Parametric Study of a Multiscale Fluidic System Using A Hybrid CFD-MD Approach

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Outline

- Introduction and Motivation
- Hybrid CFD-MD Framework:
  Application Codes and Runtime Environment
- Numerical Simulations
  - Couette Flow
  - Stokes (Oscillating) Boundary Condition
- Current Issues
  - Low-speed Flow Simulation
  - Realistic Fluid Domain
- Conclusion and Future Works

Introduction and Motivation

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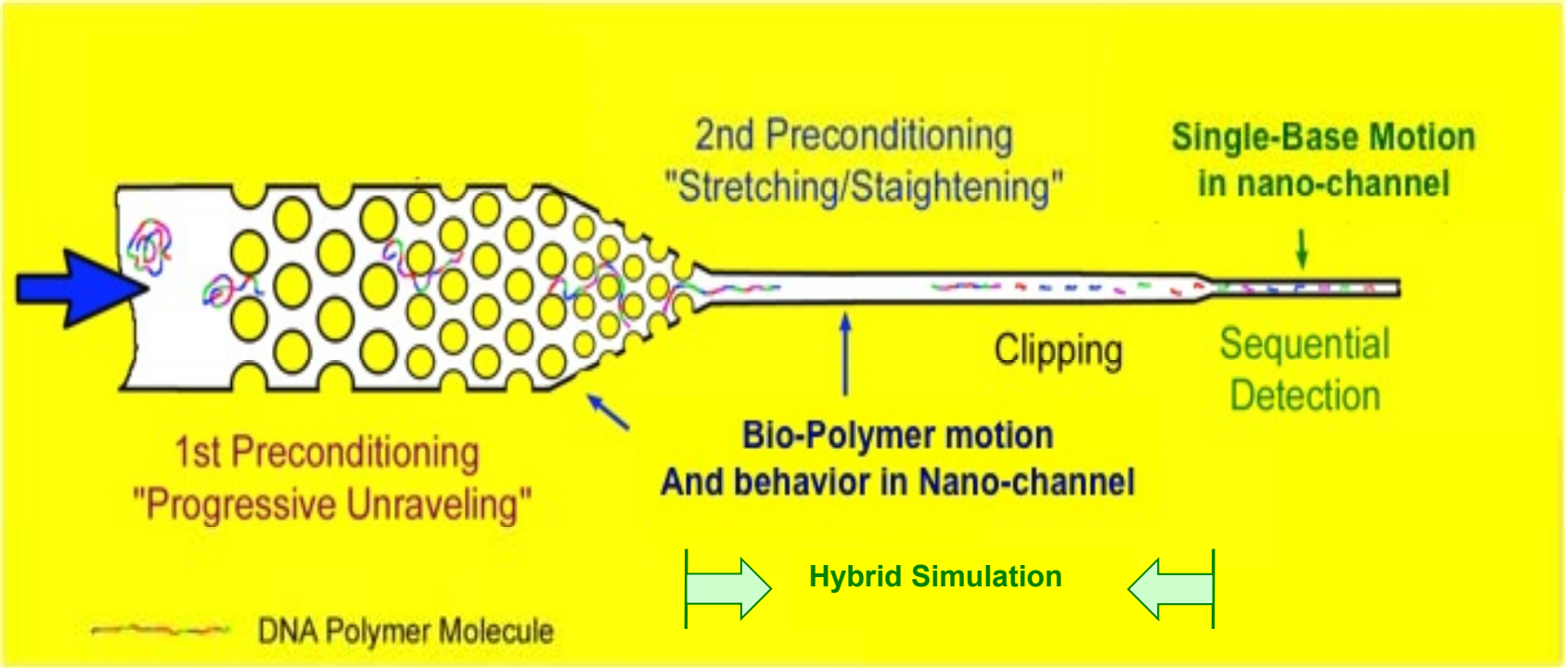
Background

- Bio-Polymer Multiscale Sensor



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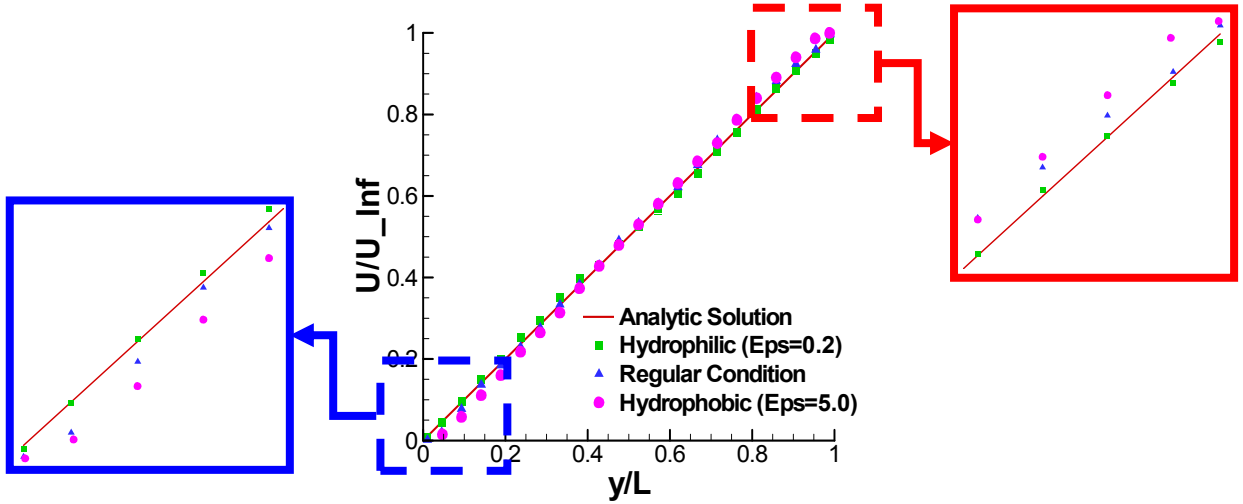
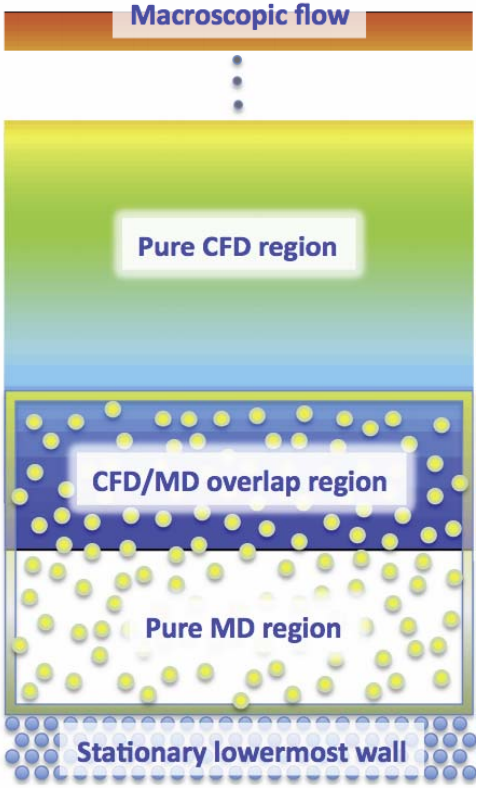
Hybrid CFD-MD Approach

