From Atomistic Simulations to Macroscopic Interfacial Response

Physical Principles of Multiscale Modeling, Analysis and Simulation in Soft Condensed Matter, Kavli Institute for Theoretical Physics, UCSB, May 3, 2012

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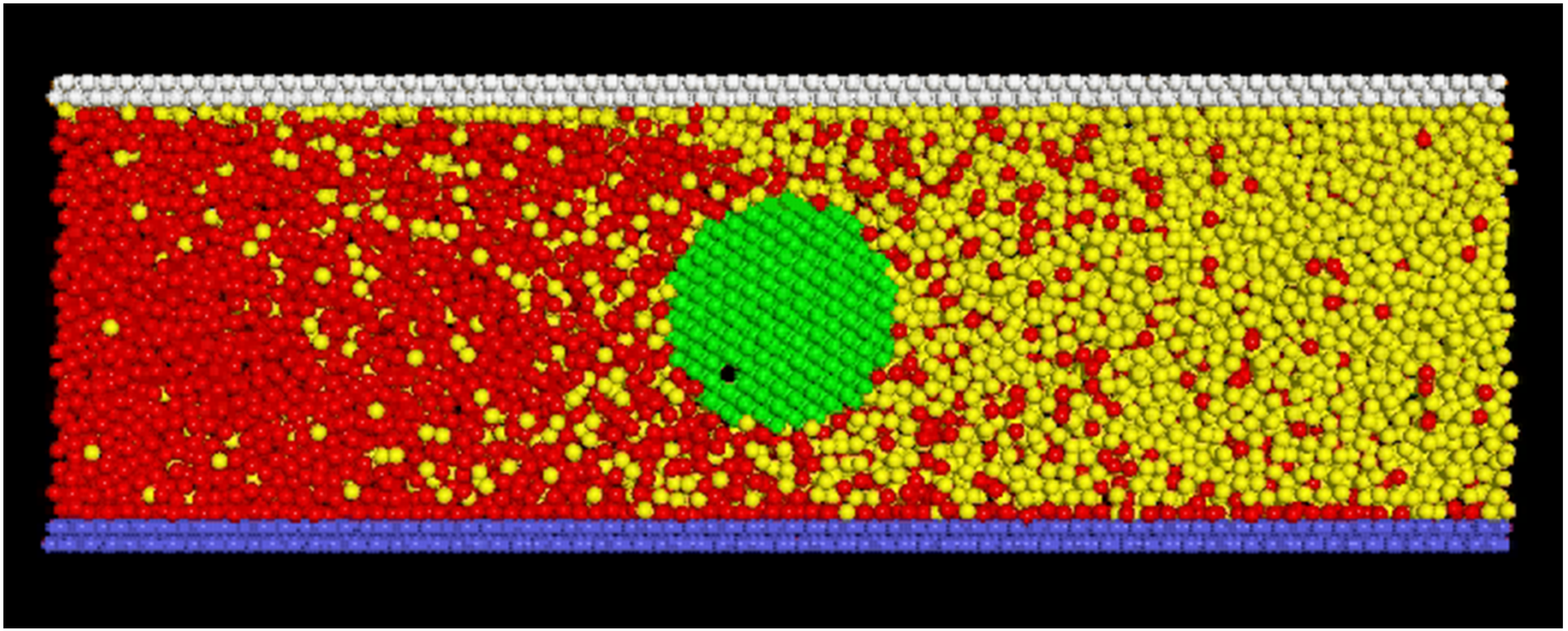
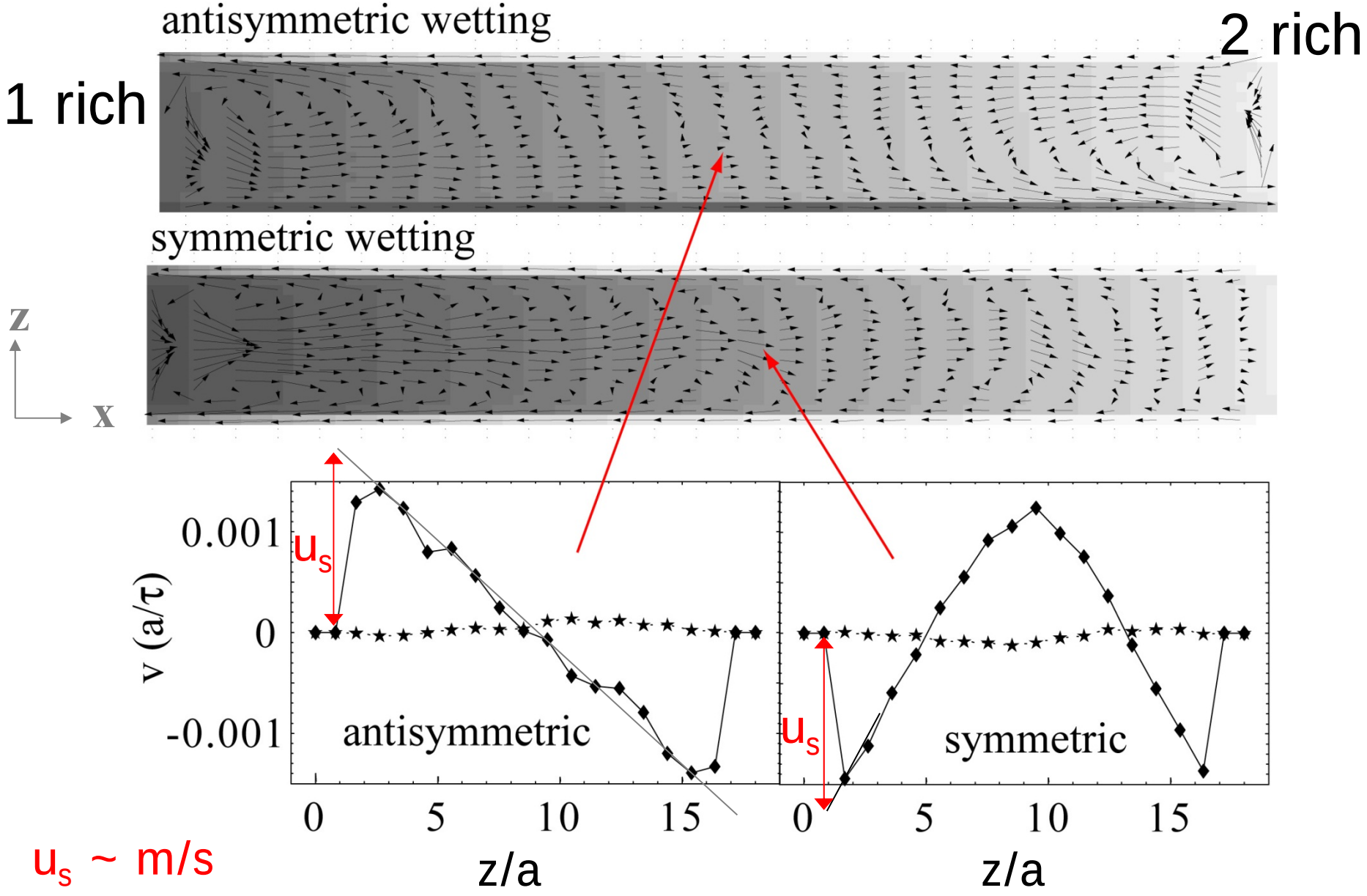
Unexpected Fine Scale Behavior

Many models coarse-grain to same equations
→Micro model constructed to give a coarse-grained eqn (LB, SPH)
can not be expected to give correct atomic and mesoscopic behavior

Nanomotor (C. Denniston & MOR, J. Chem Phys. 125, 214102, 2006)



Wetting + Conc. Gradient → Couette or Poisseuille-like flow between static walls



u_s ~ m/s

General Slip Boundary Condition

Atomistic flows fit by generalized sharp interface boundary conditions down to scales ~ a few nm

- Stress balance $\rightarrow \Delta\sigma_{xz} \equiv \sigma_{xz}^{b}(w) - \sigma_{xz}^{wall} = \partial_x \gamma$
- Slip boundary condition

$$u_s = \frac{L_s}{\eta_b}\sigma_{xz}^{b} + \frac{L_m}{\eta_b}\partial_x\gamma + \left[\frac{f_1}{c_1} - \frac{f_2}{c_2}\right] D\partial_x c_1$$

Navier Surface stress Diffusive

Can get net mass flux with no drag, negative slip lengths, ...

