Hybrid Atomistic-Continuum Approach for Handling Multi-scale Physics

Marika Buchholz[1], Kasra Fattah-Hesary[2], Dimitris Nikitopoulos[2]
[1]Louisiana School for Math, Science, and the Arts
[2]Department of Mechanical Engineering at Louisiana State University, Baton Rouge, LA 70803

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Abstract

To create a simulation of Couette flow with a hybrid atomistic-continuum approach using Python and to visualize the results using Visual Molecular Dynamics (VMD). One typical scenario in fluid dynamics is Couette flow. Couette flow was chosen for this project because of the relative ease with which it can be modeled. The continuum portion of the fluid flow was modeled using OpenFOAM, and the atomistic portion was modeled using LAMMPS.. Potential applications are numerous; for example, Couette flow simulations can be used to identify DNA bases on nucleotides. The DNA is sent into nano-channels, and based on the flight time of the nucleotide from the beginning of channel to the end, the type of base (A, C, T, or G) can be identified. The flight of the nucleotide is modeled most accurately using hybrid molecular-continuum descriptions due to the size of the channel. These simulations can also be helpful in enhanced oil recovery (EOR). Nanoparticles functionalized by chemical agents can be used to help recover hydrocarbons in the pores of rocks in the earth. Modeling the transport of these nanoparticles requires a multi-scale approach.

Using a Hybrid Approach

- Some processes cannot be represented using only continuum descriptions, since they omit important phenomena.
  - Navier-Stokes equations
  - No-slip condition breaks down at a small scale
- Purely atomistic representations are not practical since they require more particles than are computationally manageable.
- A hybrid approach uses continuum dynamics for the most of the flow and molecular dynamics only near the interface(s).
  - Continuum:
    - OpenFOAM
      - Open-source Field Operation and Manipulation
      - Free computational fluid dynamics (CFD) software package
  - Molecular:
    - LAMMPS
      - Large-scale Atomic/Molecular Massive Parallel Simulator
      - Open-source molecular dynamics program

Couette Flow Model

- Flow of fluid between two parallel, unbounded plates, one of which is moving at constant velocity U
- Fictitious force keeps molecules within the atomistic portion in place
- Buffers “reduce confusion” between molecular and continuum portions during the simulation

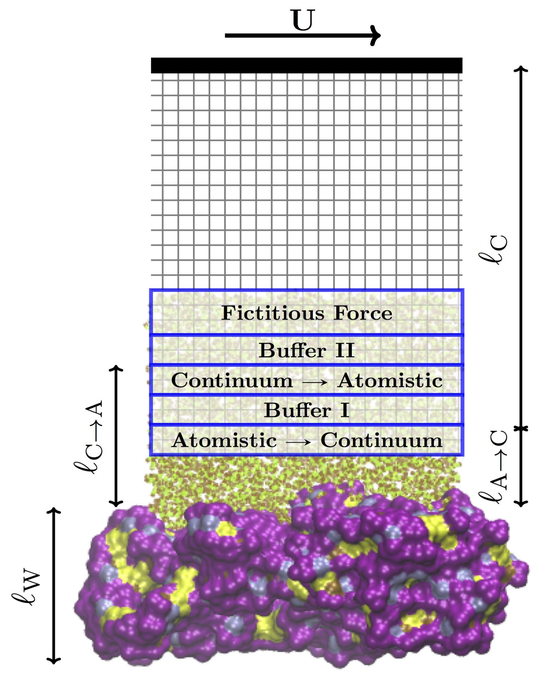


Figure 1

Visualization

- Visual Molecular Dynamics (VMD)
  - molecular modeling and visualization computer program
- Tool Command Language (Tcl)
  - used to write scripts that streamline the visualization process
- Data for the visualizations were obtained from LAMMPS.

Figure 1: a realistic model of Couette flow using water and poly (methyl methacrylate) (PMMA).

Figure 2: a VMD rendering of the flow of water, PMMA, and a nanoparticle.

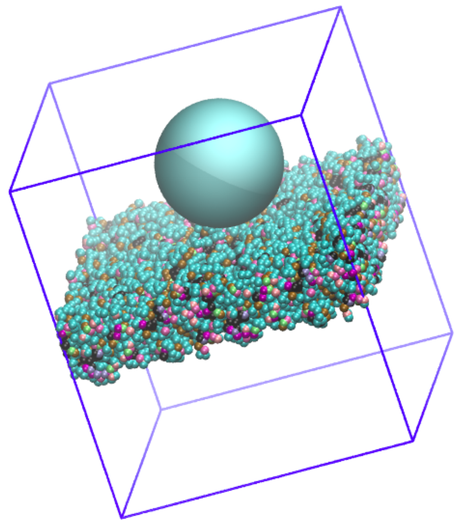
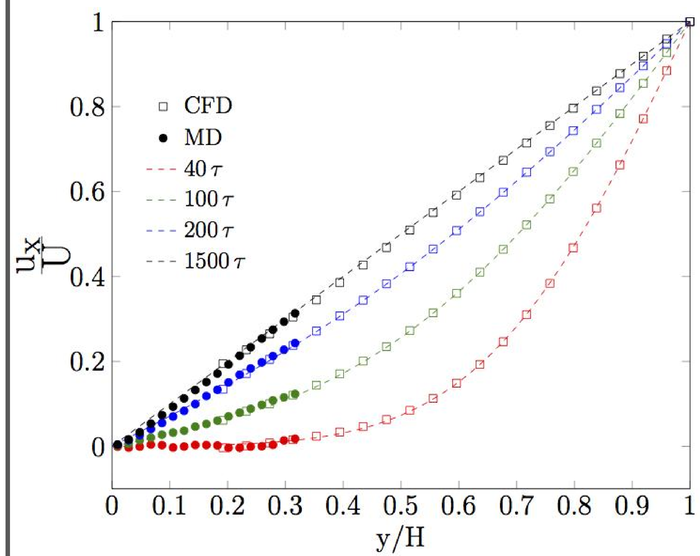


Figure 2

Results of Unrealistic System



- Output of Python script modeling Couette flow using a hybrid approach
- Shows velocity of fluid with respect to distance from bottom plate
  - This ideal system ignores intermolecular forces.
- Throughout time, the change in velocity of the particles reaches a constant.

Improving Usability

- Python script was modified so that user can input different values for the height between two plates and velocity.
- Modifications to the original code included addition of dictionaries, tests for correct input, and directions for input in the event of a user-related error.

Discussion/Future Work

- The velocity profiles show that molecular dynamics (MD) gives more accurate data, but since the computational power required to run an entire simulation using MD is so great, a hybrid continuum-atomistic approach is an adequate compromise for this situation.
- Using MD near the interfaces makes for more accurate results, because the movement of the molecules closest to the plates is most drastic and important to measure.
- Future work may include making the script even more user-friendly, rendering more visualizations of Couette flow using different materials and fluids, and creating simulations for other types of flow such as Poiseuille flow and lid-driven cavity flow.

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