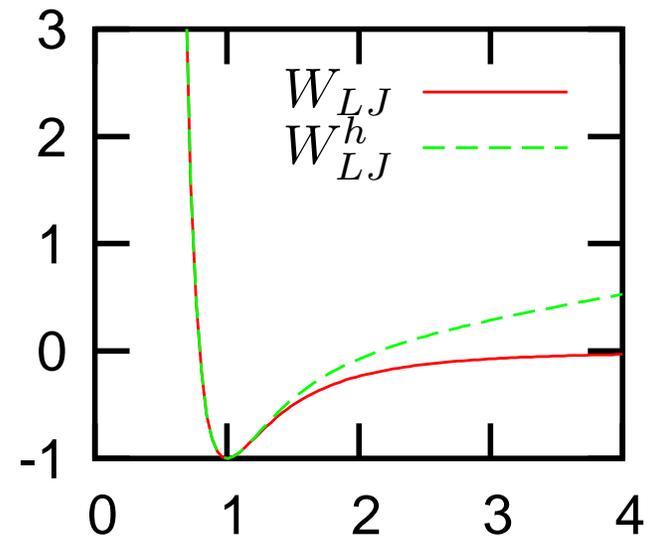
$$E_{\text{mod}}(u) = \int_{\Omega_M} W_{LJ}^h(u'(x)) - f(x) u(x) dx$$

$$+ h \sum_{i, [ih, ih+h] \subset \Omega_\mu} W_{LJ} \left( \frac{u^{i+1} - u^i}{h} \right) - h \sum_{i, ih \in \Omega_\mu} u^i f(ih)$$

$$W_{LJ}^h(r) := W_{LJ}(r) + \sqrt{h} \left( r - \frac{1+r_c}{2} \right)_+$$

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

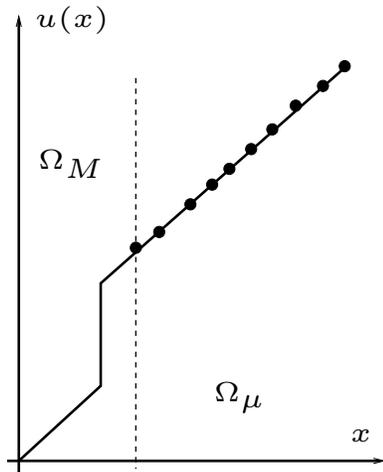
$$\lim_{h \rightarrow 0} E_{\text{mod}}(u) = E_M(u) \text{ (consistency).}$$



If  $f \equiv 0$ , does that solve the problem?

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

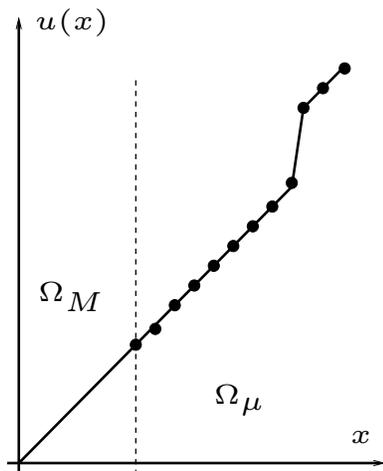
$$E_{\text{mod}}(u) = \int_{\Omega_M} \left[ W_{LJ}(u'(x)) + \sqrt{h}(u'(x) - r_0)_+ \right] dx + h \sum_{\Omega_\mu} W_{LJ} \left( \frac{u^{i+1} - u^i}{h} \right)$$



If crack localized in  $\Omega_M$ :

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

$$E_{\text{mod}}(u) = E_c(u) + \sqrt{h}(a-L) = L W_{LJ}(1) + \sqrt{h}(a-L)$$



If crack in  $\Omega_\mu$ :

$$E_{\text{mod}}(u) = E_c(u) = L W_{LJ}(1) - h W_{LJ}(1)$$

$$\sqrt{h} \gg h: \quad E_{\text{mod}}(F \in \Omega_M) > E_{\text{mod}}(F \in \Omega_\mu).$$

$f \equiv 0$ : the modified approach is ok!

