Hybrid MD-continuum simulation methodology for biomolecular systems: LAMMPS-ANSYS/Fluent coupling implementation and transition to CPU/GPU high performance computing

K. Fattah-Hesary[1], N. Kim[2], S-H. Ko[2], B. Novak[1], S. Jha[2], D. Moldovan[1], and D. Nikitopoulos[1]
[1]Mechanical Engineering Department, LSU
[2]Center for Computational & Technology, LSU

Abstract

A coupled CFD-MD scheme for simulating multi-scale (micro- and nano-) fluidic systems has been further developed. The coupling process involves three domains i.e. CFD, MD and an overlap hybrid region. A commercial continuum code, ANSYS/FLUENT is employed for the continuum part of the simulation, and LAMMPS is adopted for the MD part. Coupling schemes and data interfaces are implemented in ANSYS/FLUENT using its User Defined Function (UDF) capability. In the overlap region a file-based information exchange method is applied between atomistic and continuum fluidic information to define boundary conditions for the continuum region and the appropriate constraint for the atomistic one. This has set the stage for exchange of required information between the two pure regions. Simulation of sudden-start Couette flow shows quantitative agreement with results from analytical solutions. This work will leverage force-field development efforts also under the LaSiGMA grant to enable multi-scale simulations involving interactions between biomaterials for which such force-field are unknown.