- CFD solves macroscopic flow characteristics while MD considers intermolecular interaction in low-speed flow region
  - CFD : Increasing accuracy
    - Inter-molecular effect near the wall





  - MD : Reducing simulation time
    - Smaller MD domain for describing the global flow feature

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Former works

- References (among multiples)
  - S.T. O'Connell and P.A. Thompson (1995)
    - A constrained particle dynamics with an empirical coupling parameter
  - N.G. Hadjiconstantinou and A.T. Patera (1997)
    - Coupling by Schwartz alternating method
  - Flekkoy et al. (2000) and G. Wagner et al. (2004)
    - Direct flux exchange in the hybrid interface
  - X. Nie et al. (2004)
    - External force to trap the particles
  - R. Delgado-Buscalioni and P.V. Coveney (2004)
    - Coupling strategy in time and unsteady simulation
  - T.H. Yen et al. (2007)
    - Hybrid simulation on large scale domains
  - R. Steijl and G.N. Barakos (2009)
    - Parallel computational framework and parametric study of coupling conditions

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Research Goals

- Development of a hybrid CFD-MD framework
  - Development of application codes with hybrid interfaces
  - Runtime environment for efficient computing
- Coupling conditions
  - Position and thickness of hybrid layer, MD system size, time scale, sampling time interval and duration
- Unsteady flow simulation
  - Time-accurate problems
    - Coupling scheme in time
- Flow simulation in moderate condition
  - Fluid materials, velocity, system scale
    - More time to converge on bigger systems
    - Inherent Brownian motion and resultant noise becomes dominant on low-speed flow
    - Modeling for polyatomic molecules: considering Coulomb force, improving constrained MD equation of motion

Hybrid CFD-MD Framework

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Baseline Code

- CFD
  - In-house code (3-D incompressible N-S, pseudo-compressibility)
    - Osher's flux scheme
    - LU-SGS (Lower-Upper Symmetric Gauss-Seidel)
    - Incorporated with application-level checkpointing and general domain partitioning for use in runtime environment
- MD
  - LAMMPS (Large-scale Atomic/Molecular Massively Parallel Simulator) by Sandia Lab
    - Truncated Lennard-Jones potential was used for calculating the interactions between atoms

$$V^{Tr\_LJ}(r) \Rightarrow \begin{cases} 4\varepsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right] & when \quad r \le r_c \\ 0 & when \quad r > r_c \end{cases}$$

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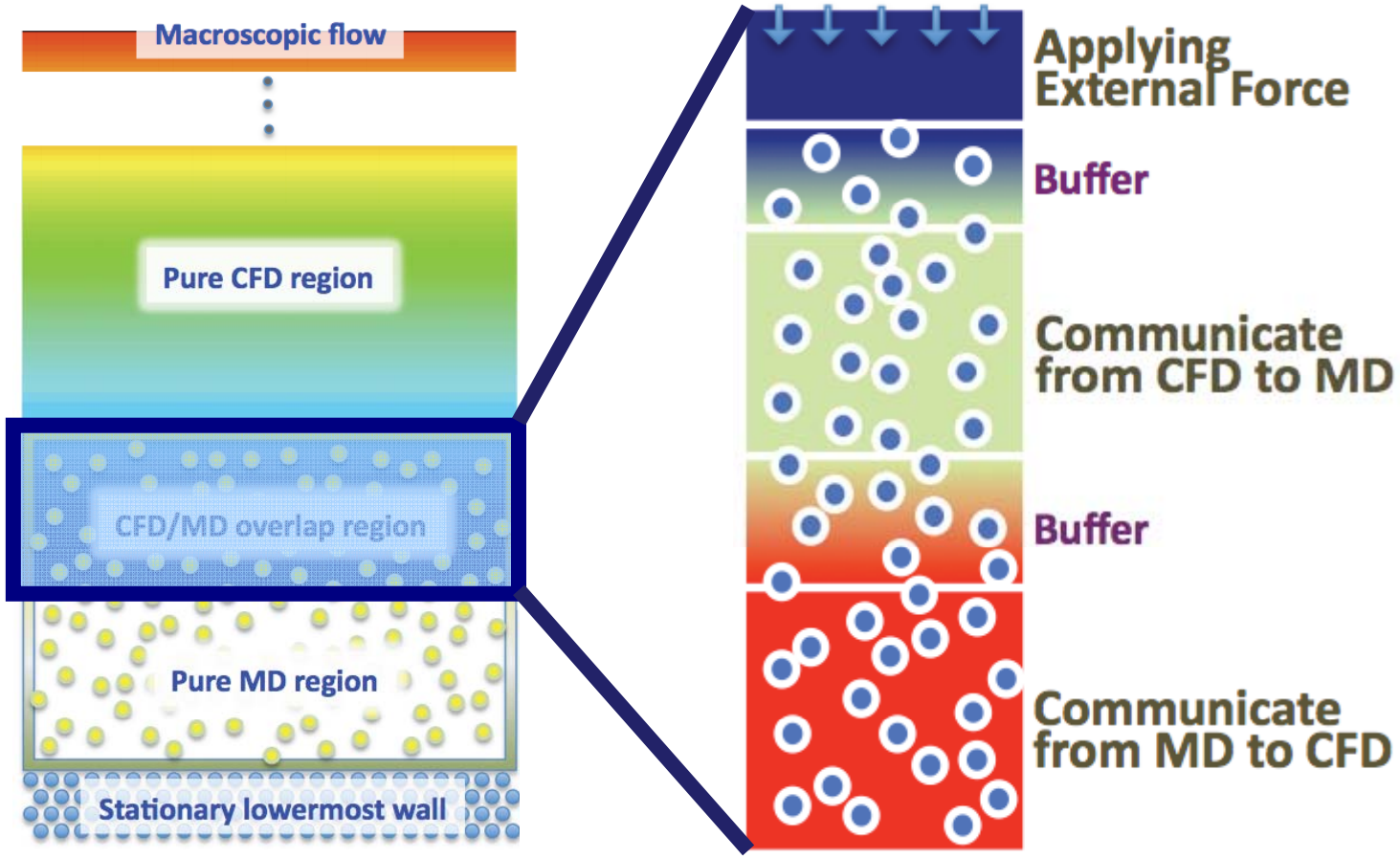
Hybrid Interfaces