Velocities ~ m/s , stresses ~ MPa

Phase-Field Model of Fluid-Fluid Interface

- If ξ » a $\rightarrow$ coarse-grained F functional of ρ, ϕ
- Square-gradient theories

$$F = \int \left\{ \psi(\rho,\phi,T) + \tfrac{1}{2} K_\rho (\nabla\rho)^2 + \tfrac{1}{2} K_\phi (\nabla\phi)^2 + \tfrac{1}{2} K_{\rho\phi} (\nabla\rho \cdot \nabla\phi) \right\}$$

Usually ignore $K_{\rho\phi}$ (odd in ϕ), assume $K_{\rho\rho}>0$
Often fix ρ, expand ψ as quartic polynomial in ϕ

$\rightarrow$ None of these assumptions is good

- Obtain ψ and K's from MD measurements of coexistence line, and pressure and linear response near coexistence
- Fit gives surface tension and width that agrees with MD results although not fit to them

Denniston & Robbins, Physical Review E69, 021505 (2004)

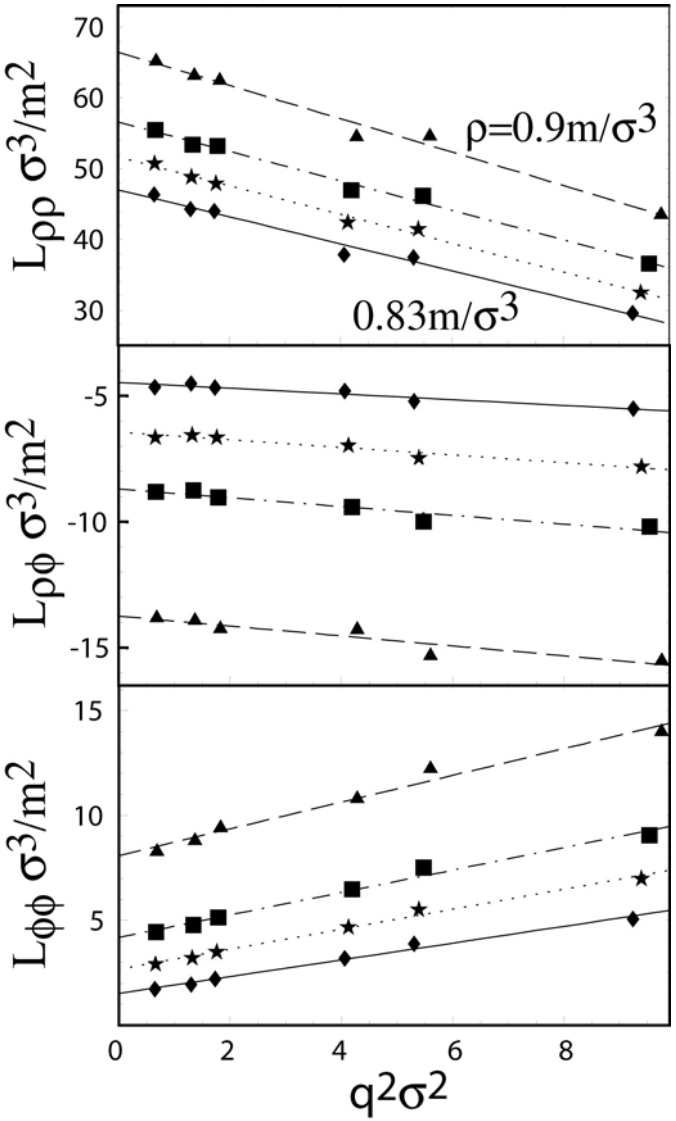
Linear Response

- Apply perturbation: $\delta\mu_\rho = -\mu_{\rho\theta}\ \sin qx$, $\delta\mu_\phi = -\mu_{\phi\theta}\ \sin qx$
- Measure resulting ρ_q, ϕ_q

$$\begin{pmatrix} L_{\rho\rho} & L_{\rho\phi} \\ L_{\rho\phi} & L_{\phi\phi} \end{pmatrix} \begin{pmatrix} \rho_q \\ \phi_q \end{pmatrix} = \begin{pmatrix} \mu_{\rho q} \\ u_{\phi q} \end{pmatrix}$$

$L_{\rho\rho} = \partial^2\psi/\partial\rho^2 + K_{\rho\rho}\, q^2$, ...

- Find L's linear in q^2 to $2\pi/q \approx 2\sigma$, but $K_{\rho\rho}, K_{\rho\phi} < 0$
- Usual to add q^4 terms if $K_{\rho\rho} < 0$ but expect $K_{\rho\rho} \to 0$ as $q \to \infty$ since cost of forcing atoms onto arbitrarily fine lattice $\to 0$



Electro-Wetting on Dielectric (EWOD)

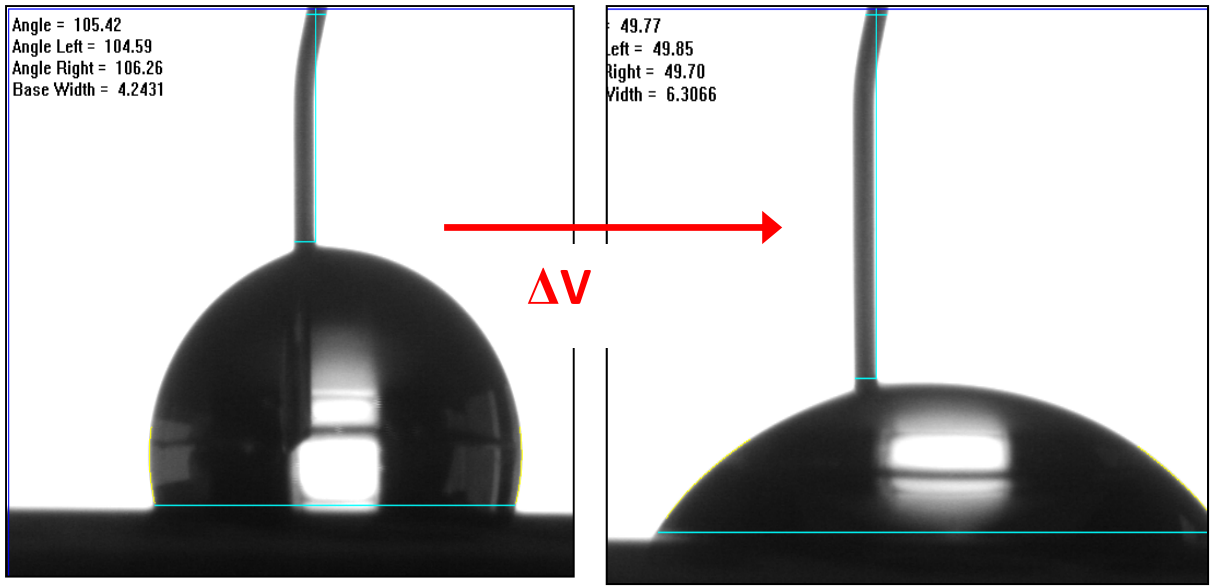
Electrowetting → Change in contact angle with voltage

Allows: Fluid drops to be guided on surface

Drop shape to be changed – active lenses

Questions: Can mechanism be used at nanometer scale?

