

A time-parallel continuum-kinetic-molecular interaction algorithm for nonequilibrium phenomena

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A parallel-in-time, multiscale interaction procedure is introduced for systems described at molecular scales by time-dependent random variables that obey Langevin dynamics. At larger, kinetic scales, the system is described by a probability distribution function that obeys an associated Fokker-Planck equation. At even larger scales a continuum formulation resulting from conservation laws is valid. It is assumed that the main quantity of interest is at the continuum scale, and that there is separation of space scales between the molecular, kinetic and continuum descriptions. Time scale separation is not assumed and the algorithm is suitable for nonequilibrium phenomena.

The kinetic-molecular interaction procedure is an iterative refinement predictor-corrector algorithm similar to the parareal method, but with different physical models used in each stage. In the predictor stage, a partial differential equation solver is used to obtain estimates of the probability distribution function on a subdivision of a time interval. At the starting time of each subinterval, the predicted probability distribution function is used to initialize an ensemble of random variables that are subsequently evolved forward in time by the Langevin dynamics. A probability distribution function estimate is constructed from the Langevin time evolution at the molecular scale and compared to that from the kinetic scale Fokker-Planck equation to determine whether further iterative refinement is needed. The molecular-scale computations are executed on highly parallel graphics processor units, while the kinetic-scale simulation is running on central processing units.

An important aspect of the kinetic-continuum interaction procedure is to establish procedures to update the kinetic probability distribution function to include data from the continuum scale. Minimal entropy modification and optimal transport theory is applied to provide a mapping of probability distribution functions between continuum time steps.

The overall performance of the algorithm is tested on bead-chain models from polymer flow.

Short Bio :

Dr. Mitran obtained his Aerospace Engineering Degree and PhD from the Politehnica University Bucharest. He has worked as a visiting researcher at the Department of Aeronautics and Astronautics at the University of Tokyo, the Institute of Reactor Safety, Karlsruhe Research Center, and the Department of Applied Mathematics, University of Washington. He has been on the faculty of the Department of Mathematics, University of North Carolina since 2002. Dr. Mitran's main research interest is the development of computational algorithms for simulation of multiscale, multiphysics phenomena.

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