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ANALYSIS OF A VARIATIONAL METHOD COUPLING DISCRETE AND CONTINUUM MECHANICS

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Summary 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 some 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 adaptative criterion in order to split the computational domain into two subdomains, that are described at different scales.

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 boudaries 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 analyse a method initially proposed in [1] that couples these two models into a single one. Other coupling methods have been proposed in [2], [3]. Another possibility 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 [4], or to add a surface energy [5]. Time-dependent methods based on mixed hamiltonians have also been proposed in [6].

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

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

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

$$\inf\left\{E_\mu(u^0, \dots, u^N),\ u^0 = 0,\ u^N = a\right\}. \tag{2}$$

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

$$E_M(u) = \int_\Omega W(u'(x))\, dx - \int_\Omega f(x)\, u(x)\, dx. \tag{3}$$

The equilibrium of the solid is defined by the minimization problem

$$\inf\left\{E_M(u),\ u(0) = 0,\ u(L) = a\right\}. \tag{4}$$

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 can be shown [7] that the microscopic energy $E_\mu(u(0), u(h), \dots, u(Nh))$ 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, $Nh = L$. Thus, solving (3)-(4) gives a good approximation of the solution of the atomistic problem, when the equilibrium deformation is smooth.

A coupled model

When non regular deformations are expected to play a role, following [1], 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

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

The equilibrium of the solid is given by the minimization problem

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

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?

RESULTS

We study both the general case of a convex energy density W, and a specific example of non convex energy, the Lennard-Jones case.

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. Essentially, the subdomain Ω_M (in which the continuum mechanics model will be used) is the part of the domain 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 displacement u_c and the strain given by the coupled model converge to the displacement u_μ and the strain given by the atomistic model.

A non convex 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 macroscopic model and the atomistic model solutions exhibit a fracture. 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

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

with $W_h(t) = W(t) + \rho_h(t-t_0)_+$, where t_0 is some threshold and ρ_h goes to 0 when h goes to 0. Several choices are possible for ρ_h. 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 will 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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