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A Fractional Step Method for Coupling Molecular Dynamics and Finite Element Models of Thermal Transport

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In this work, we develop and implement a combined time integration and constraint enforcement scheme to couple dynamic simulations of particle and continuum mediated thermal transport. Our previous work in atomistic-to-continuum (AtC) modeling [1] developed a framework for performing multiscale modeling with combined finite element (FE) and molecular dynamics (MD) systems in the MD code LAMMPS (http://lammps.sandia.gov). The basis for that work focused on lattice-based calculations using the kinetic definition of temperature to understand thermal transport in solids. Extending the AtC method to more general situations requires a overcoming several challenges. Most importantly, more general temperature definitions do not have time derivatives that can be directly evaluated, such as definitions based on the potential energy or with extra degrees of freedom for complex molecules. Eulerian frame calculations have similar issues, particularly if discontinuous shape functions are used. A numerical drawback is that slow drift can occur between the FE and MD temperature fields due to integration errors, which can lead to numerical instabilities in the coupling scheme.

To enhance the AtC method, we introduce a time integration algorithm based on the fractional step method. FE Time advancement is handled using standard methods (e.g., Gear) while the MD contributions to the temperature field are determined by only using changes in the MD state, eliminating potential drift between the two fields. In doing so, much more general temperature definitions are allowed because their time derivatives are no longer required. Similarly, changes in the shape function at an atom due to atomic motion can be evaluated based on their changes, and shape functions need not be updated every time step for improved efficiency. A result of this formulation is that the constraint-based equations that must be solved for the coupling thermostat include both first and second order terms in the time step. We introduce an iterative method to solve for the thermostat parameters and identify a criterion to evaluate if the time step is sufficiently small for the coupling method to be stable. The method is evaluated in several target applications AtC approaches: nanoscale heat transfer devices connecting hot and cold reservoirs and NEMD calculations of fluid thermal conducitivity.

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References

[1] G. J. Wagner, R. E. Jones, M. P. Parks, and J. A. Templeton. An atomistic-to-continuum coupling method for heat transfer in solids. *Computer Methods in Applied Mechanics and Engineering* 197, 2008.