## 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**

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

## Modified coupled problem: error estimates

There exists a threshold  $\theta_M$  such that:

- if  $a \leq \theta_M$  (no crack case):  $\exists!$  **solution**  $u_{\text{mod}}$ , estimates similar to the convex case ones:  $\|u_{\text{mod}} - u_\mu\|_{W^{1,\infty}} \leq Ch\kappa_f$ .
- If  $a > \theta_M$ : There are one or many minimizer(s) for  $\inf E_{\text{mod}}$ .
  - For any minimizer  $u_{\text{mod}}$ , a **“crack” nucleates in  $\Omega_\mu$**  at some bond  $i_{\text{mod}}$ . There is **no crack in  $\Omega_M$** .
  - Let  $u_\mu$  be a minimizer of the atomistic model with “crack” in  $i_\mu$ .

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

$$u_{\text{mod}}^{i_{\text{mod}}+1} - u_{\text{mod}}^{i_{\text{mod}}} \underset{h \rightarrow 0}{\sim} a - \theta_M, \quad u_\mu^{i_\mu+1} - u_\mu^{i_\mu} \underset{h \rightarrow 0}{\sim} a - \theta_M,$$

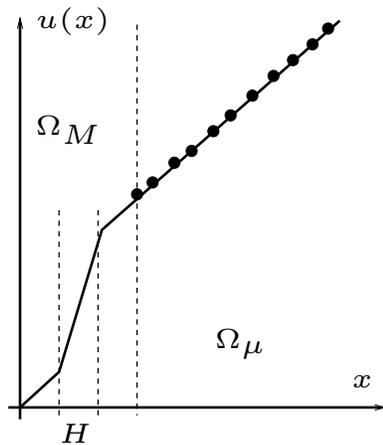
$$\left| (u_{\text{mod}}^{i_{\text{mod}}+1} - u_{\text{mod}}^{i_{\text{mod}}}) - (u_\mu^{i_\mu+1} - u_\mu^{i_\mu}) \right| \leq Ch, \quad |I_{\text{mod}} - I_\mu| \leq Ch.$$

## In practice ...

$$E_c^H(U, u|_{\Omega_\mu}) = \int_{\Omega_M} W \left( \sum_k U_k N'_k(x) \right) dx + h \sum_{\Omega_\mu} W \left( \frac{u^{i+1} - u^i}{h} \right)$$

## In practice ...

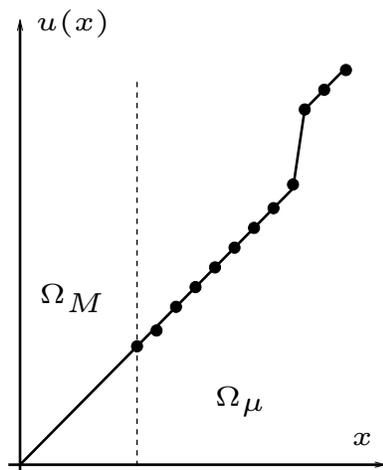
$$E_c^H(U, u|_{\Omega_\mu}) = \int_{\Omega_M} W \left( \sum_k U_k N'_k(x) \right) dx + h \sum_{\Omega_\mu} W \left( \frac{u^{i+1} - u^i}{h} \right)$$



If crack localized in  $\Omega_M$ :

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

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



If crack in  $\Omega_\mu$ :  $\sum U_k N'_k(x) = 1; \frac{u^{i+1} - u^i}{h} = 1 (i \neq i_\mu)$

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

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

## Conclusions on the Lennard-Jones case

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

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

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

- in a code, people work with  $E_c^H \implies$  good results.
- if  $H \rightarrow 0$ ,  $E_c^H(u) \rightarrow E_c(u)$ . However,  $\inf E_c$  and  $\inf E_c^H$  have qualitatively **different** behaviours.
- the problem  $\inf E_c$  has some flaws,  $\inf E_{\text{mod}}$  has a better behaviour.
- $\inf E_c^H$  is not the discretized version of  $\inf E_c$ , but of  $\inf E_{\text{mod}}$ .

# Conclusions

We have studied 1D materials described by **NN pair interatomic potential**, and looked at their **equilibrium** at **zero temperature**:

- **Convex** potential: one can define a partition of  $\Omega$  based only on the body forces  $f$ .
- **Lennard-Jones potential**: there are issues with the natural coupling. These issues disappear when FE discretization.
- We propose another (consistent) definition for the coupling energy and a strategy to partition  $\Omega$ .

X. Blanc, C. Le Bris, F. Legoll, *Analysis of a prototypical multiscale method coupling atomistic and continuum mechanics*, *Mathematical Modelling and Numerical Analysis*, vol. 39 (2005).