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A parallel fluid solid coupling model using *LAMMPS* and *Palabos* based on the immersed boundary method

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Abstract

The study of viscous fluid flow coupled with rigid or deformable solids has many applications in biological and engineering problems, e.g., blood cell transport, drug delivery, and particulate flow. We developed a partitioned approach to solve this coupled Multiphysics problem. The fluid motion was solved by *Palabos* (Parallel Lattice Boltzmann Solver), while the solid displacement and deformation was simulated by *LAMMPS* (Large-scale Atomic/Molecular Massively Parallel Simulator). The coupling was achieved through the immersed boundary method (IBM). The code modeled both rigid and deformable solids exposed to flow. The code was validated with the Jeffery orbits of an ellipsoid particle in shear flow, red blood cell stretching test, and effective blood viscosity flowing in tubes. It demonstrated essentially linear scaling from 512 to 8192 cores for both strong and weak scaling cases. The computing time for the coupling increased with the solid fraction. An example of the fluid-solid coupling was given for flexible filaments (drug carriers) transport in a flowing blood cell suspensions, highlighting the advantages and capabilities of the developed code.

Keywords: Lattice Boltzmann Method, Palabos, LAMMPS, Immersed Boundary Method, Parallel Computing

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