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ABSTRACT. *The description and computation of fine scale localized phenomena arising in a material (during nanoindentation, for instance) is a challenging problem that has given birth to many multiscale methods. In this work, we propose an analysis of a simple one-dimensional method that couples two scales, the atomistic one and the continuum mechanics one. The method includes an adaptive criterion in order to split the computational domain into two subdomains, that are described at different scales.*

RÉSUMÉ. *Pour décrire des solides qui subissent des déformations peu régulières, mais dont les irrégularités sont localisées, beaucoup de méthodes multi-échelles ont été développées. Elles s'attachent en général à coupler un modèle continu (ou macroscopique), qui décrit les zones où la déformation est régulière, et un modèle discret (ou atomique), qui décrit les zones où la déformation présente des singularités. Nous présentons ici une étude théorique et une analyse d'erreur de ce type de méthode en dimension un.*

KEYWORDS: *Multiscale methods, variational problems, continuum mechanics, discrete mechanics.*

MOTS-CLÉS : *Méthodes multi-échelles, problèmes variationnels, mécanique du continuum, mécanique discrète.*

1. Introduction

The traditional framework in mechanics is the continuum description. However, when nanoscale localized phenomena arise, the atomistic nature of material cannot be ignored: for instance, to understand how dislocations appear under a nanoindenter, one has to describe the deformed atomistic lattice. The situation is the same when one wants to have a detailed understanding of the behaviour of grain boundaries in a polycristal. In all these examples, an appropriate model to describe the localized phenomena is the atomistic model, in which the solid is considered as a set of discrete particles interacting through given interatomic potentials.

However, the size of materials that can be simulated by only using the atomistic model is very small in comparison to the size of the materials one is interested in. Fortunately, in the situations we considered above, the deformation is smooth in the main part of the solid. So, a natural idea is to try to take advantage of both models, the continuum mechanics one and the atomistic one, and to couple them. In this work, we analyze a method that couples these two models into a single one, and which is a toy example for more advanced methods such as the Quasi-Continuum Method (Knap *et al.,* 2001, Miller *et al.,* 2002, Shenoy *et al.,* 1999, Tadmor *et al.,* 1996). A recent overview of some mathematical results on atomistic to continuum limits for crystalline materials can be read in (Blanc *et al.,* 2007b). Other coupling methods have been proposed in (Ben Dhia, 1998, Ben Dhia *et al.,* 2005, E *et al.,* 2003, Feyel *et al.,* 2000, Park *et al.,* 2005, Van Vliet *et al.,* 2003, Zhang *et al.,* 2002). See also the monographs (Bulatov *et al.,* 1999, Liu *et al.,* 2004, Raabe, 1998).

An alternative to multiscale methods is to use continuum mechanics models in which the elastic energy depends not only on the strain, but also on higher derivatives of the displacement (Triantafyllidis *et al.,* 1993), or to add a surface energy (Del Piero *et al.,* 2001). Another alternative way consists in the approximation of the variational problems with a Γ-limit approach (Braides *et al.,* 1999). Time-dependent methods based on mixed hamiltonians have also been proposed in (Broughton *et al.,* 1999).

1.1. *The atomistic and continuum mechanics models*

Let us consider a one-dimensional material occupying in the reference configuration the domain $\Omega = (0, L)$, submitted to body forces f and fixed displacement boundary conditions on $\partial\Omega$. In the atomistic model, the solid is considered as a set of $N+1$ atoms, whose current positions are $(u^i)_{i=0}^N$. The energy of the system is given by

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

where W is an interacting potential between atoms, and h is the atomic lattice parameter, which is linked to the number of atoms and the size of the solid by $L = Nh$.

We have assumed only nearest neighbour interaction. The potential W is such that its minimum is attained at 1, so, at equilibrium without body forces and boundary conditions, the interatomic distance is h. The microscopic equilibrium configuration is a solution of the variational problem

$$\inf \left\{ E_\mu(u^0, \ldots, u^N),\ u^0 = 0,\ u^N = a,\ \forall i, u^{i+1} > u^i \right\}. \qquad [2]$$

Note that we look here for a global minimizer of the energy. Another approach would be to look at local minimizers (see for instance (E *et al.*, 2007, Rieger *et al.*, 2007)).

In the continuum mechanics model, the solid deformation is described by the map $u : \Omega \to \mathbb{R}$, and the elastic energy associated with the deformation u reads

$$E_M(u) = \int_\Omega W(u'(x))\, dx - \int_\Omega f(x)\, u(x)\, dx. \qquad [3]$$

The equilibrium of the solid is defined by the minimization problem

$$\inf \left\{ E_M(u),\ u \in H^1(\Omega),\ u(0) = 0,\ u(L) = a,\ u \text{ is increasing on } \Omega \right\}. \qquad [4]$$

We assume here that the energy $E_M(u)$ is well defined as soon as $u \in H^1(\Omega)$.