Why does contact angle saturate before perfect wetting?



Electro-Wetting on Dielectric (EWOD)

Equilibrium: $\theta_0 \rightarrow$ balance between interfacial tensions

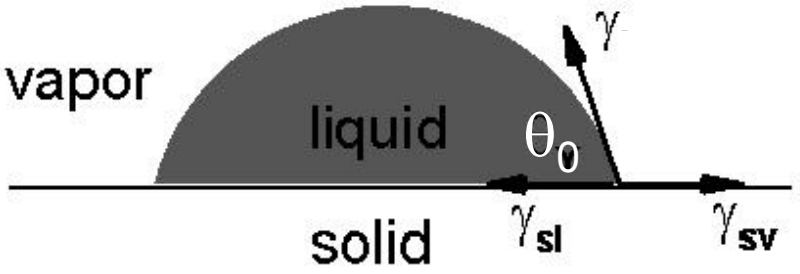
Young's eqn: $\gamma \cos \theta_0 + \gamma_{sl} = \gamma_{sv}$

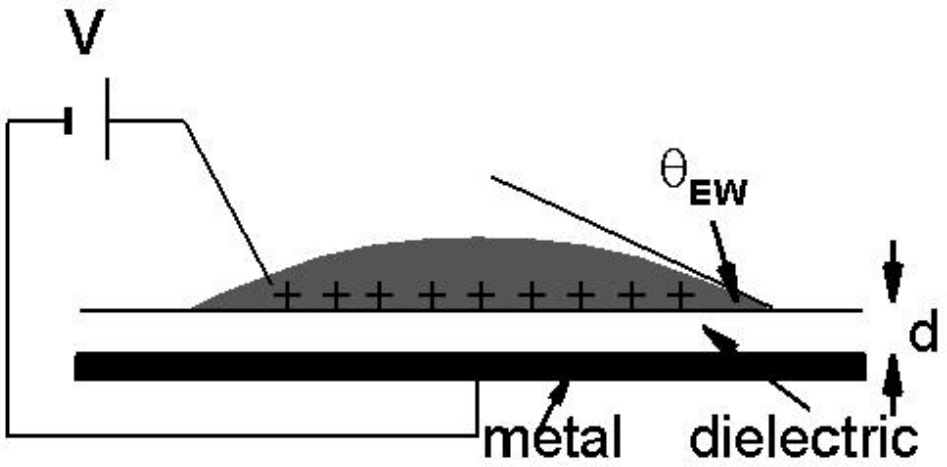
Apply V: Must add effect of electrostatic energy

Lippmann's eqn.: $\cos \theta - \cos \theta_0 = \epsilon_0 \epsilon_r V^2/2d\gamma = cV^2/2\gamma$

c=capacitance per unit area

Electrocapillary view $\rightarrow$ surface tension reduced by electric energy per unit area: $\gamma_{sl} \rightarrow \gamma_{sl} - cV^2/2$





Experiments: Saturation at High Voltage

Proposed explanations:

Negative effective tension $\rightarrow \gamma_{sl} - cV^2/2 < 0$

Quinn et al., J. Phys. Chem. B**109**, 6268 (2005).

Field diverges as approach contact line

Dielectric breakdown $\rightarrow$ Charging of dielectric

Papathanasiou et al., J. Appl. Phys**. 103**, 034901, (2008)

Micro-droplet ejection

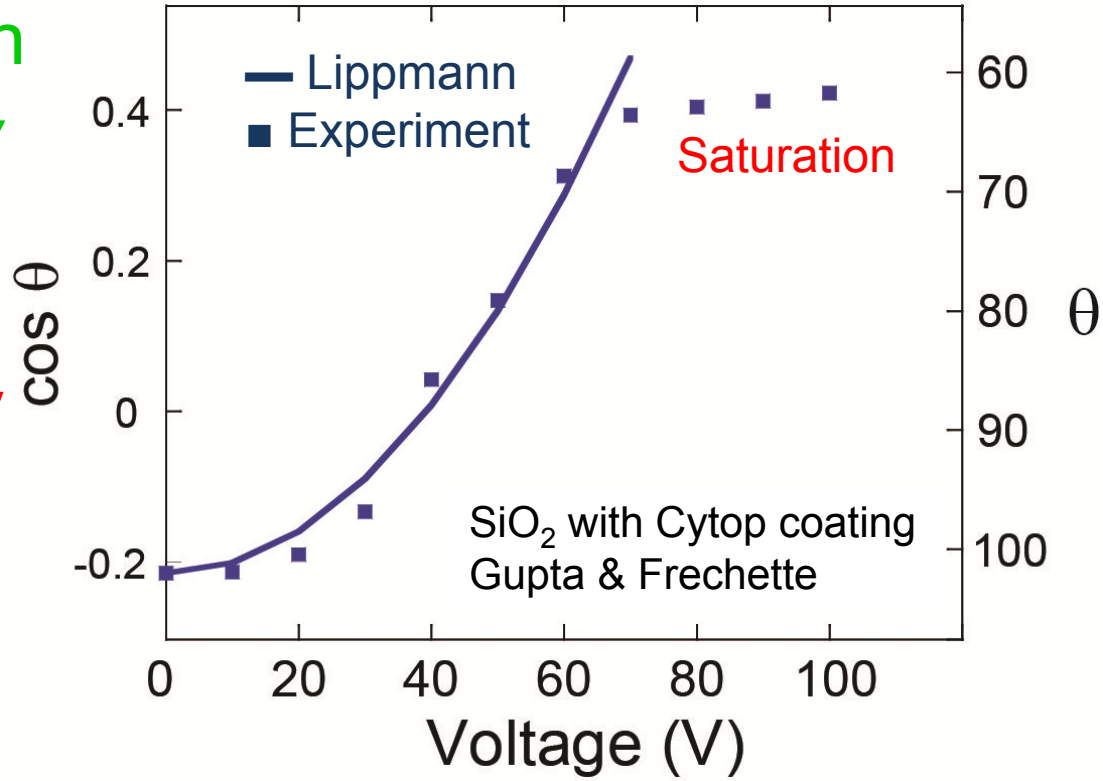
$\rightarrow$ Field overcomes γ

Vallet et al. Eur. Phys. J. B11, 583 (1999)