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Hybrid Interfaces

CFD	MD
- Overset mesh scheme	
	- External force to trap particles inside
- Big enough not to directly interfere effects of upper and lower layers (height > cut off length)	
- File interface: Sender	- File interface: Receiver - Constrained MD eqn.
Big enough not to direc and lower layers (h	
- File interface: Receiver	- File interface: Sender

$$F_y = -\alpha p_0 \sigma \frac{(y - y_2)}{1 - (y - y_2)/(y_3 - y_2)}$$

where, p_0 is the average pressure

$$\frac{x(t + \Delta t_{MD}) - 2x(t) + x(t - \Delta t_{MD})}{\Delta t_{MD}^2} =$$

$$\frac{F_i}{m} - \frac{1}{N_J m}\sum_{i=1}^{N_J} F_i - \frac{1}{\Delta t_{MD}}\left(\frac{1}{N_J}\sum_{i=1}^{N_J} v_i(t) - u_J(t + \Delta t_{MD})\right)$$

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Runtime Environment for Coupled Applications

- Necessities
  - Co-scheduling of distinct codes
  - Load balancing and more resource allocation
- Runtime environment using SAGA (Simple API for Grid Application) and BigJob abstraction
  - Python script submits a container job and distributes allocated processors to application codes
  - Load balancing changes allocated processors to each application and restarts using its checkpointing data

	Waiting	Inactive	Runtime
Convectional Job (32 + 32 PEs)	83102	47488	39595
BigJob with LB (64 PEs)	**76645**	**0**	**34350**

- S.-H. Ko, etc., "Efficient Runtime Environment for Coupled Multi-Physics Simulations: Dynamic Resource Allocation and Load-Balancing," CCGrid 2010

Numerical Results

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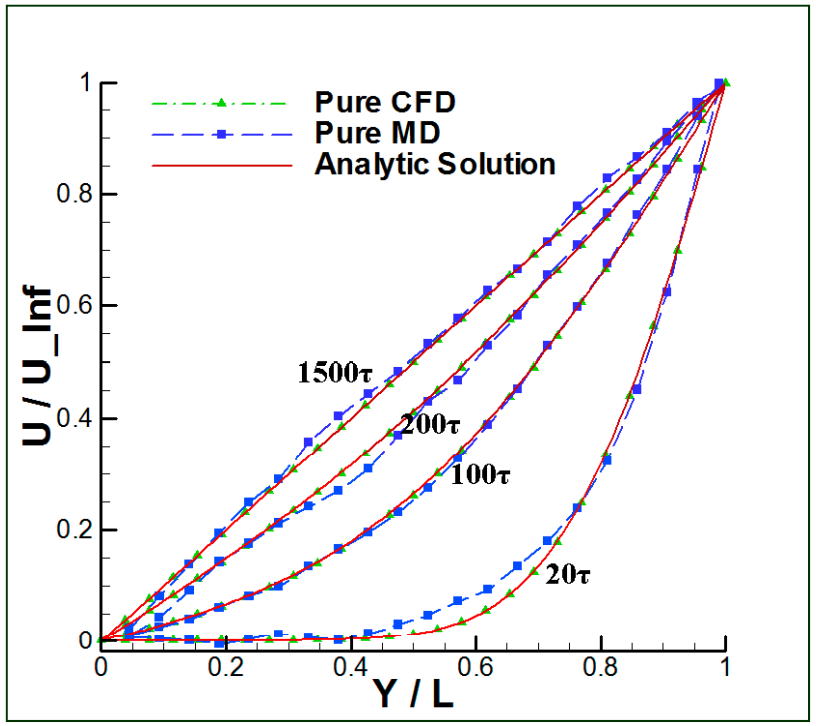
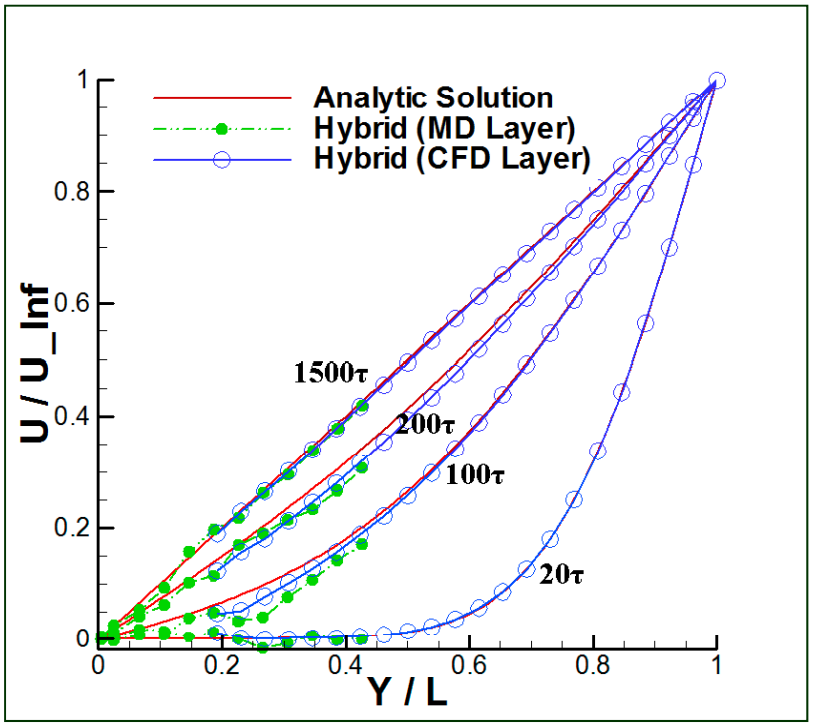
Validation

- Couette flow simulation
  - Liquid Argon (characteristic time scale $\tau=2.2*10^{-12}$ sec)
  - Nano-scale channel ($52\sigma \approx 176$Å)
  - Velocity of upper plate ≈ 155m/s





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Coupling Conditions

- Pure MD simulation (relaxation process)
  - Imp $\Delta t=10^{-3}\tau$, Lx=160σ, Lz=15σ dary conditions and run
  - On sys
    -
    -
    - $\Delta t=10^{-4}\tau$, Lx=40σ, Lz=5σ ection was more effective than increase in periodic direction

	1 tau	2 tau	4 tau	8 tau	16 tau	32 tau
0.1 sigma	0.023577	0.016684	0.012762	0.012421	0.009154	0.008156
0.2 sigma	0.020196	0.013967	0.011196	0.01178	0.008802	0.007972
0.4 sigma	0.016701	0.011753	0.010209	0.011346	0.008688	0.007916
0.8 sigma	0.015342	0.01064	0.009327	0.010793	0.00838	0.007766
1.6 sigma	0.01419	0.009834	0.009285	0.010468	0.008115	0.007672
3.2 sigma	0.011073	0.008635	0.00795	0.009958	0.008115	0.007405