In principle, the equilibrium configuration of the solid is given by (1)-(2), but the huge number of particles to be considered makes the problem impossible to solve in practice. For a given smooth deformation u, it has been shown in (Blanc *et al.*, 2002) that the microscopic energy $E_\mu(u(0), u(h), \ldots, u(Nh))$ converges to $E_M(u)$ when the atomic lattice parameter h goes to 0 and the number of atoms goes to infinity such that Nh remains constant, $Nh = L$ (see (Arndt *et al.*, 2005) for some other possible ways for deriving continuum energies from the atomistic level). Thus, solving (3)-(4) gives a good approximation of the solution of the atomistic problem, when the equilibrium deformation is smooth.

1.2. *A coupled model*

When non regular deformations are expected to play a role, following (Tadmor *et al.*, 1996), we approximate the solution of the atomistic problem with the solution of a coupled model. A partition $\Omega = \Omega_M \cup \Omega_\mu$ of the domain being given, a natural expression for a coupled energy reads

$$\begin{aligned} E_c(u) &= \int_{\Omega_M} \left[W(u'(x)) - f(x)u(x) \right] dx \\ &+ h \sum_{i;\, ih, ih+h \in \Omega_\mu} W\left(\frac{u^{i+1} - u^i}{h} \right) - h \sum_{i; ih \in \Omega_\mu} f(ih) u^i. \end{aligned} \qquad [5]$$

The equilibrium of the solid is given by the minimization problem

$$\inf \left\{ \begin{array}{c} E_c(u),\ u_{|\Omega_M} \in H^1(\Omega_M),\ u_{|\Omega_\mu} \text{ is the discrete set of variables} \\ (u^i)_{ih \in \Omega_\mu}, u \text{ is continuous at the interface } \partial\Omega_M \cap \partial\Omega_\mu, \\ u(0) = 0,\ u(L) = a,\ \text{u is increasing on } \Omega \end{array} \right\} \qquad [6]$$

The questions we address here are:

– is the previous definition (5) of the coupled energy always the most appropriate?

– how to (adaptively) define the partition $\Omega = \Omega_M \cup \Omega_\mu$ such that the solution of the coupled problem (5)-(6) is a good approximation of the solution of the atomistic problem (1)-(2)?

– can error bounds be derived?

The error analysis of such coupled models has also been addressed in (Lin, 2003, Lin, 2007).

2. Results

We study both the general case of a convex energy density W, and a specific example of nonconvex energy, the Lennard-Jones case. More precise and detailed statements of the following results are given in (Blanc *et al.*, 2005) and (Blanc *et al.*, 2007a).

2.1. *The convex case*

In this case, we propose an *a priori* definition for the partition which is only based on properties of the body forces f. Vaguely stated, the subdomain Ω_M (in which the continuum mechanics model will be used) is the part of the domain Ω where the body force f and its derivative f' are small.

With this definition, we show that the solution of the coupled problem (5)-(6) is a good approximation of the solution of the atomistic problem (1)-(2): when the atomic lattice parameter h goes to 0, the deformation u_c and the strain given by the coupled model converge to the deformation u_μ and the strain given by the atomistic model.

2.2. *A nonconvex case: the Lennard-Jones case*

In this case, we show that expression (5) for the coupled energy might be inappropriate, and we thus propose a modified expression.

If the material is submitted to an extensional loading (i.e., if $u(L) = a > L$ in the case of no body forces), the displacement at equilibrium is discontinuous both with the macroscopic model and with the atomistic model (there is a fracture in the solid). With the natural coupled model (5)-(6), the equilibrium also exhibits a fracture, but this fracture is always located in the macroscopic subdomain Ω_M. However, we would rather like the atomistic subdomain Ω_μ to contain the fracture. To solve this issue, we propose to work with the coupled energy

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

with $W_{\mathrm{LJ}}^h(t) = W_{\mathrm{LJ}}(t) + h^\alpha (t-t_0)_+$, where W_{LJ} is the Lennard-Jones potential, t_0 is some threshold and α is any real number in $(0,1)$. Finally, the algorithm we propose consists in two steps:

– compute a solution u_M of the macroscopic problem (3)-(4), and from the properties of u_M, define a partition $\Omega = \Omega_M \cup \Omega_\mu$.

– with this partition, minimize the coupled energy $E_c^h(u)$ to find u_c.

We show that the resulting solution u_c is a good approximation of the atomistic solution. In particular, if the solid is submitted to extensional loadings, the atomistic subdomain Ω_μ contains the fracture.

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