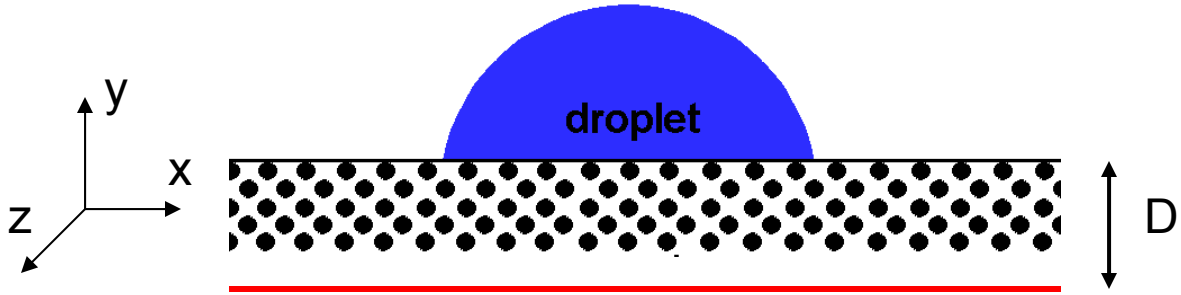
If continuum $\rightarrow$ singularity

$\rightarrow$ atoms may matter

Moving contact lines, cavity flow, …

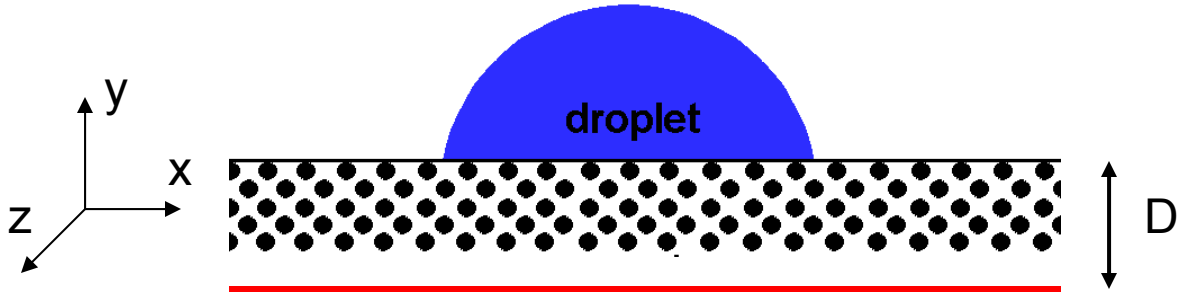


Nanoscale Simulations of EWOD



- Fluid – short bead-spring chains 4 to 8 beads at $T \sim 2T_g$
  Covalent bonds on chain → $U_{FENE} = 0.5kR_0^2 \ln[1-(r/R_0)^2]$
  Interchain → Lennard-Jones (LJ) $U_{LJ} = 4u[(\sigma/r)^{12}-(\sigma/r)^6]$
- Rigid solid substrate, discrete atoms $\rho_w = 0.61m\sigma^{-3}$
- Change solid-fluid binding energy u_{sf} to change θ_0
- Charge one monomer on some chains to increase V
- Perfect conductor at depth D via image charges, uniform ε
- Periodic boundary conditions: $L_x = 114.6\sigma$, $L_z = 10.6\sigma$, $L_y = 2L_x$
  Correct to remove effect of periodic images along y
- Measure γ, $\gamma_{sv}-\gamma_{sl}$, capacitance c for uniform films – not fit

Nanoscale Simulations of EWOD



Can express parameters in terms of key lengths normalized by molecular diameter σ

Interface width $\xi \sim 3\sigma$

$\rightarrow$Bjerrum length $l_B = e^2/\varepsilon k_B T \rightarrow$ at l_B interaction = $k_B T$

Gouy-Chapman screening length

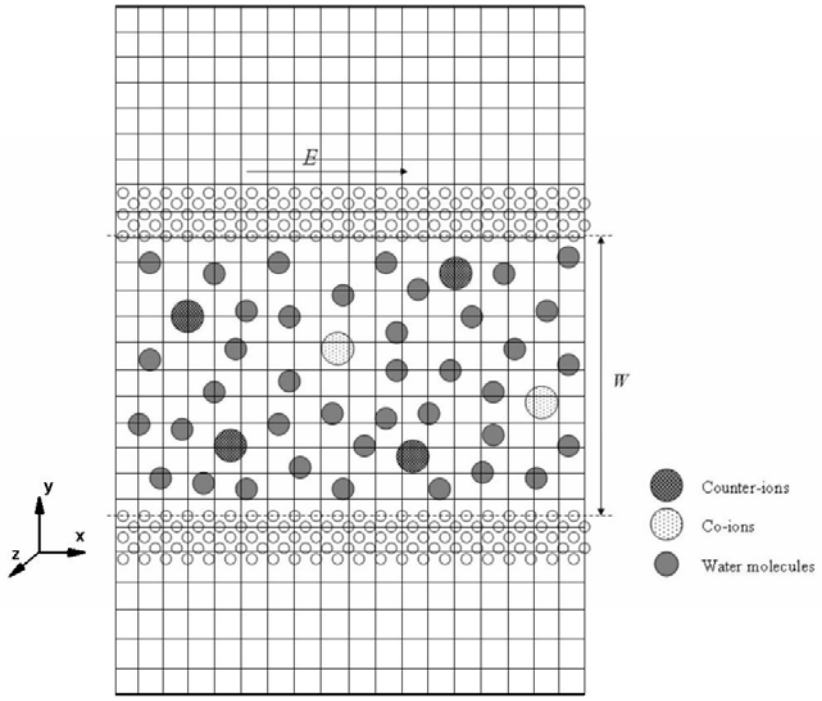
$\lambda_{GC} = e/2\pi l_B cV$ where cV is surface charge density

