

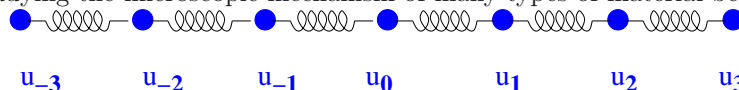
Upscaling molecular models to PDEs

Research Project for Math 497A, Spring 2008.
Mentor: Xiantao Li

March 3, 2008

1 Introduction

In this project, we consider systems at the molecular scale, where the structure is modeled through the interaction between the atoms making up the material. Such models, typically referred to as molecular mechanics and molecular dynamics, provide a description with great details. They have been very useful in studying the microscopic mechanism of many types of material behavior.



As an example, we consider a one-dimensional model, in which the atoms are connected by springs. The potential energy is given by,

$$V = \frac{1}{2} \sum_i \sum_{0 < |j| \leq 2} \varphi(r_{i+j} - r_i). \quad (1)$$

Here, r_i is the current position of atom i ; the first sum is over all the atoms in the system, and the second summation collects the neighbors of the atom i . We restrict the interaction within the nearest two neighbors. The potential energy is of the Lennard-Jones type, i.e.

$$\varphi(r) = \frac{1}{r^{12}} - \frac{1}{r^6} \quad (2)$$

with the equilibrium atom spacing $a_0 = \sqrt[6]{2}$. The equilibrium position is denoted by $X_i = ia_0$, and r_i indicates the current position with the displacement,

$$u_i = r_i - X_i. \quad (3)$$

The equilibrium is defined as the state for which the total stress is zero. For this 1D problem, it will be an equally spaced configuration, but an equally spaced state might not be an equilibrium. To define the equilibrium more specifically,

let $r_j = ja$, then the energy becomes a function of a , then for the equilibrium state,

$$\frac{d}{da}V = 0.$$

For molecular mechanics, we seek a state of lowest energy,

$$\min_u V, \quad (4)$$

which implies that,

$$\varphi'(u_{i+1}-u_i+a_0)+\varphi'(u_{i+2}-u_i+2a_0)-\varphi'(u_i-u_{i-1}+a_0)-\varphi'(u_i-u_{i-2}+2a_0) = 0. \quad (5)$$

For molecular dynamics, we use the Newton's second law,

$$m\ddot{u}_j = \varphi'(u_{i+1}-u_i+a_0)+\varphi'(u_{i+2}-u_i+2a_0)-\varphi'(u_i-u_{i-1}+a_0)-\varphi'(u_i-u_{i-2}+2a_0). \quad (6)$$

2 The macroscale description.

Assuming that the discrete displacement field corresponds to a continuous one, which is smooth, one can view the molecular models as a discretization of some continuous PDEs. For molecular mechanics, this amounts to defining,

$$W(\epsilon) = \varphi(a_0(1 + \epsilon)) + \varphi(2a_0(1 + \epsilon)), \quad (7)$$

where $\epsilon = u'$ is the deformation gradient. The force balance implies that,

$$\frac{d}{dx}\sigma(u'(x)) = 0, \quad \sigma = W'(\epsilon),$$

subject to suitable boundary conditions.

For dynamics, the corresponding PDE is,

$$\rho_0 \frac{\partial^2}{\partial t^2} u = \frac{d}{dx} \sigma(u'(x)). \quad (8)$$

3 Research topics

The calculation shows that when the displacement of the atoms is smooth, the molecular model can be replaced by a set of macroscopic equations. This can be extremely useful in practice because the molecular models usually have many variables due to the microscopic nature, making the computation very expensive.

In this project, we will study several issues that arise in the upscaling procedure,

1. The accuracy of such approximation

2. Higher order approximations
3. The coupling between regions that can be upscaled and regions that can not
4. Stability of the microstructure.