A Coupling Strategy between CFD and MD Codes for Hybrid Simulations

Nayong Kim[1], Soon-Heum Ko[1], Kasra F. Hesary[2,3], Dimitris E. Nikitopoulos[2,3], Shantenu Jha[1], Dorel Moldovan[2,3],

[1] Center for Computation and Technology, Louisiana State University, 216 Johnston Hall, Baton Rouge, LA 70803
[2] Department of Mechanical Engineering, Louisiana State University
[3] Center for Bio-Modular Multi-Scale Systems, Louisiana State University

Abstract. A coupled CFD-MD scheme for simulating multi-scale (micro- and nano-) fluidic systems has been developed. This research is motivated by the need to accurately represent molecular-level effects on material surfaces and interfaces in flow and transport domains within which continuum formulations of the conservation equations are valid. As the coupling process involves three domains i.e. CFD, MD and an overlap hybrid region, accurate CFD and MD codes should be developed in advance of designing and developing a coupling algorithm between two domains. Currently, an incompressible in-house code based on artificial compressibility approach is employed for the continuum CFD simulation, and a famous LAMMPS package is adopted for the MD part. Also, coupling schemes and data interfaces are implemented on these two codes to conduct a hybrid CFD-MD simulation.

The coupling algorithm is embedded in Figure 1, which also illustrates the communications between the constituents of the hybrid code. MD simulation is conducted near the solid material boundary where the interaction between the solid material and the fluid is on the molecular level. The macroscopic features are governed by the continuum equations solved through the CFD solver. A hybrid region is positioned between these regions to let the two domains exchange information. This hybrid region minimally consists of five subzones. The CFD boundary grid region is positioned near the pure MD region. Velocities of particles within this zone are averaged and imposed as CFD boundary conditions for the corresponding computational cells. The MD boundary zone is placed above the CFD boundary zone. Here, velocities from the CFD grid are imposed on the MD through dynamically constrained MD equations. The dynamic constraint is introduced as a source term to the particle equation of motion which is appropriate to ensure that a macroscopic velocity from CFD and an averaged particle velocity from MD will eventually be the same. Between these zones, a buffer layer exists to transition the differences between the MD boundary and CFD boundary zones without direct influence of one on the other. On the top of the domain, an artificial force is applied to prevent particles from escaping from the hybrid region. A buffer layer is also placed between the constrained MD and the "retaining" force regions.

Keywords: CFD, MD, Hybrid, Coupling Scheme, Constrained Dynamics, Artificial Compressibility, LAMMPS

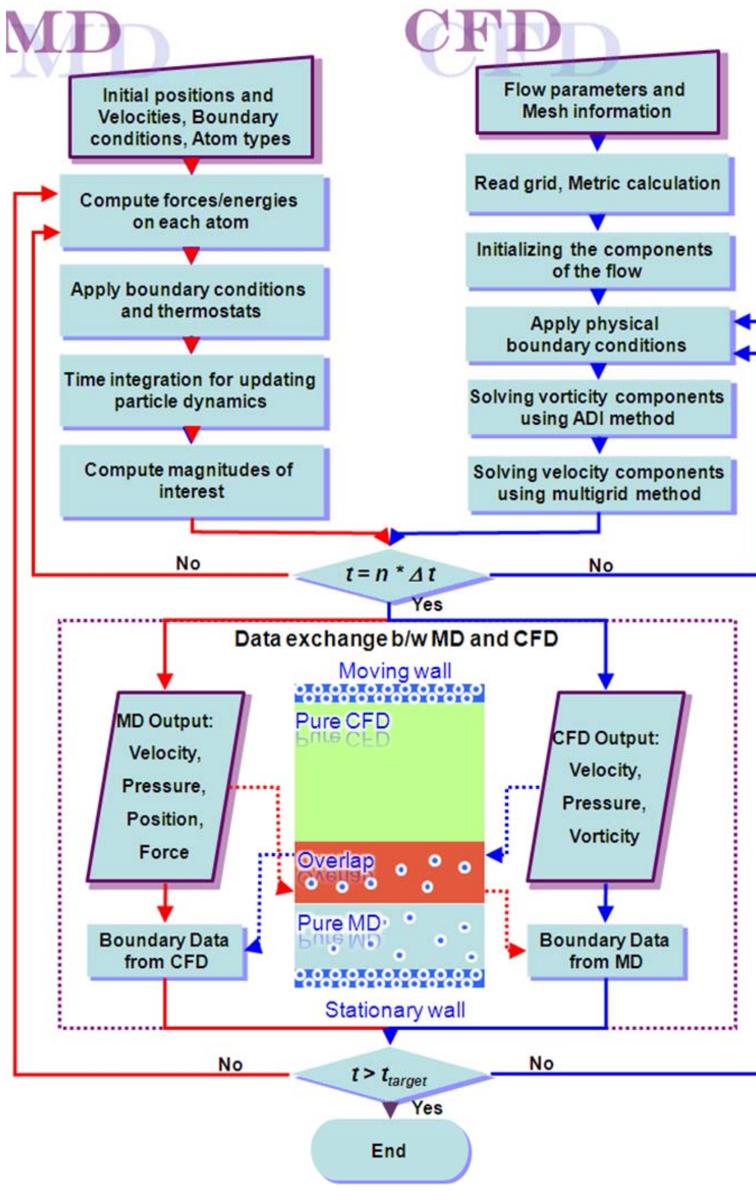

Fig. 1. Designed Schematic of a Cactus CFD Toolkit and Diffusion Simulation on a Multi-block Domain