

TEMPLE UNIVERSITY

Department of Mathematics

Applied Mathematics and Scientific Computing Seminar

Room 617 Wachman Hall

Wednesday April 25, 2007 at 4 p.m.

*Analytical and numerical study of coupled
atomistic-continuum methods for fluids*

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Several coupled atomistic-continuum methods have been proposed in recent years for the modeling of fluid systems which possess disparate length scales. These methods couple a continuum model with molecular dynamics (MD) through the exchange of boundary conditions in the continuum-particle overlapping region: The boundary condition for the continuum model is provided by the molecular model, and vice versa. Two fundamental issues have to be addressed in this domain-decomposition type of multiscale methods. The first is what kind of boundary condition we should impose on each model. Typical choices are velocity and fluxes. The second question is how to accurately impose a specified boundary condition on each model. In this talk, I discuss the stability and convergence issues of different coupling schemes. We also analyze the error introduced from the imposition of boundary conditions in MD.