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A smooth dissipative particle dynamics method for domains with arbitrary-geometry solid boundaries

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ABSTRACT

A smooth dissipative particle dynamics method with dynamic virtual particle allocation (SDPD-DV) for modeling and simulation of mesoscopic fluids in wall-bounded domains is presented. The physical domain in SDPD-DV may contain external and internal solid boundaries of arbitrary geometries, periodic inlets and outlets, and the fluid region. The SDPD-DV method is realized with fluid particles, boundary particles, and dynamically allocated virtual particles. The internal or external solid boundaries of the domain can be of arbitrary geometry and are discretized with a surface grid. These boundaries are represented by boundary particles with assigned properties. The fluid domain is discretized with fluid particles of constant mass and variable volume. Conservative and dissipative force models due to virtual particles exerted on a fluid particle in the proximity of a solid boundary supplement the original SDPD formulation. The dynamic virtual particle allocation approach provides the density and the forces due to virtual particles. The integration of the SDPD equations is accomplished with a velocity-Verlet algorithm for the momentum and a Runge–Kutta for the entropy equation. The velocity integrator is supplemented by a bounce-forward algorithm in cases where the virtual particle force model is not able to prevent particle penetration. For the incompressible isothermal systems considered in this work, the pressure of a fluid particle is obtained by an artificial compressibility formulation for liquids and the ideal gas law for gases. The self-diffusion coefficient is obtained by an implementation of the generalized Einstein and the Green–Kubo relations. Field properties are obtained by sampling SDPD-DV outputs on a post-processing grid that allows harnessing the particle information on desired spatiotemporal scales. The SDPD-DV method is verified and validated with simulations in bounded and periodic domains that cover the hydrodynamic and mesoscopic regimes for isothermal systems. Verification of the SDPD-DV is achieved with simulations of transient, Poiseuille and Couette isothermal flow of liquid water between plates with heights of 10^{-5} m and 10^{-3} m. The velocity profiles from the SDPD-DV simulations are in very good agreement with analytical estimates and the field density fluctuation near solid boundaries is shown to be below 5%. Verification of SDPD-DV applied to domains with internal curved solid boundaries is accomplished with the simulation of a body-force driven, low-Reynolds number flow of water over a cylinder of radius $R = 0.02$ m. The SDPD-DV field velocity and pressure compare favorably with those obtained by FLUENT. The results from these benchmark tests show that SDPD-DV is effective in reducing the density fluctuations near solid walls, enforces the no-slip condition, and prevents particle penetration. Scale-effects in SDPD-DV are examined with an extensive set of SDPD-DV isothermal simulations of liquid water and gaseous nitrogen in mesoscopic periodic domains. For the simulations of liquid water the mass of the fluid particles is varied between 1.24 and 3.3×10^7 real molecular masses and their corresponding size is between 1.08 and 323 physical length

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scales. For SDPD-DV simulations of gaseous nitrogen the mass of the fluid particles is varied between 6.37×10^3 and 6.37×10^6 real molecular masses and their corresponding size is between 2.2×10^2 and 2.2×10^3 physical length scales. The equilibrium states are obtained and show that the particle speeds scale inversely with particle mass (or size) and that the translational temperature is scale-free. The self-diffusion coefficient for liquid water is obtained through the mean-square displacement and the velocity auto-correlation methods for the range of fluid particle masses (or sizes) considered. Various analytical expressions for the self-diffusivity of the SDPD fluid are developed in analogy to the real fluid. The numerical results are in very good agreement with the SDPD-fluid analytical expressions. The numerical self-diffusivity is shown to be scale dependent. For fluid particles approaching asymptotically the mass of the real particle the self-diffusivity is shown to approach the experimental value. The Schmidt numbers obtained from the SDPD-DV simulations are within the range expected for liquid water.