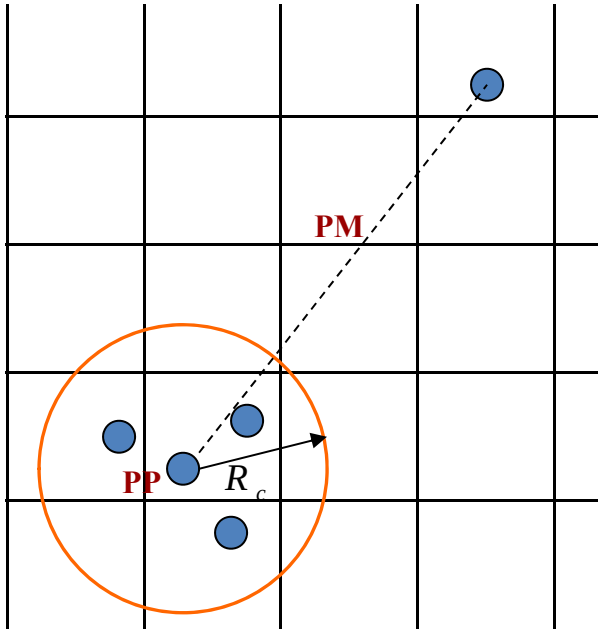
Continuum theory assumes all lengths ~0

Electroosmotic Flow & Electrowetting

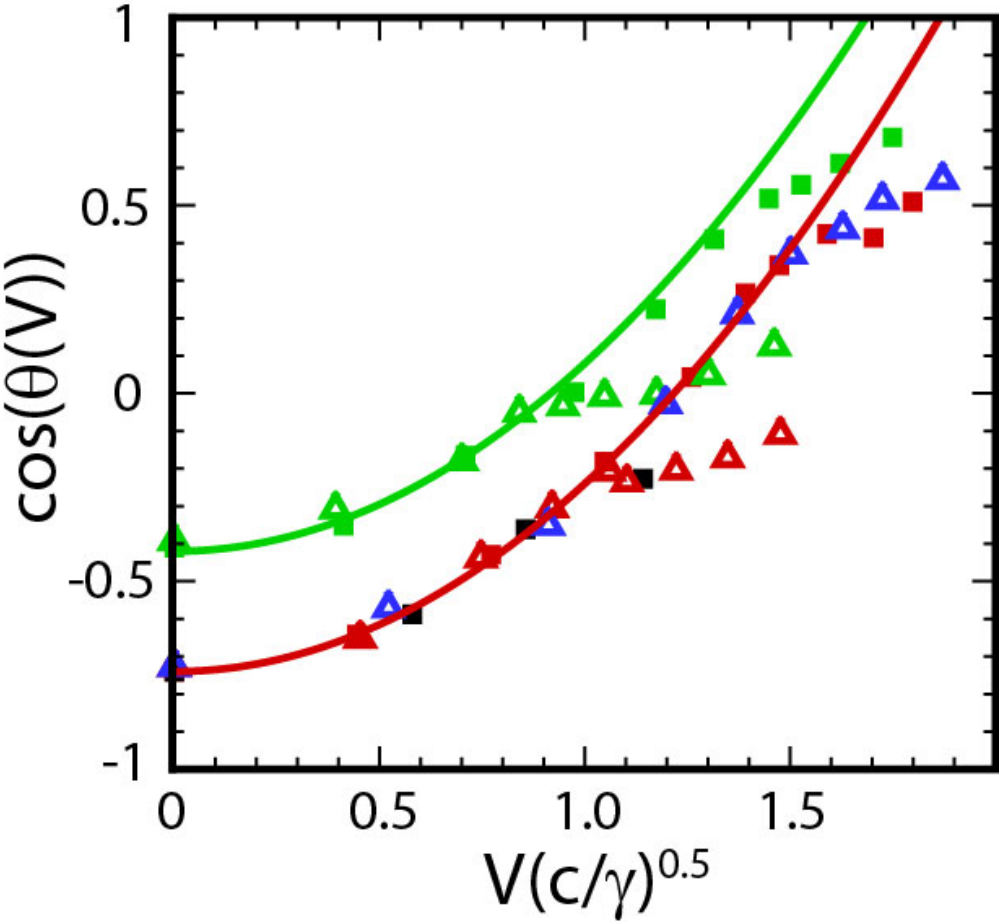
- Direct summation of long range interactions is prohibitive for large systems.
- Use particle-particle particle-mesh with multigrid method for solving Poisson equation

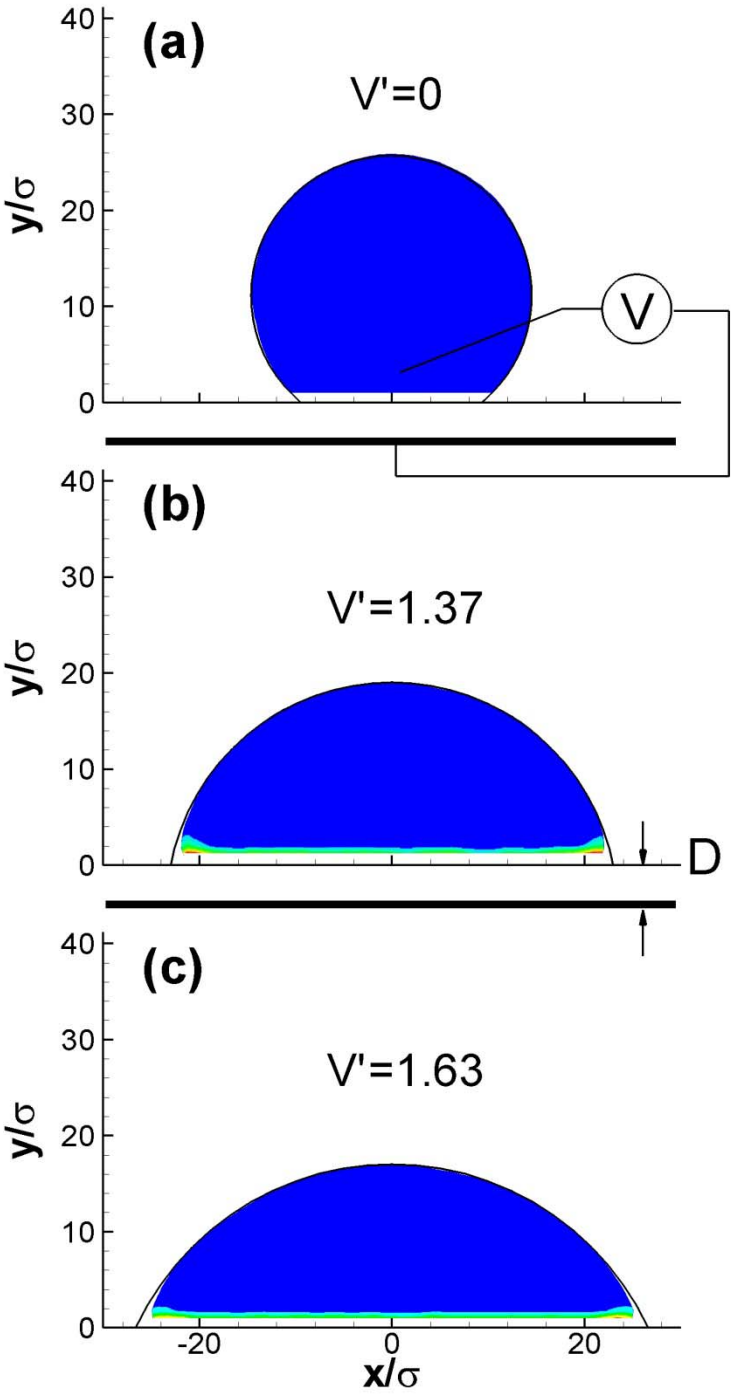
  Liu, Wang, Chen and Robbins, J. Comput. Phys. **229**, 7834-7847 (2010)



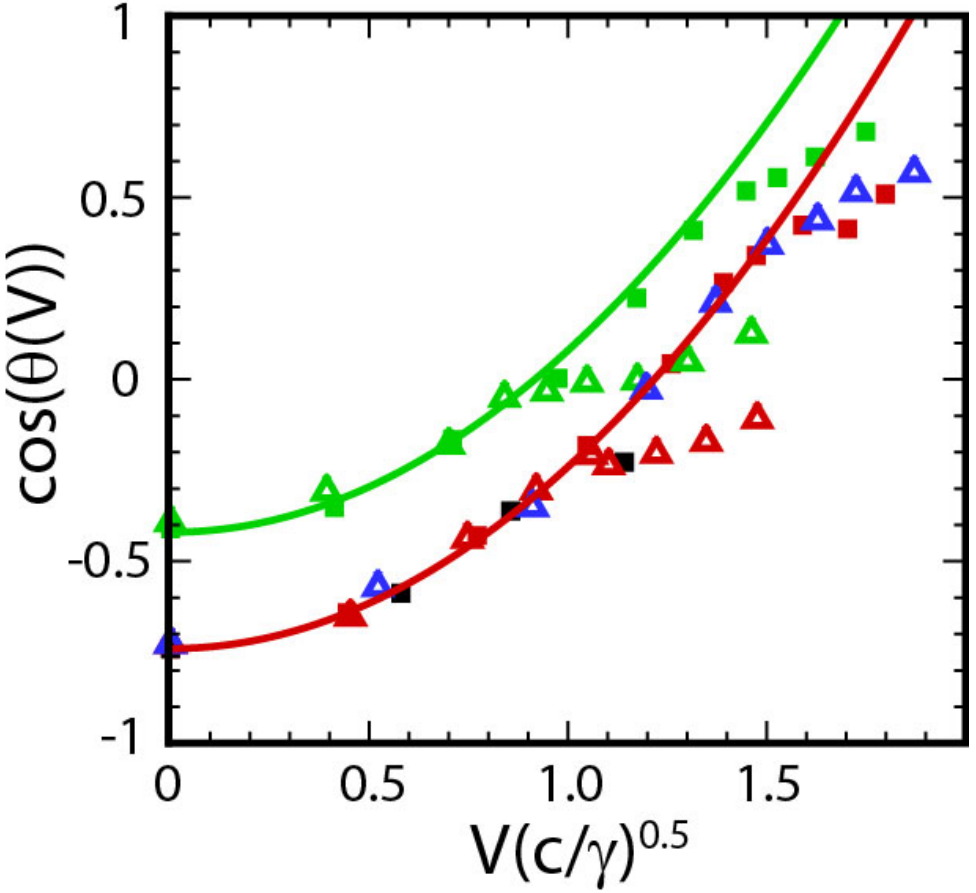


Behavior Like that in Macroscopic Experiments





Comparison to Lippmann Equation



Lines – Lippmann with no fit params.

