TEMPLE UNIVERSITY
Department of Mathematics

Applied Mathematics and Scientific Computing Seminar

Room 617 Wachman Hall

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Energy-Stable Numerical Schemes for Multiscale Simulations of Polymer-Solvent Mixtures

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Abstract.

A second order energy dissipative numerical scheme is presented, which treats macroscopic equations aiming at the modeling of the dynamics of complex polymer-solvent mixtures. These partial differential equations are the Cahn-Hilliard equation for diffuse interface phase fields and the Oldroyd-B equations for the hydrodynamics of polymeric mixtures. A second order combined finite volume / finite difference method is applied for the spatial discretization. A complementary approach to study the same physical system is realized by simulations of a microscopic model based on a hybrid Lattice Boltzmann / Molecular Dynamics scheme. These latter simulations provide initial conditions for the numerical solution of the macroscopic equations. This procedure is intended as a first step towards the development of a multiscale method that aims at combining the two models.