Time-parallel continuum-kinetic-microscopic computation of non-equilibrated phenomena

Modeling and Algorithmic Approaches to Constitutively-Complex Microstructured Fluids

Sorin Mitran
University of North Carolina
CB3250, Chapel Hill, NC 27599-3250

Abstract

Multiple levels in the physical description of natural phenomena can be used to significantly accelerate the computation of systems with responses on a large range of space and time scales. This talk presents a combined continuum, kinetic, microscopic computational procedure with two embedded predictor-corrector steps: (1) The continuum level is used as a predictor of a few moments of the probability density function (PDF) describing the phase space statistics of the system; (2) The time evolution of the PDF is seen as a kinetic-level predictor of the microscopic evolution. Corrections from microscopic simulations are incorporated in an overall Bayesian framework that allows quantitative assessment of the validity of an assumed continuum closure.

Several novel mathematical concepts are introduced in the context of multiscale computation. The continuum predictor does not fully determine the microscopic PDF. The concept of an optimal Bregman divergence is introduced to measure differences in information content of PDFs at different time levels. Minimization of the optimal Bregman divergence subject to continuum constraints is shown to produce PDFs that closely conform to the microscopic dynamics. Optimal transport theory is another useful concept that is applied to the problem of approximation of the phase-space trajectory of the system.

Applications of the overall framework to the problem of polymeric flow are presented. In particular, it is shown how including statistical concepts in multiscale computation can be used to ascertain regions of validity of Oldroyd-B, FENE-P and Rolie-Poly viscoelastic flow models.