	1 tau	2 tau	4 tau	8 tau	16 tau	32 tau
0.1 sigma	0.077729	0.062558	0.048524	0.037529	0.03156	0.023296
0.2 sigma	0.068395	0.054294	0.044798	0.034836	0.029806	0.02243
0.4 sigma	0.058948	0.050013	0.042595	0.033129	0.028392	0.021704
0.8 sigma	0.052668	0.046317	0.040927	0.031329	0.02829	0.021028
1.6 sigma	0.04457	0.040083	0.039038	0.029542	0.028054	0.020911
3.2 sigma	0.035236	0.029713	0.030352	0.026632	0.027042	0.019317

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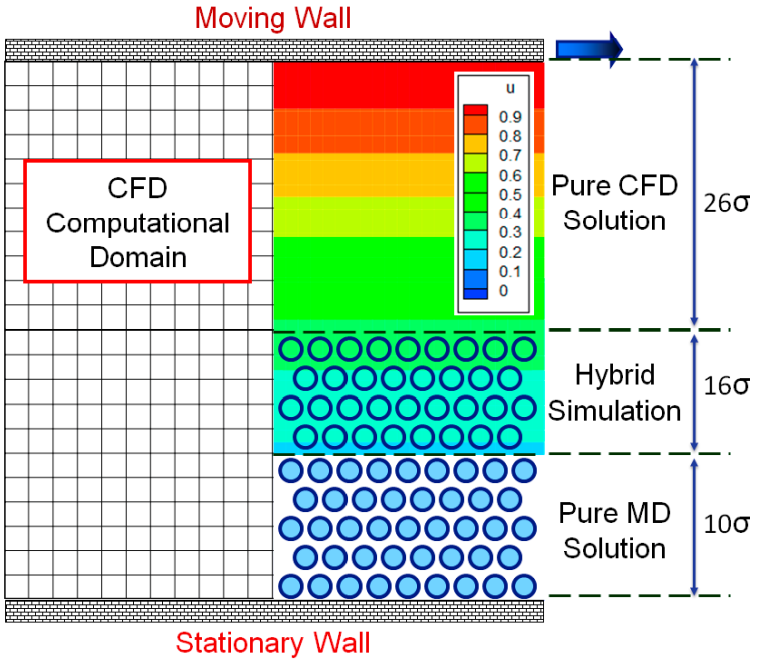
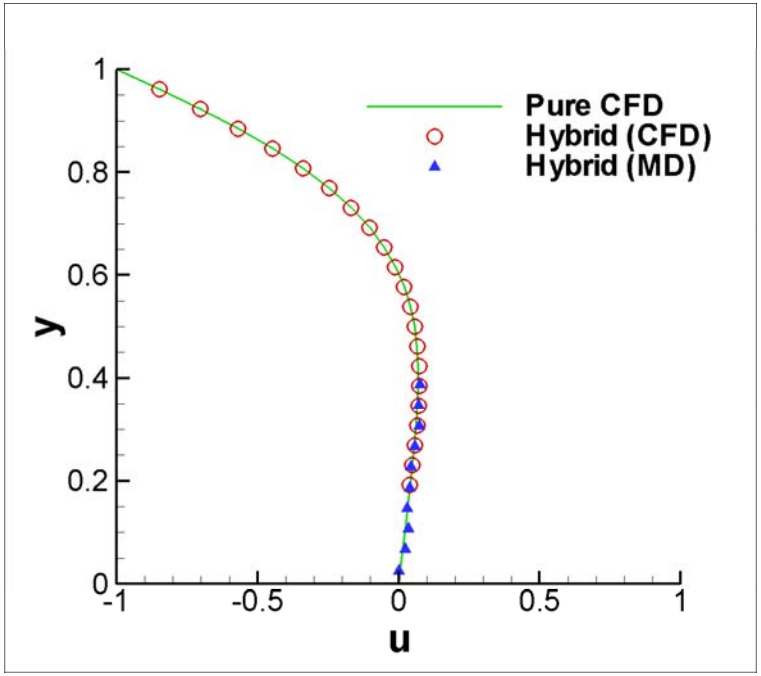
Oscillating Boundary Problem

- The same conditions as Couette flow simulation except harmonic oscillation of upper plate with $T=4.4*10^{-10}$ seconds
  - Liquid Argon, 52σ height, maximum velocity of 155m/s
  - $\Delta t_{MD}=1*10^{-3}\tau$, layer size of 2σ, sampling for 10τ
  - X ≈ 200σ, two ghost layers in overlapping boundary





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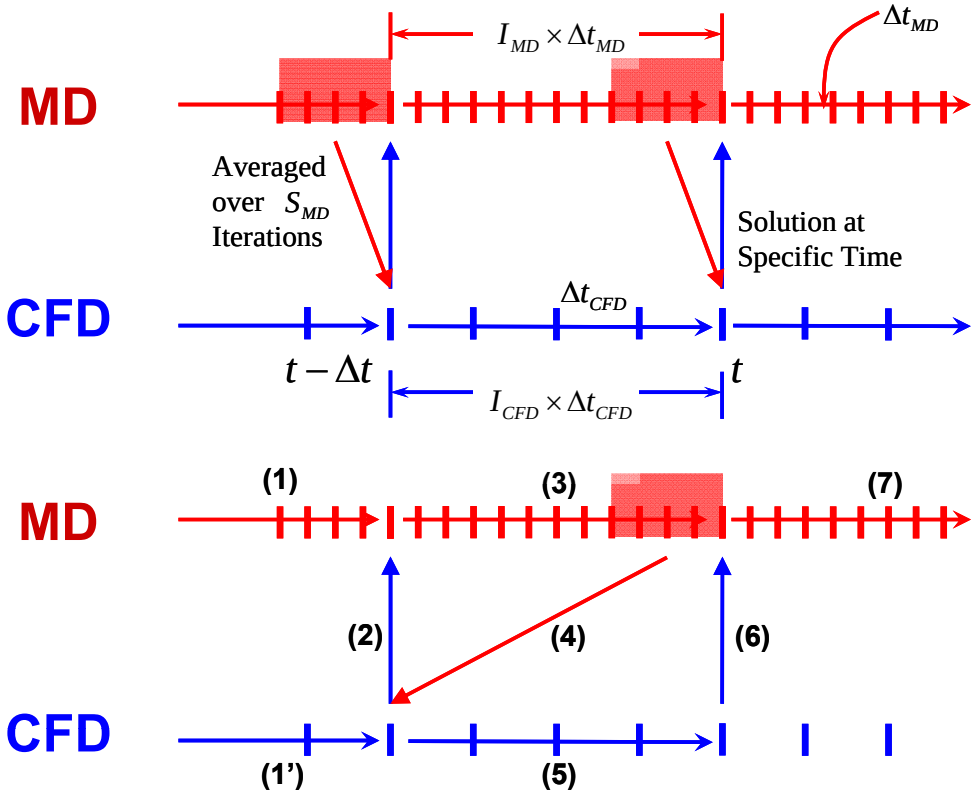
Time Coupling Strategies

