Hybrid flow simulations in confined geometries using MD-data

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ABSTRACT

Hybrid flow simulations of complex fluids are performed. The incompressible form of the macroscopic governing equations, which are the momentum and continuity equations, are considered. The equations are discretized using the dG method with a high-order polynomial representation of the solution. To compute the viscous terms in the momentum equations, which are divergence of the stress tensor, the regularized data from Molecular Dynamics (MD) simulations are employed. Here, we adopt the approach of the Heterogeneous Multisacle Method (HMM), where we use the MD-data at each quadrature point to compute the required volume and face integrals on the discrete domain. In order to account for the Dirichlet (no-slip) boundary condition on the macroscopic level, we add a penalty term (containing the jump in the velocity) to the discrete form for divergence of the stress tensor. The governing equations are solved in the non-dimensional form. Therefore, proper rescaling must be performed when exchanging data between the MD and macroscopic simulations. The strain tensor is transformed to a 1D shear field, which is considered as the Lees-Edwards boundary condition for the MD simulations. The non-equilibrium MD simulations are performed using the Weeks-Chandler-Andersen (WCA) potential. Using the Irving-Kirkwood formula the stress tensor is found and transformed back to the macroscopic level. As test cases, 2D simulations for the Couette-Poiseuille flows are performed. Although the flow is incompressible on the macroscopic scale, the pressure difference along the stream-wise direction in the Poiseuille flow means having different densities at the MD simulations. Therefore, we regularized the data for the stress tensor versus the density as well as the shear rate. The regularization of the data is performed within an optimization procedure based on the Greedy sampling to reduce the number of the MD simulations required.

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