Reduced-order hybrid multiscale method combining the Molecular Dynamics and the Discontinuous-Galerkin method

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ABSTRACT

We present a new reduced-order hybrid multiscale method to simulate complex fluids. The method combines the continuum and molecular descriptions. We follow the framework of the heterogeneous multi-scale method (HMM) that makes use of the scale separation into macro- and micro-levels. On the macro-level, the governing equations of the incompressible flow are the continuity and momentum equations. The equations are solved using a high-order accurate discontinuous Galerkin Finite Element Method (dG) and implemented in the BoSSS code. The missing information on the macro-level is represented by the unknown stress tensor evaluated by means of the molecular dynamics (MD) simulations on the micro-level. We shear the microscopic system by applying Lees-Edwards boundary conditions and either an isokinetic or Lowe-Andersen thermostat. The data obtained from the MD simulations underlie large stochastic errors that can be controlled by means of the least-square approximation. In order to reduce a large number of computationally expensive MD runs, we perform on-line/off-line coupling. Numerical experiments confirm the robustness of our newly developed hybrid MD-dG method.

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