Hybrid MD-continuum simulation methodology for multiphase biomolecular systems

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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. The coupling is applied to a one-phase plane Couette flow where the fluid-solid interface is modeled at molecular level and by choosing suitable fluid-solid interaction parameters, the results are validated by comparing with analytical solution. Then, we study the physics of fluid-fluid planar interfaces under shear by modeling an atomistic binary liquid Couette flow to set the stage for applying the hybrid scheme to multiphase-multiscale systems. Discrepancies between available semi-analytic solution and atomistic results in two-phase simulation are explained by interfacial viscosity. 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.

MD Code

Adapted LAMMPS for the MD/CFD Toolkit

- Atomistic approach which can deal with flow phenomena in nano domains.
- Equations of motion solved for all atoms with intermolecular potentials.
- LAMMPS ("Large-scale Atomic/Molecular Massively Parallel Simulator")
  - Efficient and fast parallel MD computing
  - Broad spectrum of available force-fields to satisfy geno/single-molecule sensor needs
  - Open source and widely used
- First tests using Lennard-Jones intermolecular potential model

Continuum Navier-Stokes Code

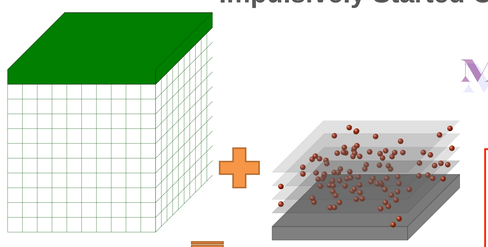
Adapted ANSYS/FLUENT for the MD/CFD Toolkit Overview

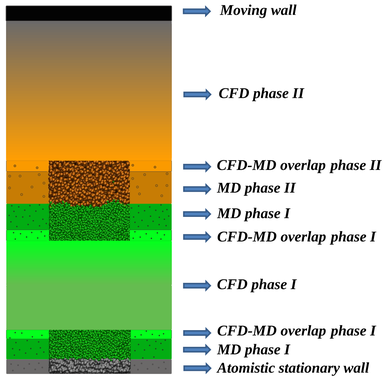
- ANSYS/FLUENT
  - Advanced solver technology provides fast, accurate CFD results
  - Thousands of companies throughout the world benefit from the use of ANSYS FLUENT software as an integral part of their design
  - User-defined functions allow the implementation of new user models and the extensive customization of existing ones
  - Delivers powerful and scalable high-performance computing (HPC) options
- Incompressible Navier-Stokes equations
  - Momentum $\rho\left(\frac{\partial \vec{v}}{\partial t} + \vec{v}\cdot\nabla\vec{v}\right) = -\nabla p + \rho\vec{g} + \mu\nabla^2\vec{v}$
  - Continuity $\nabla\cdot(\rho\vec{v}) = 0$
- Solution Procedure
  - Using Fractional Step Method (good for transient incompressible flows)
  - Developing a User Defined Function for updating boundary conditions received from MD during the simulation

