Hybrid atomistic?continuum method for the simulation of dense fluid flows

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We present a hybrid atomistic?continuum method for multiscale simulations of dense fluids. In this method, the atomistic part is described using a molecular dynamics description, while the continuum flow is described by a finite volume discretization of the incompressible Navier?Stokes equations. The two descriptions are combined in a domain decomposition formulation using the Schwarz alternating method. A novel method has been proposed in order to impose non-periodic velocity boundary conditions from the continuum to the atomistic domain, based on an effective boundary potential, consistent body forces, a particle insertion algorithm and specular walls. The extraction of velocity boundary conditions for the continuum from the atomistic domain is formulated by taking into account the associated statistical errors. The advantages and drawbacks of the proposed Schwarz decomposition method as compared to related flux-based schemes are discussed. The efficiency and applicability of the method is demonstrated by considering hybrid and full molecular dynamics simulations of the flow of a Lennard?Jones fluid past a carbon nanotube.

Author Name:
Thomas Werder
Jens H. Walther
Petros Koumoutsakos
Industries:
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