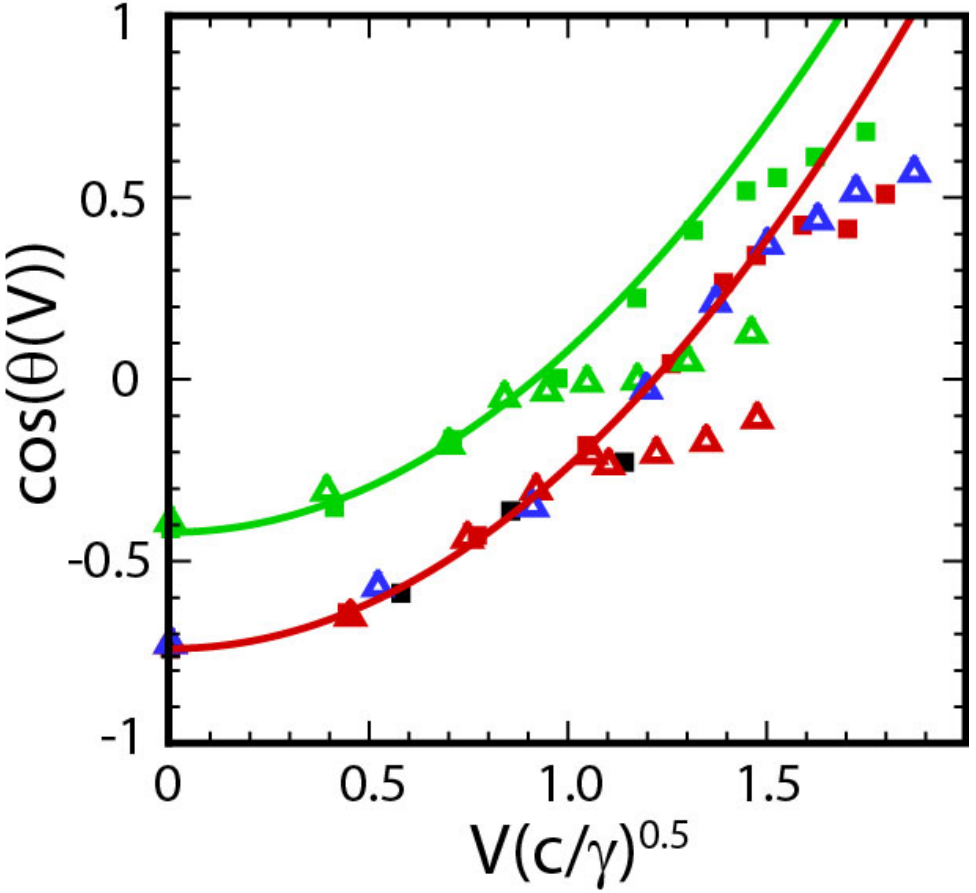
Δ chain length 4
■ chain length 8

Green: diff. $u_{sf} \rightarrow \theta_0$

Black $l_B=96\sigma$
Red $l_B=12.32\sigma$
Blue $l_B=4\sigma$

As in experiment, θ follows Lippmann at small V then saturates
Saturation delayed for longer chains
since γ not changed by length $\rightarrow$ molecular effect
Stronger screening, shorter l_B, delays saturation

Comparison to Lippmann Equation



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Green: diff. $u_{sf} \rightarrow \theta_0$

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Not negative effective tension $\gamma_{sl} - cV^2/2 < 0$ (Quinn et al., 2005).
γ_{sl} ~ independent of chain length, arbitrarily large
No dielectric breakdown (Papathanasiou et al., 2008)
Not related to γ as expected if microdroplet ejection (Vallet et al., '99)

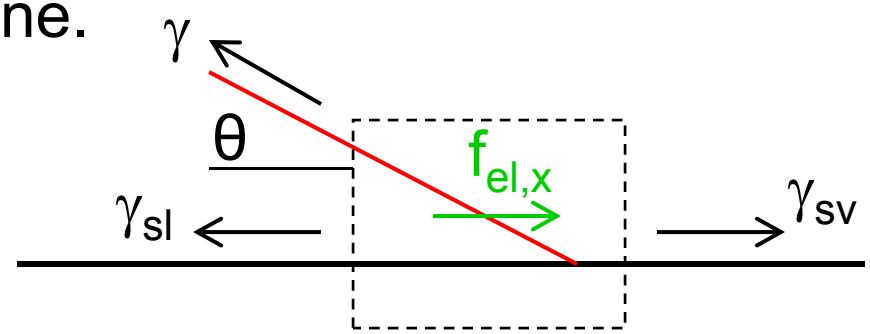
Microscopic Force Balance Equation

Lippmann Equation derived from energy minimization with assumed geometry. May be violated.

Forces must balance everywhere in simulation

Consider region around contact line.

