**8th. World Congress on Computational Mechanics (WCCM8)**
**5th. European Congress on Computational Methods in Applied Sciences and Engineering (ECCOMAS 2008)**
**June 30 – July 5, 2008**
**Venice, Italy**

# AN ATOMISTIC-TO-CONTINUUM COUPLING METHOD FOR NON-EQUILIBRIUM HEAT TRANSFER IN SOLIDS

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**Key Words:** *Atomistic-to-Continuum Coupling, Heat Transfer, Multi-Scale Simulations.*

## ABSTRACT

As device sizes are driven to the nanoscale by technological advances, traditional continuum descriptions of heat transfer based on bulk material properties become less applicable. Surface effects, grain boundaries, defects, and other deviations from a perfect continuum can have a large effect on phonon propagation, and therefore heat transfer, at these scales. Simulation techniques based on descriptions at the atom scale, such as molecular dynamics (MD), have become an important part of the computational toolbox, but these methods are in general limited to length scales too small to allow the study of the micro-to-macroscale interactions that must be captured in the simulation of most typical real devices. A method to couple atomistic and continuum descriptions of heat transfer in a single simulation, similar to other efforts to couple mechanical deformation problems [1, 2], is desirable. These earlier coupling approaches have for the most part focused on coupling the static or dynamic forms of the momentum equation in the two regions, and where temperature effects are considered, an equilibrium thermal state is usually assumed [3].

In this work we present a seamless, energy-conserving method to couple thermally the atomistic and continuum representations of material for non-equilibrium, time-dependent heat transfer [4]. This method allows MD simulation to be used in localized regions of a computational domain, surrounded and overlaid by a continuum finite element representation. We begin by rigorously defining the relationship between the continuum temperature field, defined through nodal degrees of freedom $\theta_I$, and the atomic velocity:

$$\theta_I = \left\langle \sum_\alpha \hat{N}_{I\alpha} \frac{1}{3k_B} m_\alpha v_\alpha^2 \right\rangle \tag{1}$$

where $m_\alpha$ and $v_\alpha$ are the mass and velocity of atom $\alpha$, $k_B$ is Boltzmann's constant, and $\hat{N}_{I\alpha}$ is a normalized shape function associated with node $I$ and evaluated at atom $\alpha$. Angle brackets denote a time filtering operation. We use this temperature definition to write a heat equation for the combined system. By enforcing total energy conservation, we derive a coupling term that relates the continuum and atomistic systems through the

heat flux at the interface, giving a system of ODEs for atom positions and velocities and nodal temperatures that is straightforward to solve numerically.

One difficulty with distilling temperature information from a set of atom velocities is that fluctuations in space and time give a field that may be difficult to couple to a continuum. In our technique we use time filtering to obtain a smooth temperature field, and show how filtering can be embedded in the coupling scheme in a natural way. We also demonstrate how atoms in the MD region can be used for numerical quadrature in computing volume and surface integrals in the finite element formulation, allowing the solution of MD domains that do not necessarily align with element boundaries. This ability to handle very general MD domain shapes and finite element meshes is one of the key advantages of our method, and the techniques we use have applicability to more traditional atomistic-to-continuum coupling methods for material deformation.

Our method and its properties are demonstrated on a series of example problems, including conduction through a quasi-1D bar, spreading of an initial "hot spot" in a material, and measurement of thermal resistance across a grain boundary (Fig. 1). Current work includes topics such as thermal-elastic coupling for atomistic-to-continuum simulations, electron-phonon coupling for heat transfer simulation in metals and semi-conductors, adaptive methods, and large-scale parallel implementation in production codes.

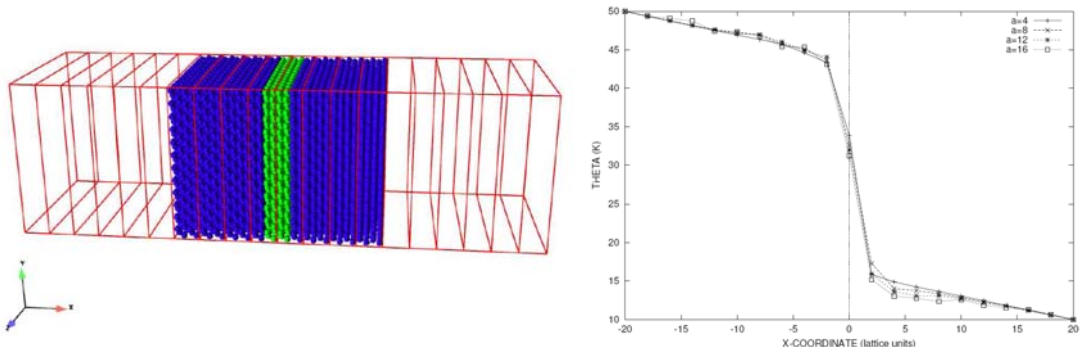


**Figure 1: Left: coupled MD-FEM geometry to simulate heat transfer across a grain boundary. Right: temperature plots showing temperature drop across grain boundary for different values of *a*, the size of the MD simulation region in lattice unit cells**


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