- Synchronized and sequential coupling
  - Better parallel performance by synchronized coupling / time lagging in the boundary



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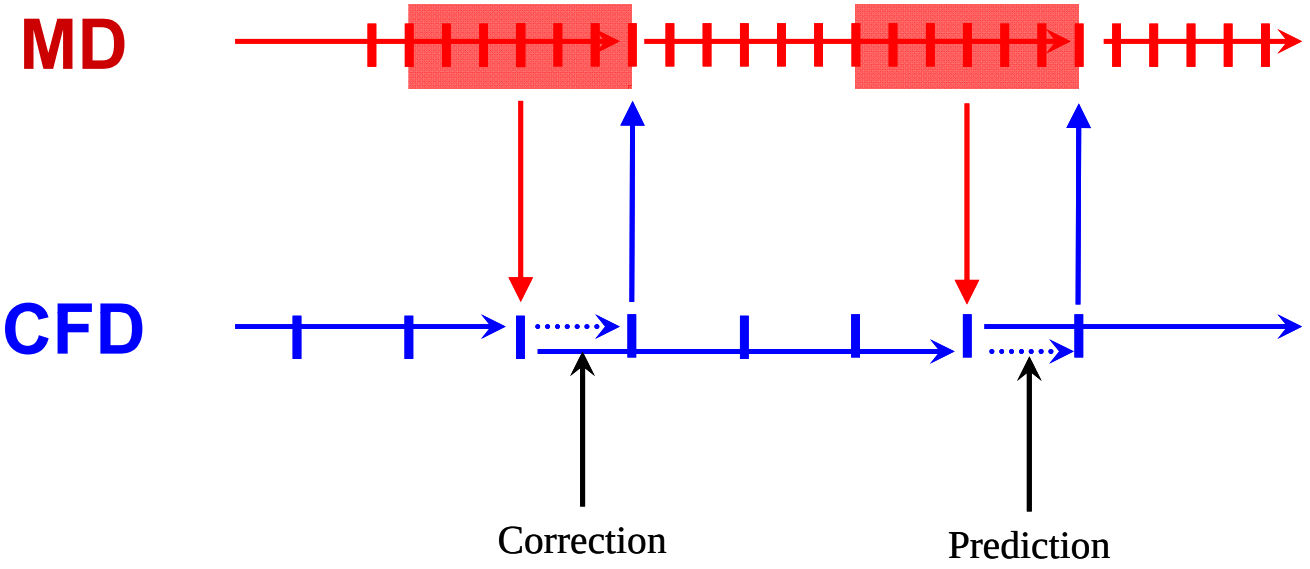
Time Coupling Strategies

- Synchronized and sequential coupling
  - Better parallel performance by synchronized coupling / time lagging in the boundary
- Prediction-correction approach
  - CFD advances to one time step for data exchange and re-computes from the former time step after communication



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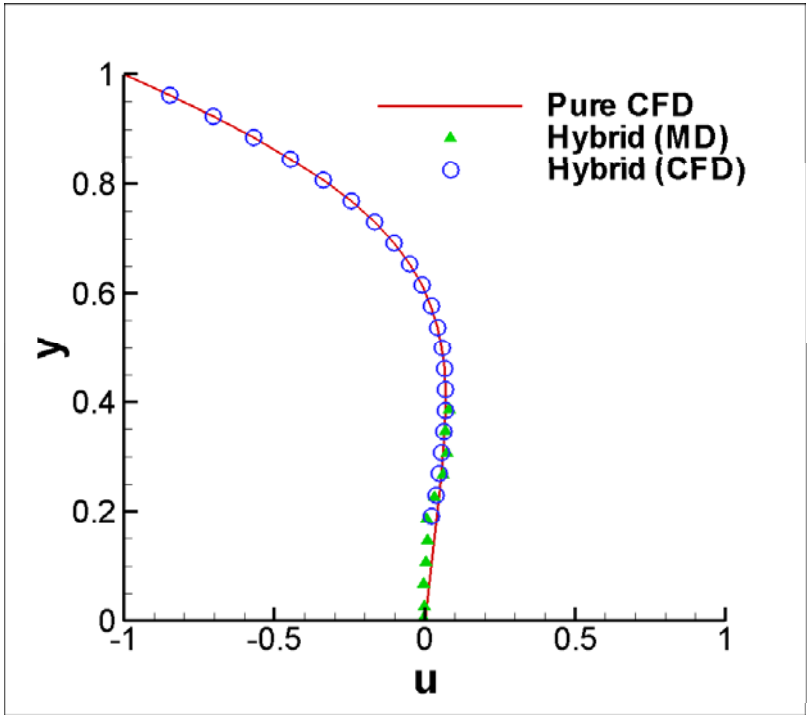
Unsteady Simulation

- Oscillating Boundary Problem
  - Reduces the time-lagging between CFD and MD domains in the overlapping region



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Parametric Study for Real-scale Simulations

- Relaxation simulation
  - System size: 10 times bigger in height (520σ)
  - Fluid element: Liquid argon
    - Time to set up real-molecular domain (water) and improvement of constrained MD equation

$\Delta t=10^{-3}\tau$, Lx=200σ, Lz=5σ

	10tau	20tau	40tau	80tau	160tau	320tau	640tau
1sigma	0.009766	0.007459	0.006626	0.005798	0.004694	0.004736	0.003083
2sigma	0.009166	0.006908	0.006421	0.005716	0.00462	0.004671	0.003038
4sigma	0.008217	0.006337	0.006024	0.005558	0.004402	0.004615	0.002981
8sigma	0.006713	0.005089	0.005213	0.00509	0.004233	0.004549	0.002928
16sigma	0.004899	0.003684	0.003196	0.003785	0.003721	0.003861	0.002733
32sigma	0.002313	0.002249	0.002399	0.003086	0.003127	0.003493	0.002617

