A Numerical Study of Force-Based Boundary Conditions in Multiparticle Collision Dynamics

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Abstract : We propose a new alternative method for imposing fluid-solid boundary conditions in simulations of Multiparticle Collision Dynamics. Our method is based on the introduction of an explicit potential force acting between the fluid particles and a surface representing a solid boundary. We show that our method can be used in simulations of plane Poiseuille flows. Important quantities characterizing the flow and the fluid-solid interaction like the slip coefficient at the solid boundary and the effective viscosity of the fluid, are measured in terms of the set of independent parameters defining the numerical implementation. We find that our method can be used to simulate the correct hydrodynamic flow within a wide range of values of these parameters.

Keywords : Multiparticle Collision Dynamics, fluid-solid, boundary conditions, molecular dynamics

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