$f_{el,x}$ = Force per length from electric field on charge within region

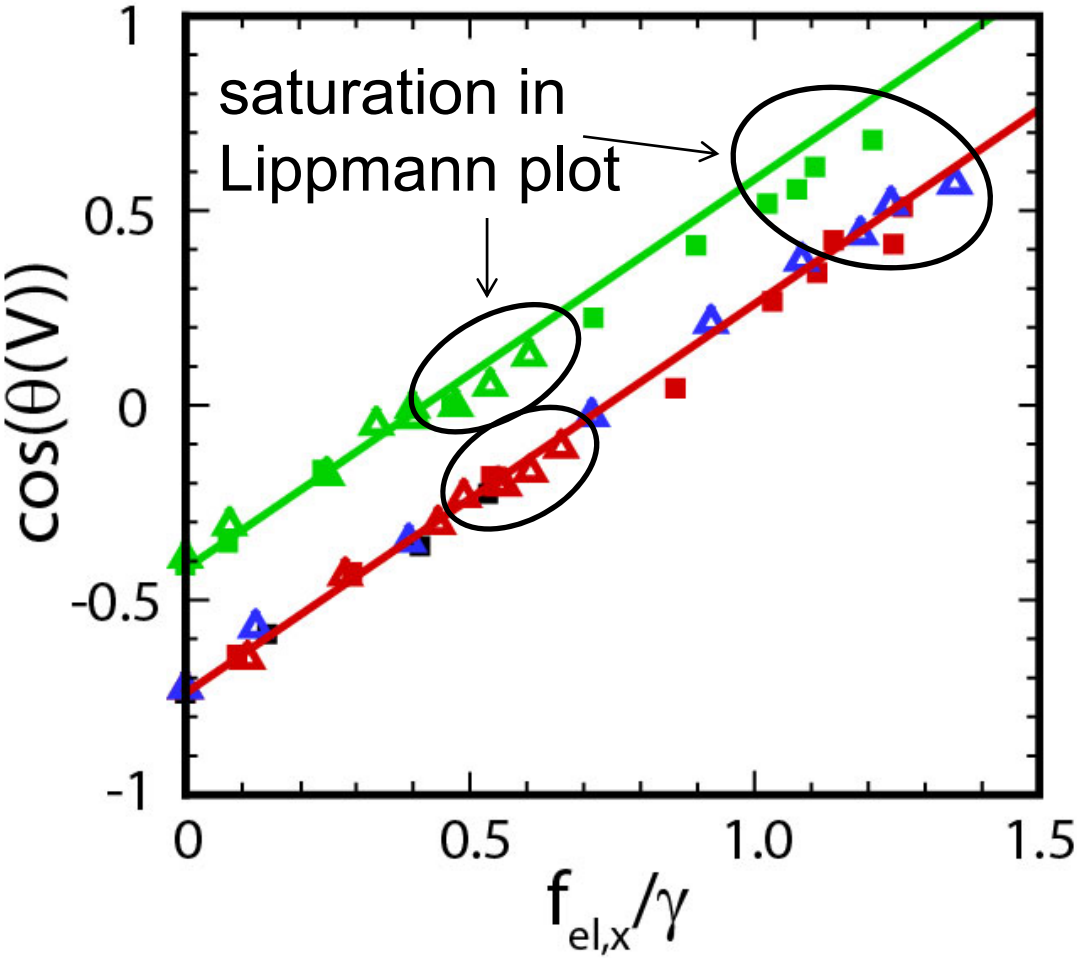


Net force must be zero $\rightarrow f_{el,x} = \gamma\,[\cos\theta - \cos\theta_0]$

Reduces to Lippman if fringing fields don't change
Then only change with position of edge is increase in area with energy $cV^2/2 \rightarrow f_{el,x}$

Choose region big enough to include most of electric field ~5σ
Bigger than interface width ~3σ → capture entire surface tension

Test of Force Balance Equation



Δ chain length 4
■ chain length 8

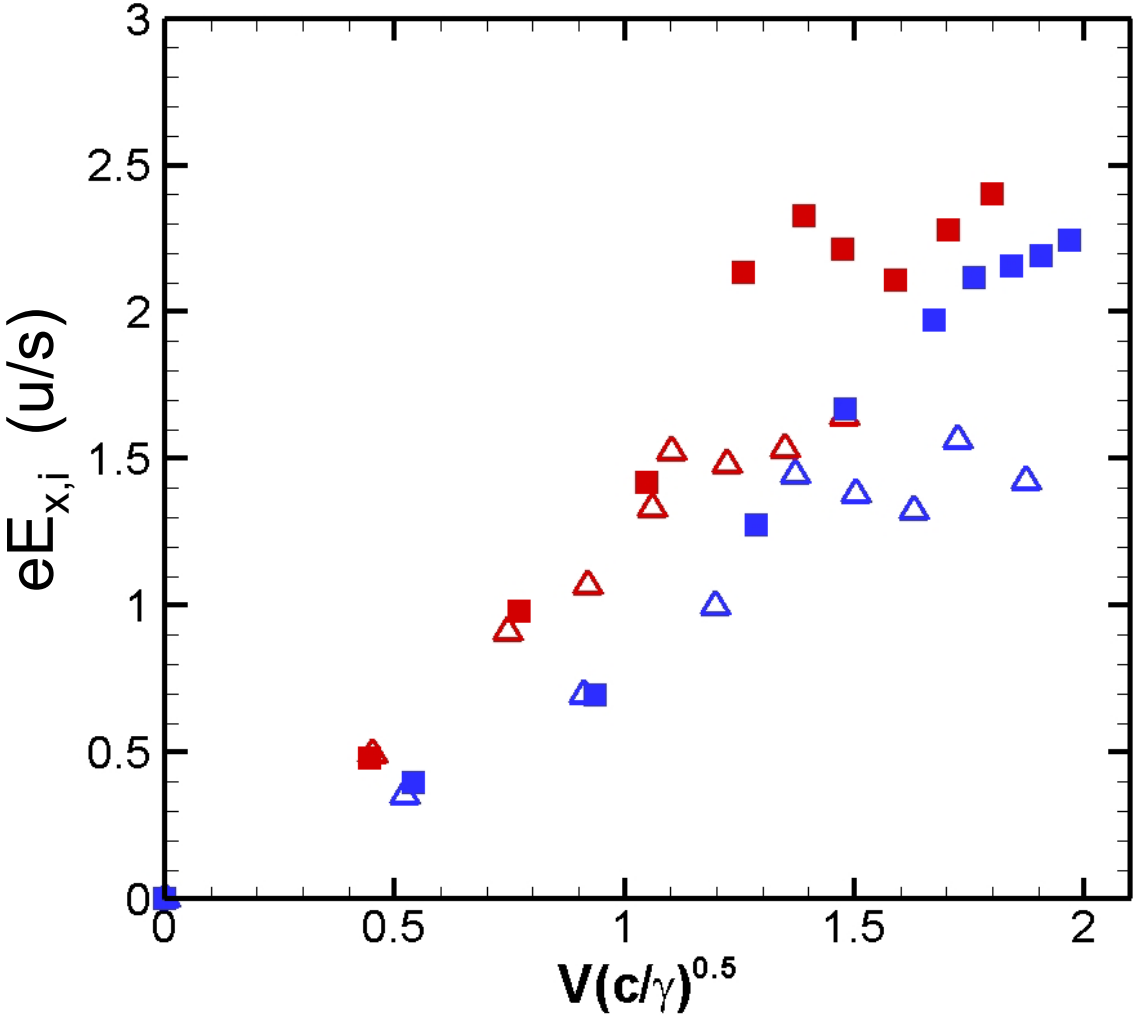
Green: diff. $\varepsilon_{sf} \rightarrow \theta_0$

Black $l_B=96\sigma$
Red $l_B=12.32\sigma$
Blue $l_B=4\sigma$

Lines assume bulk surface tensions.

Force balance holds at all voltages BUT $f_{el,x}$ saturates.
Saturation depends on chain length.
At high field molecules leave drop, screen field at drop edge

Maximum Force on Charges at Interface



Exp.: Saturation delayed for larger ions (Heikenfeld)
Saturation delayed for ac voltage (Ralston)

Δ chain length 4
■ chain length 8

Red $l_B=12.32\sigma$
Blue $l_B=4\sigma$

Lateral interfacial field $E_{x,i}$ rises at different rates for different l_B, D, …

Saturates at value that only depends on chain length
Constant in saturation region of electrowetting

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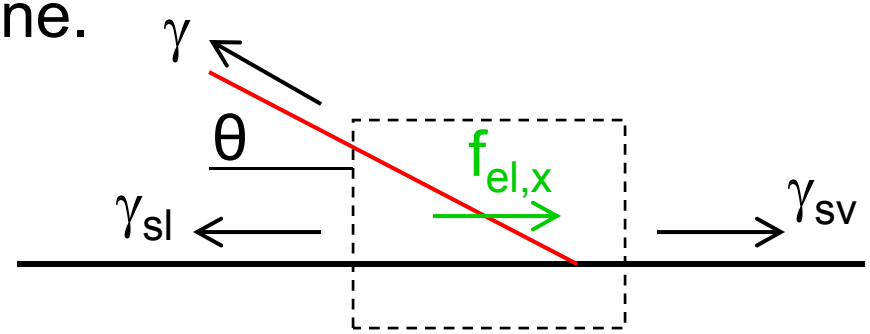


Net force must be zero $\rightarrow f_{el,x} = \gamma\,[\cos\theta - \cos\theta_0]$