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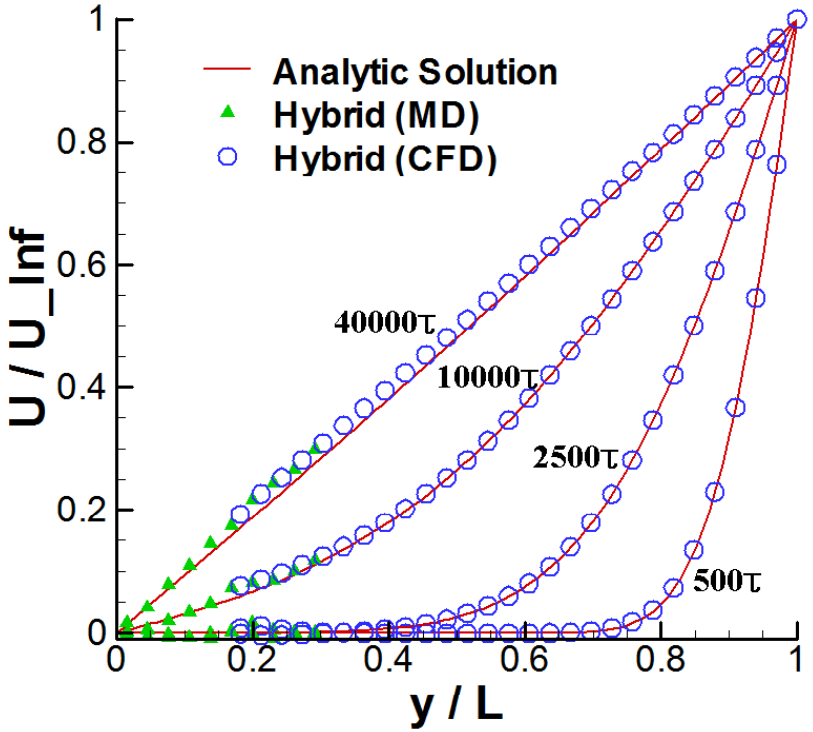
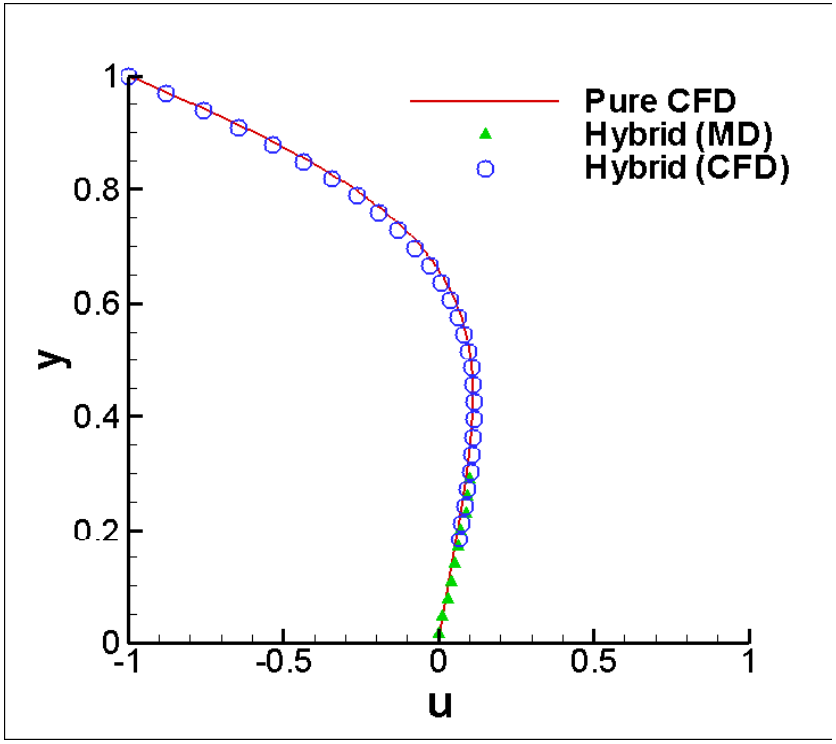
Simulations on Larger Domain

- Simulation conditions
  - Same Δt_{MD} and velocity, layer size of 16σ, sampling for 100τ
  - Far longer time until convergence



Couette Solution



Unsteady Oscillation

Current Issues

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Agenda

- Simulation on low-speed flow system
  - Parametric study on coupling condition
- Realistic flow simulation (water filled in carbon tube)
  - Improvement of a constrained MD equation
  - Accurate solution on interaction between fluid and solid domains expected

