Abstract Submitted
for the DFD17 Meeting of
The American Physical Society

**Coupling molecular dynamics with lattice Boltzmann method based on the immersed boundary method.**[1] JIFU TAN, TALID SINNO, SCOTT DIAMOND, University of Pennsylvania — 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 classic problem of rigid ellipsoid particle orbit in shear flow, blood cell stretching test and effective blood viscosity, and demonstrated essentially linear scaling over 16 cores. 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.

[1]NIH 1U01HL131053-01A1

Jifu Tan
University of Pennsylvania

Date submitted: 01 Aug 2017 Electronic form version 1.4