Coupling molecular dynamics with finite elements. Projective methods issues at finite temperature

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CSMA 2011
10e Colloque National en Calcul des Structures
9-13 Mai 2011, Presqu'île de Giens (Var)

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Projective methods issues at finite temperature

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Résumé — In the context of coupling methods that match molecular dynamics with finite elements, we focus on the finite temperature and heat rates treatment done by Bridging Domain approaches. The energy dissipation occurring due to the projection of the fine scale onto the coarse scale is demonstrated during a sliding simulation of contacting surfaces. We describe the problems brought by the dissipation and propose a method that does not alter the temperature of the atoms in the coupling region. A coupling of the thermal fluxes with a continuum temperature field is also introduced and tested on simple examples.
Mots clés — finite elements, molecular dynamics, finite temperature, coupling.

1 Introduction

The main motivation for multiscale methods in the context of condensed matter simulations is to reduce MD simulation times. In many cases, such as realistic indentation simulation, a full atomistic model is out of reach ($0.1\mu m^3 \simeq 10^9$ atoms for crystalline copper). Thus a multiscale approach is mandatory as well as Parallel High Performance Computing efforts. A large body of work exists [1] to circumvent the difference in nature between molecular dynamics and continuum models, naturally inducing pathological wave reflections at the coupling interface. For instance, the *Bridging Domain* method consists in having an overlap region where the degrees of freedom have a mixed dynamic evolution. These methods have the merit to deal with wave reflections that occur because of the change of scales. In the overlap zone, the formulation of the *Bridging Domain* method damps (with an acceptable control) the kinetic energy not forwarded to the continuum. It has been proven [2] that some parameters, such as element sizes, allow to damp problematic waves in order to ameliorate the reflective behavior of coupling interfaces. Thus, the coupling region can be seen as a parameterizable filter.

Nevertheless, a critical issue of coupled multiscale methods for solid mechanics appears in finite temperature configurations. Because temperature plays an important role in material response, efforts have been made to extend to finite temperature the Quasi-continuum method [3], CGMD [4], and the Bridging scale [5]. But these techniques only provide a correct accounting of the local temperature with no fluctuations between the two models. To the best of our knowledge, only few methods allow a two-way coupling of thermal fluxes with thermal energy provided by MD [6, 7, 8].

In this presentation, we will focus on the Bridging domain method and more generally on the direct coupling that uses an overlapping with a projection of the fine solution onto the coarse finite element mesh. There are two problems concerning this approach. First it is hardly acceptable to loose energy when the molecular dynamics ensemble (NVE) should be conservative. Secondly, the damping has a dramatic effect on the temperature field. Indeed, the Bridging Domain strategies are very efficient in dissipating the waves that are not representable by the coarse mesh. However it always brings the atoms in the coupling area to a temperature very close to absolute zero which creates very steep temperature gradients. We will demonstrate this behavior on a sliding contact simulation [9] at low temperature. Because heat is generated at an important rate during the sliding motion of two contacting surfaces, the damping effect of the enforced Bridging Domain coupling is particularly evidenced. Thus thermal fluxes were not playing the important role we are emphasizing now.

2 A method with no projection

We will present a much simpler coupling strategy with no projection of the atomic part onto the smooth mesh field. The simple idea is to separate spatially the overlapping zone in two as plotted on figure 1. In Ω_1, the atoms are dictating the nodal fields in least square sense whereas in Ω_2 the atoms have displacement and velocities interpolated from the embedding finite elements. The idea is that no dissipation of the lattice vibrations should be imposed. Such a method shall not introduce any spurious temperature gradient or ghost forces.

We demonstrate the effectiveness of the approach by using the simple coupled situation. Boundary conditions are periodic on the lateral sizes whereas fixed Dirichlet conditions are imposed on the top and bottom boundaries. Atoms are positioned with taking into account the thermal expansion coefficients ensuring a thermodynamic equilibrium with no pressure acting on the walls. When no load is applied, it is clear that equilibrium should remain stable during a dynamic simulation. In order to test these points the *LibMultiScale* (`http://libmultiscale.gforge.inria.fr/`) parallel framework which is an investigation tool for 3D parallel concurrent coupling approaches was used. With a Bridging Domain method, a strong gradient is created in the entire domain while our approach allows to maintain the thermodynamic equilibrium. The absence of projection of fine to coarse scale leads to this improvement. The crucial conclusion is that damping strategies, as efficient as they can be in limiting wave reflections at low temperature, are inaccurate in the context of finite temperature simulations.

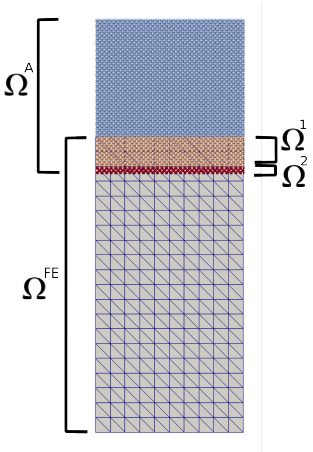

FIGURE 1 – Schematic of the overlap regions when no projection is introduced.

Still, wave reflections need a specific treatment so that the energy flux due to the highest frequency modes is not trapped in the atomistic region. Thus, in order to recover a proper energy balance, a coupling of the thermal energy flux with a continuum temperature field is introduced. As a pure phonon heat transport is assumed (dispersion heat equation) within the body, a set of thermostat can be used to drive the energy exchange between molecular dynamics and finite elements. An energy balance equation allows to derive the scaling parameters of such thermostats. Finally we will validate the methodology by the analysis of a coupled domain with heat flows and mechanical waves passing through the overlapping region.

Références

[1] W A Curtin and Ronald E. Miller. Atomistic/continuum coupling in computational materials science. *Modelling and simulation in materials science and engineering*, 11 :R33–R68, April 2003. Topical Review.

[2] G. Anciaux, O. Coulaud, J. Roman, and G. Zerah. Ghost force reduction and spectral analysis of the 1d bridging method. INRIA report, HAL http ://hal.inria.fr/inria-00300603/fr/.

[3] L. Dupuy, E. B. Tadmor, R. E. Miller, and R. Phillips. Finite-temperature quasicontinuum : Molecular dynamics without all the atoms. *Physical Review Letters*, 95, 2005.

[4] Jeremy Q. Broughton and Robert E. Rudd. Coarse-grained molecular dynamics : Nonlinear finite elements and finite temperature. *Physical review. B, Condensed matter and materials physics*, 72(14) :144104.1–1441040.32, 2005.

[5] Gregory J. Wagner and Wing Kam Liu. Coupling of atomistic and continuum simulations using a bridging scale decomposition. *Elsevier Science*, 190(1) :249–274, 2003.

[6] Gregory J. Wagner, R.E. Jones, J.A. Templeton, and M.L. Parks. An atomistic-to-continuum coupling method for heat transfer in solids. *Computer Methods in Applied Mechanics and Engineering*, 2008.

[7] Y. Kulkarni, J. Knap, and M. Ortiz. A variational approach to coarse graining of equilibrium and non-equilibrium atomistic description at finite temperature. *Journal of Mechanics and Physics of Solids*, 56(4) :1417–1449, 2008.

[8] N. Mathew, R.C. Picua, and M. Bloomfieldb. Concurrent coupling of atomistic and continuum models at finite temperature. *JMPS*, 2010.

[9] G. Anciaux and JF. Molinari. Contact mechanics at the nanoscale, a 3d multiscale approach. *International Journal for Numerical Methods in Engineering*, 79(9) :1041–1067, 2009.