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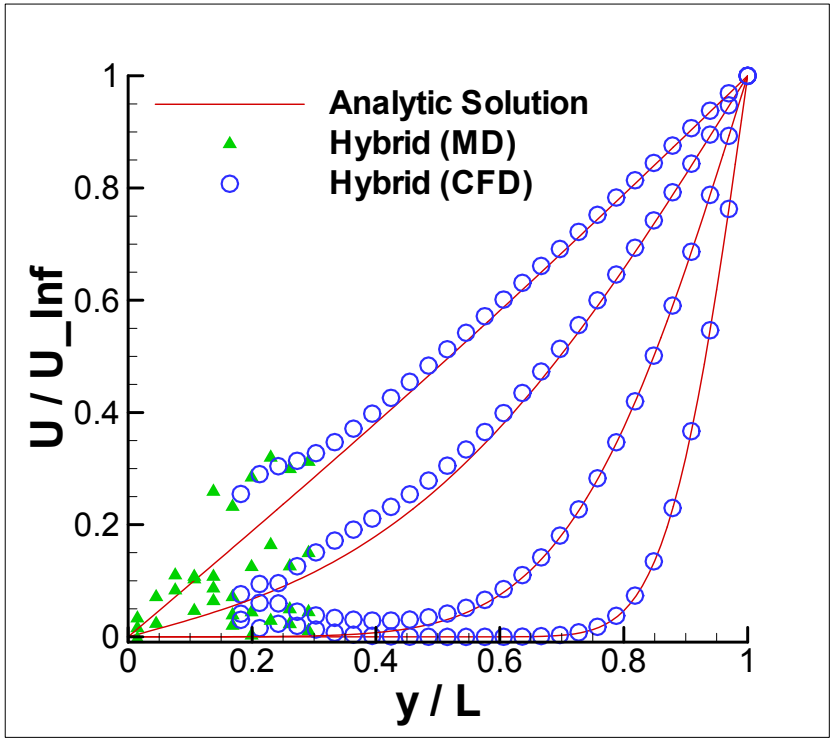
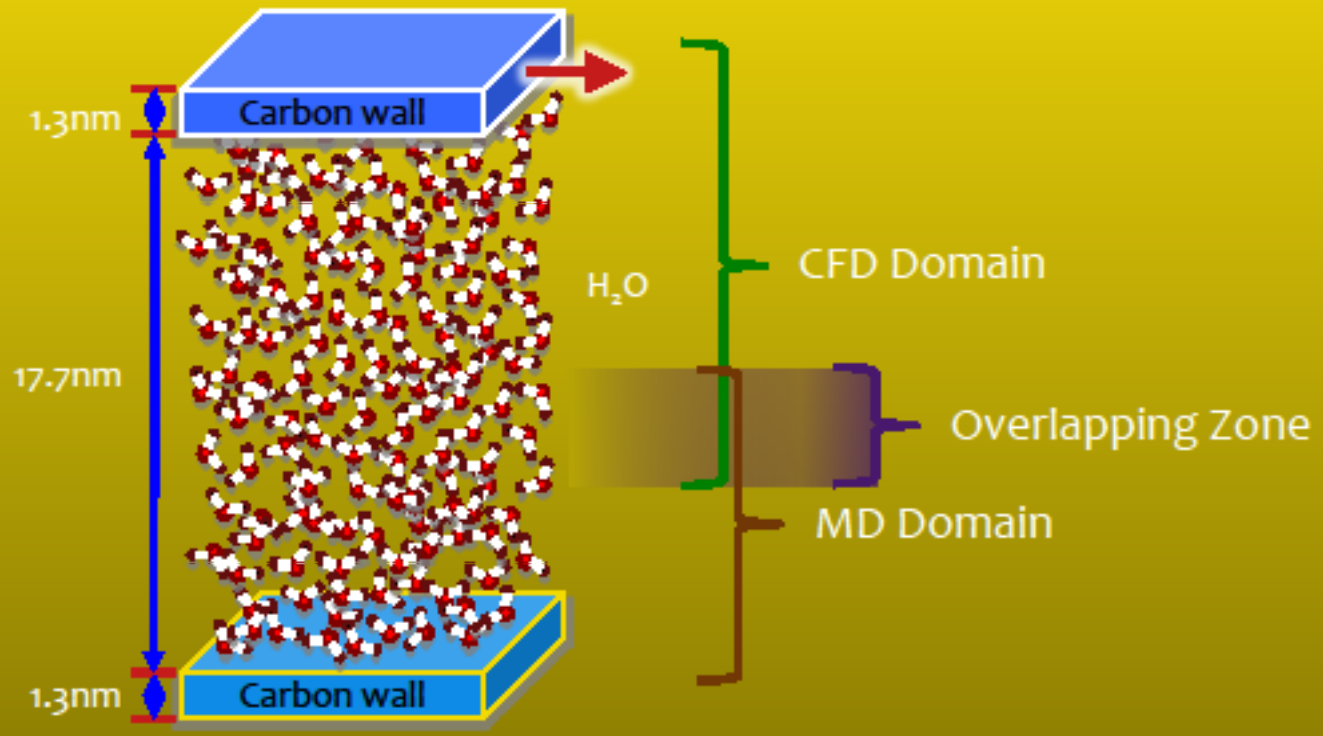
Low-speed Flow Simulation

- O(10) Velocity
  - Strong noise from MD solution
    - Need to increase sampling duration



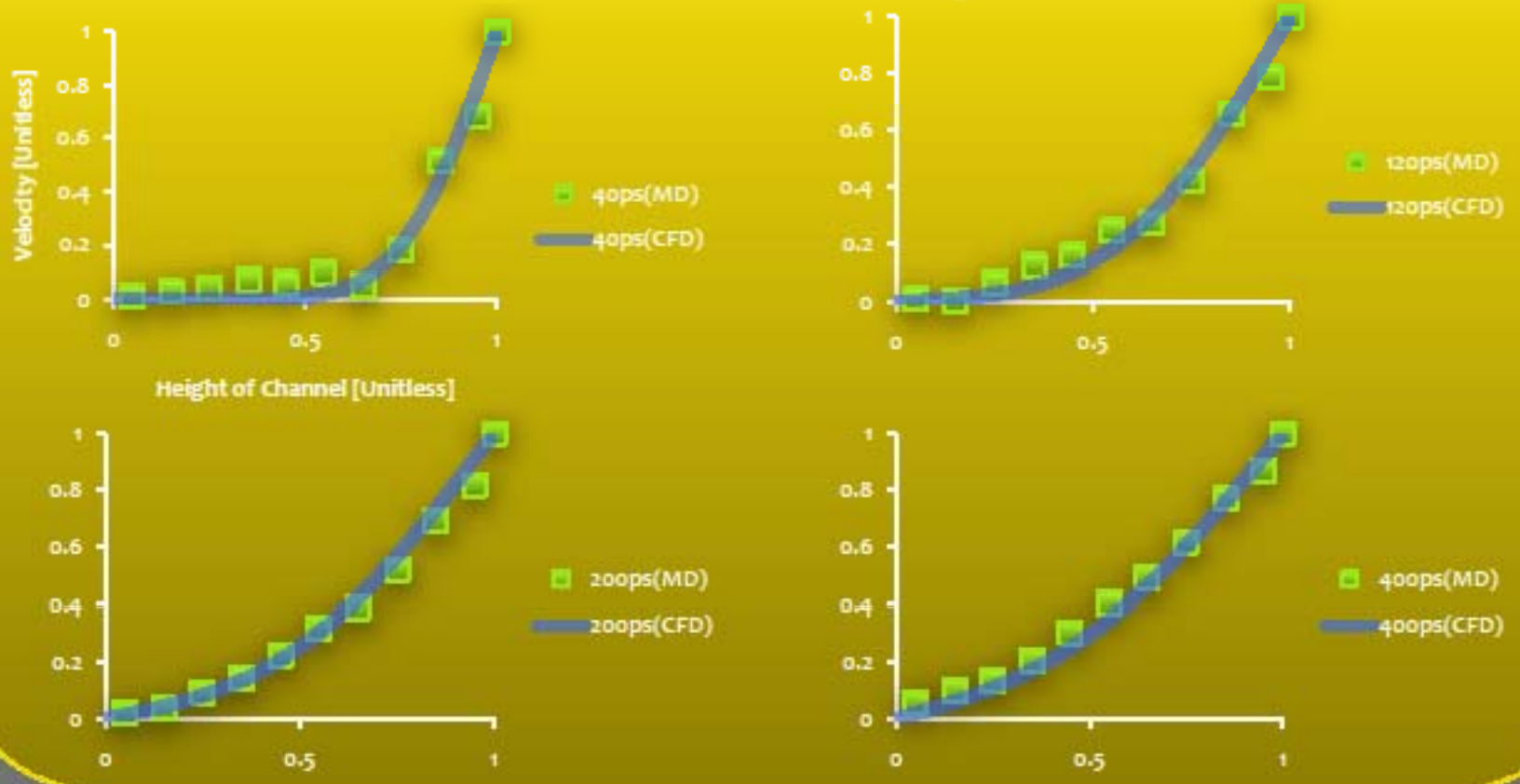
Hybrid Model to Polyatomic Molecular Fluid

