Hybrid Atomistic-Continuum Approach for Handling Multi-scale Physics

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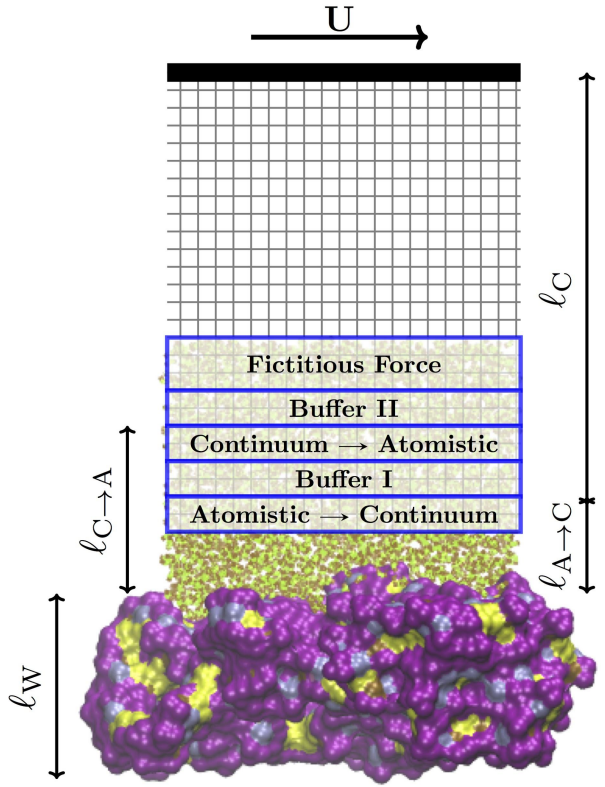
Couette Flow Model

- 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

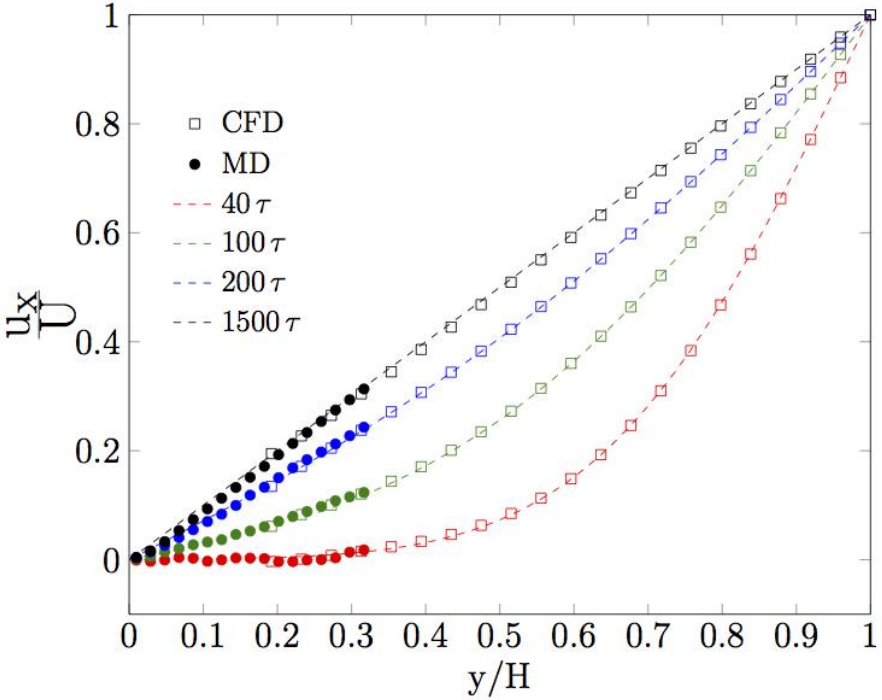


Using a Hybrid Approach

- 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).

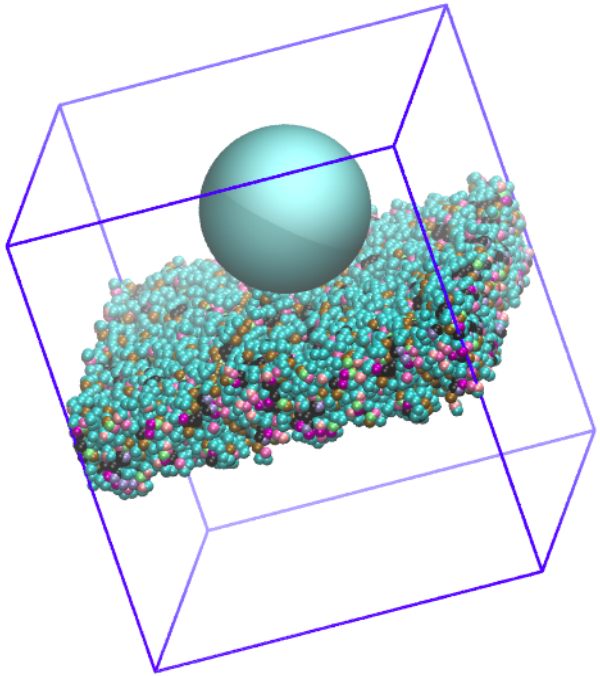
Results of Unrealistic System

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



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.

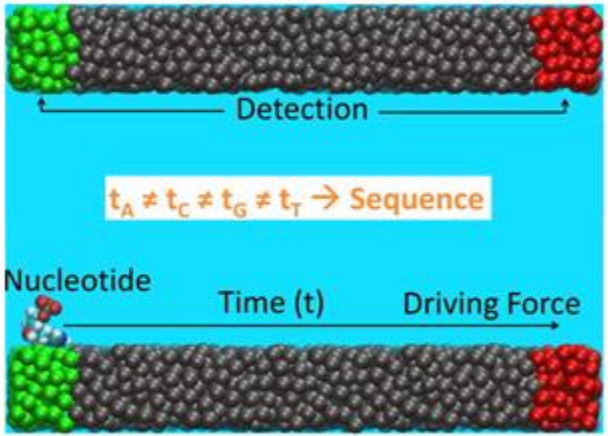


Improving Usability

- 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/Applications

- Applications:
  - Identification of DNA bases on nucleotides
  - Enhanced oil recovery (EOR)
- 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:
  - Rendering more visualizations of Couette flow using different materials and fluids
  - Creating simulations for other types of flow such as Poiseuille flow and lid-driven cavity flow



Source: http://www.chem.unc.edu/people/faculty/soper/index.html?display=research_display&show=all

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