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Wall Boundary Conditions in 3D Smooth Dissipative Particle Dynamics Simulations[1] JUN YANG, RAFFAELE POTAMI, NIKOLAOS GATSONIS — The mesh-free thermodynamically consistent smooth dissipative particle dynamics (SDPD) method is implemented in 3D using a block structure to minimize computational time and the Verlet neighbor-list algorithm for efficient search of particles. A new method for solid wall boundary conditions is presented that enforces non-penetration and minimizes the density fluctuations. The geometry of the wall is described using wall pseudo-particles. This geometry is used to generate a set of ghost fluid particles obtained by mirroring the neighbor particles of a given fluid particle in the proximity of a boundary. The ghost particles are used for minimizing the density fluctuations near walls, for generating the repulsive force that ensures the impenetrability condition, and for generating a dissipative force that ensure the no slip condition. Numerical results for isothermal flows show only minimal density fluctuations in the proximity of the solid wall and an overall good agreement between the velocity profiles from numerical simulations and analytical results.

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Jun Yang

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