❖ **Hybrid Coupling Simulation w/ Realistic Materials and Structure**

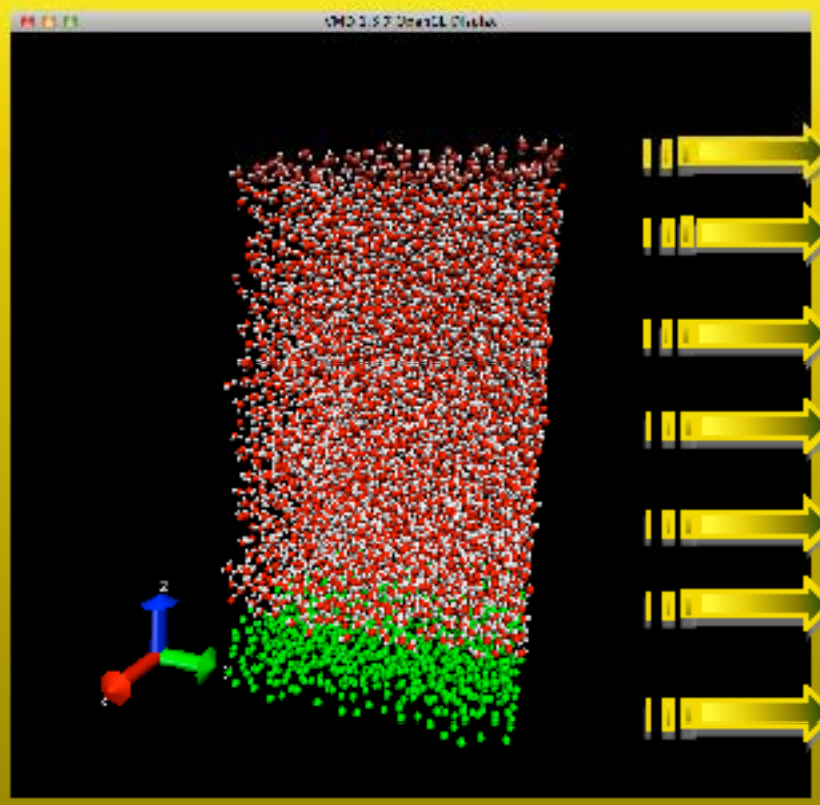


Pure CFD vs. Pure MD

❖Results from CFD & MD using Water Molecules



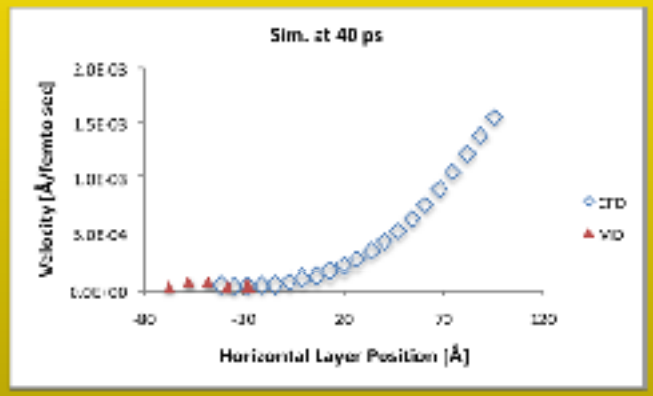
Hybrid Schemes (MD + Hybrid Region)

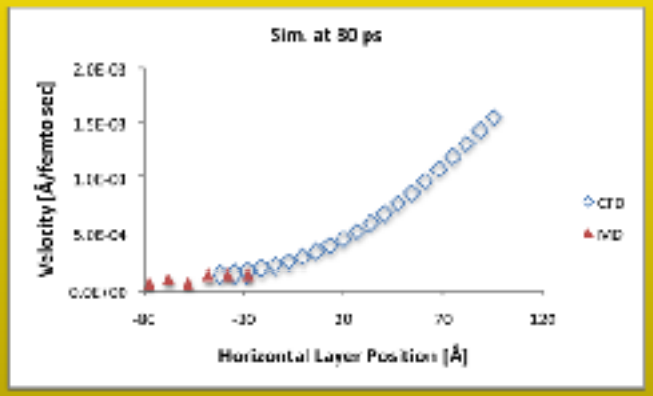


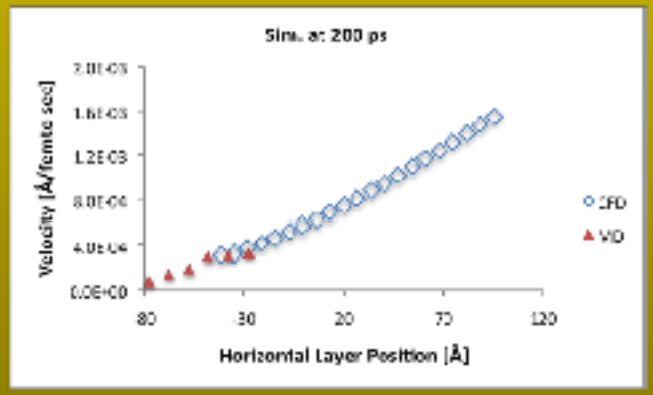
Schematic diagram of the channel flow model using polyatomic molecular fluids

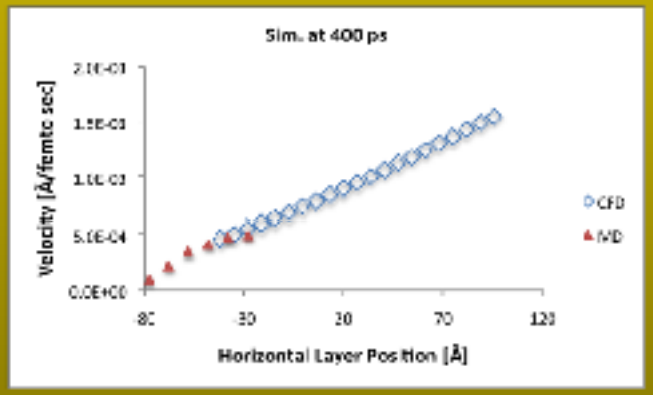
Polyatomic Hybrid Simulation

❖ Hybrid Simulation using Water Molecules









Conclusion

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Conclusion

- Hybrid CFD-MD Approach
  - Better solution near the solid body with acceptable efficiency
- Development of hybrid CFD-MD framework
  - Individual codes with hybrid interface
  - Runtime environment for co-scheduling and load balancing
- Applications to nano-scale systems
  - Coupling conditions determined from relaxation process
  - Couette flow simulation and oscillating boundary problem
    - Improving time-coupling strategy
  - Simulation on larger domain
    - Larger layer with longer sampling duration
  - Low-speed flow simulation
    - Requires more sampling duration
  - Simulation of realistic fluid system
    - Solution of nano-scale Couette flow