1. Introduction

Fluids at the mesoscopic regime have spatiotemporal scales larger than atomic and smaller than hydrodynamic, and exhibit hydrodynamic fluctuations in their mean properties. These mesoscopic scales are found in many natural, biological, and engineering systems. Theoretical modeling and numerical methods appropriate for the fluctuating hydrodynamic regime have been pursued in part due to the emerging role of microscale and nanoscale applications. The Smoothed Dissipative Particle Dynamics (SDPD) [1] and the Dissipative Particle Dynamics (DPD) [2] are modeling and simulation methods developed for mesoscopic fluids. In DPD the simulation particles represent clusters of molecules interacting by means of repulsive, dissipative and random forces. This clustering permits use of larger integration time steps and allows simulation of spatial scales much larger than those covered by molecular dynamics [3–5]. There have been many additions and improvements to DPD since its introduction and the method has been applied to a variety of mesoscale systems, including binary immiscible fluids [6], colloidal behavior [7], DNA in microchannels [8,9], two phase flows [10], flow over rotating cylinder [11], nanojet breakup [12], polymers [13–15], and water in microchannels [16]. The SDPD was developed by Espanol and Revenga [1] as a top-bottom approach and thermodynamically consistent alternative to DPD. The SDPD invokes the Smoothed Particle Hydrodynamics (SPH) [17] which is applied to the discretization of the Navier–Stokes equations. By using the GENERIC framework developed by Ottinger to describe fluctuating hydrodynamic [18], Espanol and Revenga arrived to the SDPD discrete equations that include thermal fluctuations. In SDPD the independent variables are position, velocity and entropy of each fluid particle, a deviation of most mesoscopic and hydrodynamic models that involve the energy of the particle.

Several SDPD investigations have appeared since its inception. Serrano [19] compared the SDPD and the Voronoi fluid particle model in a shear stationary flow. He found the efficiency of the two methods comparable. The accuracy of the Voronoi approach was found superior for regular ordinate systems while SDPD produced more accurate results for arbitrary, disordered configurations. Litvinov et al. [20] applied SDPD to model the behavior of polymer molecules in suspensions. Their results confirmed that SDPD can be successfully used to describe such mesoscopic phenomena. Vázquez-Quesada et al. [21] investigated the scaling laws in isothermal SDPD due to fluid particle size which is related to its volume. They found that the deterministic part of SDPD is scale-free while stochastic fluctuations increase as the size of the SDPD particle decreases. Litvinov et al. [22] derived an analytical expression for the diffusion coefficient in a solvent in terms of SDPD model parameters. Their SDPD simulations with varied values of viscosity showed that the Schmidt number (Sc, defined as the ratio of kinematic viscosity over the self-diffusion coefficient) can be up to 10^6, consistent with those of real liquids. In subsequent work Litvinov et al. [23] presented a splitting integration scheme for SDPD to overcome the time-step limitations associated with highly dissipative phenomena. Bian et al. [24] applied SDPD to modeling of particles in a suspension for a range of conditions. They verified their SDPD results with analytical theories and also examined diffusion properties of a single spherical particle in a microchannel.

Among the outstanding theoretical and computational issues in SDPD is its implementation in domains with solid boundaries of arbitrary geometry. In mesh-free methods, such as DPD, SDPD, SPH, the wall and its effects on the fluid density and force of a near-wall particle, are modeled using various types or layers of particles. One of the issues is in assigning the physical properties of such ghost (or wall) particles and in defining the interaction forces with the fluid particles in the proximity of the wall. Such forces must ensure that a fluid particle does not penetrate the wall and that the no-slip condition is enforced. In SPH ghost particles can be loaded at the start of the simulation with static properties [25,17], or can be dynamically generated with properties updated during the simulation [26,27]. In general, the fluid particle force is composed of a repulsive and a dissipative term. The soft repulsive force acting on a fluid particle near a wall from the neighboring fluid particles may not be sufficiently strong to prevent wall penetration. To overcome this problem a stronger repulsive force between the fluid and the wall particles, in the Lennard–Jones form, has been used in SPH [28,17]. Different solutions have been proposed in DPD for imposing wall conditions, such as increasing the repulsive force coefficient for wall/fluid interaction [29], increasing the wall particle density [30] or imposing bounce-back and bounce-forward boundary conditions [31,29,32,33,30]. For SDPD, Litvinov et al. [20] extended the virtual particle SPH approach [26] and filled a solid