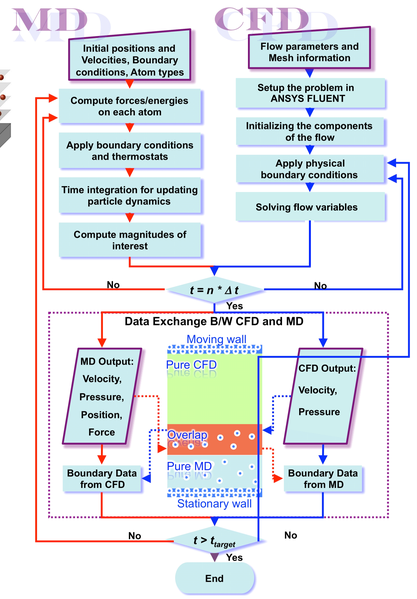
LSU

Hybrid Continuum(CFD)/MD Test Problem

Impulsively Started Couette Flow

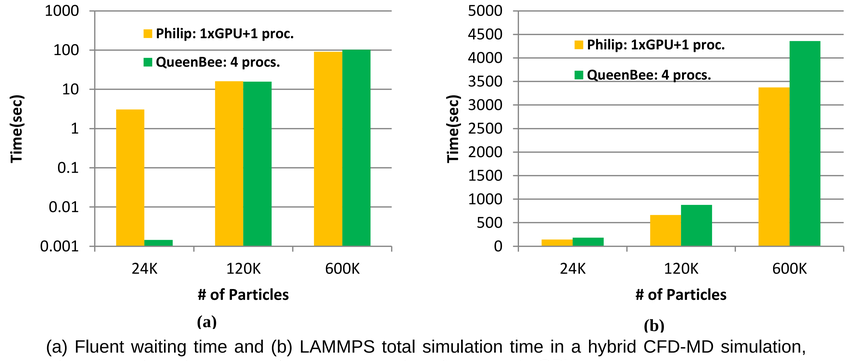






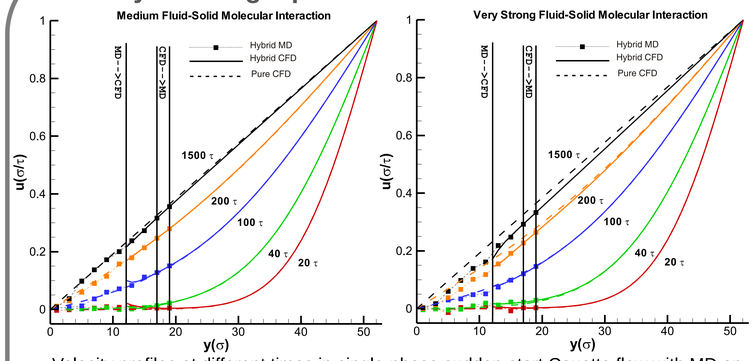
	Single-phase Hybrid Simulation	Two-phase MD Simulation	
		Phase *I*	Phase *II*
ϵ	1.0	1.0 ϵ_I	1.0 ϵ_{II}(=1.0 ϵ_I)
σ	1.0	1.0 σ_I	1.0 σ_{II}(=1.986 σ_I)
ρ	0.81 σ^3	0.7 σ_I^{-3}	0.85 σ_{II}^{-3}
T	1.1 ϵ/k_B	1.1 ϵ_I/k_B	1.1 ϵ_{II}/k_B

Performance of GPU vs. CPU



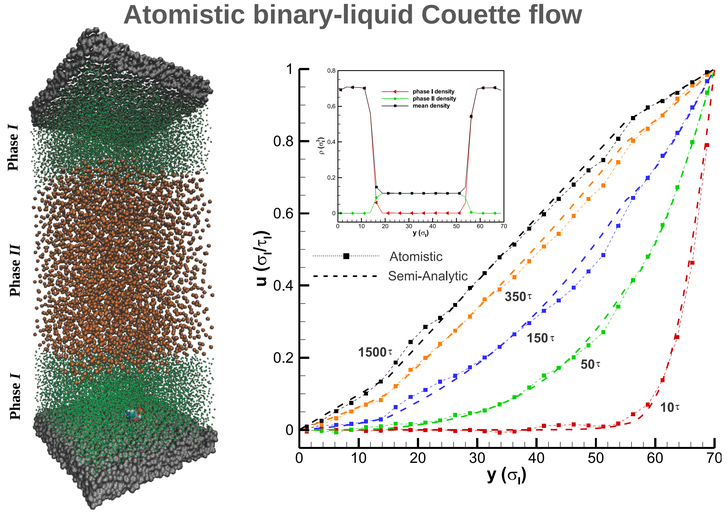
(a) Fluent waiting time and (b) LAMMPS total simulation time in a hybrid CFD-MD simulation, with different system sizes (number of particles), using 1 GPU in double precision and 1 processor for LAMMPS and 1 processor for FLUENT on Philip cluster compared with that of one CPU (4 processors) for LAMMPS and 1 processor for FLUENT on QueenBee.

Hybrid single phase Couette flow simulation



Velocity profiles at different times in single-phase sudden-start Couette flow with MD on stationary wall. $\epsilon_{wf} = 0.6$ (left) and $\epsilon_{wf} = 10.0$ (right).

Atomistic binary-liquid Couette flow



Snapshot from the MD simulation(left), time evolution of velocity profiles and steady state density profile(right) of binary liquid Couette flow. Deviations near the interfaces on velocity profiles are explained by changes (decrease) in local viscosity near the interfaces.

Conclusion & Future Plans

Hybrid CFD-MD Approach & Atomistic Multiphase Flow — Accomplished

- **LAMMPS Modification and ANSYS FLUENT Adaptation**
- **Better solution near the interfaces with acceptable efficiency**
- **Partial slip can appear at liquid-liquid interface**

Extension to hybrid/coarse-grained multiphase CFD-MD — Next

- **Simulation of multiphase flow with a mono-nucleotide**
- **Transition from atomistic to a coupled atomistic-continuum**
- **Applying coarse-grained method for complex fluids like bio-molecular assemblies**

Acknowledgements

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