Reduces to Lippman if fringing fields don't change

As region shrinks in size, $f_{el,x} \rightarrow 0$ and $\theta \rightarrow \theta_0$

although limited by finite width of interface

Electrowetting Conclusions

- Similar electrowetting in ~10nm and macroscopic drops
  $\rightarrow$ Can extend applications to nanoscales
- Lippmann equation fails as V increases, $\theta(V)$ saturates
- Lateral force balance obeyed even after saturation
  Negligible changes in γ's with V
- Saturation $\rightarrow$ molecules pulled from drop at $E_{x,l}$ that depends on molecular binding, size and not γ
  Screen fringing fields $f_{el,x}$ and limit increase in $\cos\theta$
- May control saturation by varying ionic binding

Linking Atomistic and Continuum Regions

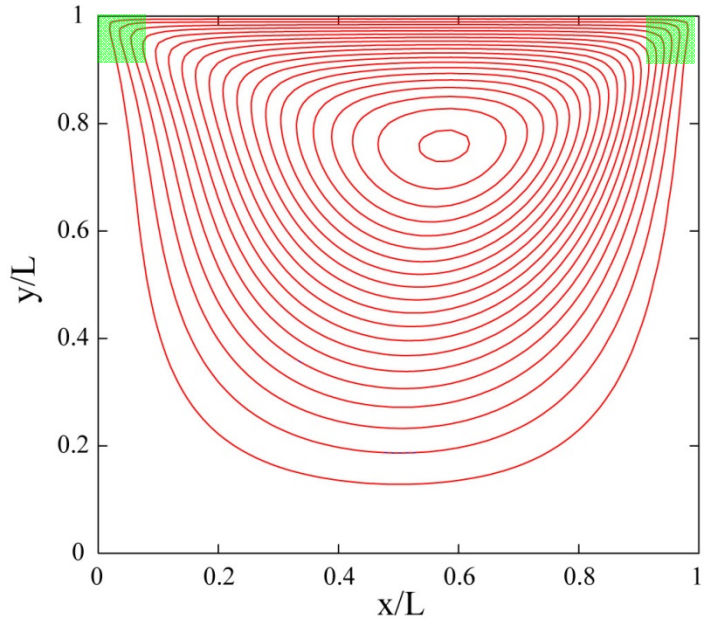
Three overlap regions where solve both continuum and MD

- Outermost → Continuum solution gives MD boundary condition
- Innermost → MD gives continuum boundary condition
- Middle → Two solutions equilibrate independently

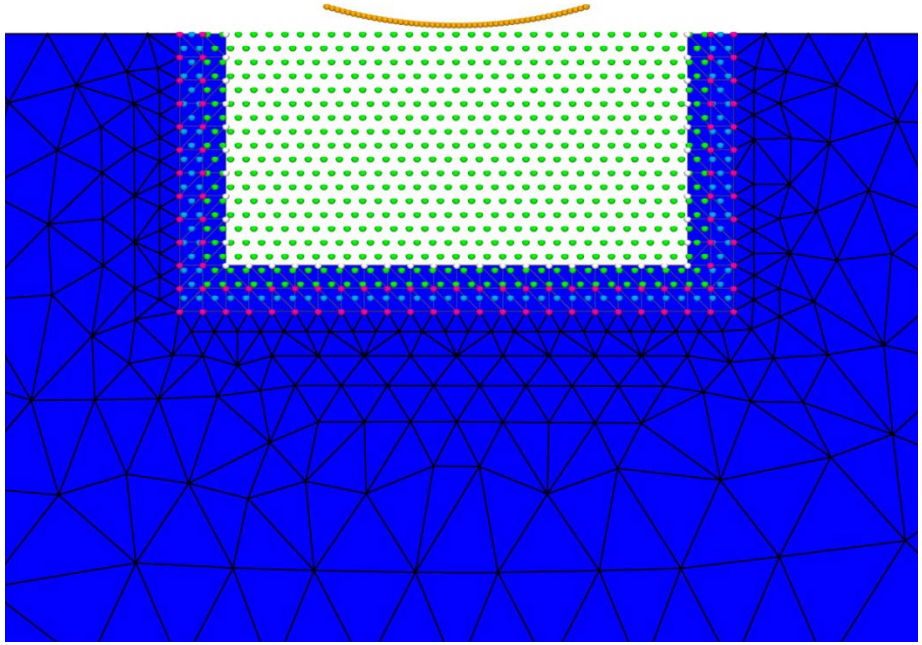
Fluids: Apply boundary conditions to velocities

Solids: Apply boundary conditions to displacements

Streamlines in L~0.3mm channel with moving top wall. Atomistic solution in <1% of area (green) removes continuum singularity



Model contact region atomistically, elastic deformations with finite-elements, constrain deformations in overlap region



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Fluids: Apply boundary conditions to velocities

Solids: Apply boundary conditions to displacements

Fluids: S. T. O'Connell & P. A. Thompson, Phys. Rev. E52, R5792, (1995)

Why not use forces instead of displacements/velocities?

E. G. Flekkoy, G. Wagner & J. Feder, Europhys. Lett. 52, 271 (2000)

Fluids – Position of boundary is undetermined

→ drifts in response to fluctuations or systematic errors

General – Any error in constitutive relation creates problems in overlap region

Less sensitive when match displacements

any global factor in stress is irrelevant

Fluid Continuum – Incompressible Navier-Stokes

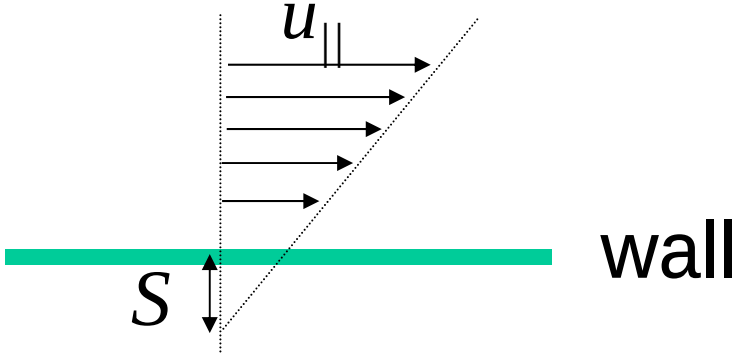
$$\partial_t \mathrm{u} + (\mathrm{u} \bullet \nabla \mathrm{u}) = -\frac{1}{\rho}[\nabla p + \mu \nabla^2 \mathrm{u}]$$

$$\nabla \bullet \mathrm{u} = 0$$

Navier slip boundary condition

$$\mathrm{u}_{\parallel}|_{\mathrm{w}} = \mathrm{S}\, \partial_{\perp} \mathrm{u}_{\parallel}|_{\mathrm{w}} \propto \text{stress}$$

Slip length



Knowledge of S, ρ and μ completely characterizes a simple fluid.

Atomistic Region → Molecular Dynamics

Truncated and shifted Lennard-Jones potential

$$V^{LJ}(r) = 4\epsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6} - \left(\frac{\sigma}{r_c}\right)^{12} + \left(\frac{\sigma}{r_c}\right)^{6}\right]$$

σ: Characteristic length, particle diameter.

ε: Characteristic energy.

$\tau \equiv (m\sigma^2/\varepsilon)^{1/2}$: Characteristic time of the potential.

r_c: Cut-off distance, usually 2.2σ for fluids

Integrate with velocity-Verlet, time step $\Delta t_{MD} = 0.005\tau$

Determine parameters for fluid continuum model:

Temperature $1.1\varepsilon/k_B$, density $\rho = 0.81 m\sigma^{-3}$, viscosity $\mu = 2.14\varepsilon\tau\sigma^{-3}$.

Wall (111) surface of fcc crystal

Wall-fluid interaction ε_{wf} controls flow boundary condition (BC)

$\varepsilon_{wf} = 0.95\varepsilon \rightarrow$ no-slip BC, S=0

Hybrid Algorithm Applied to Fluids

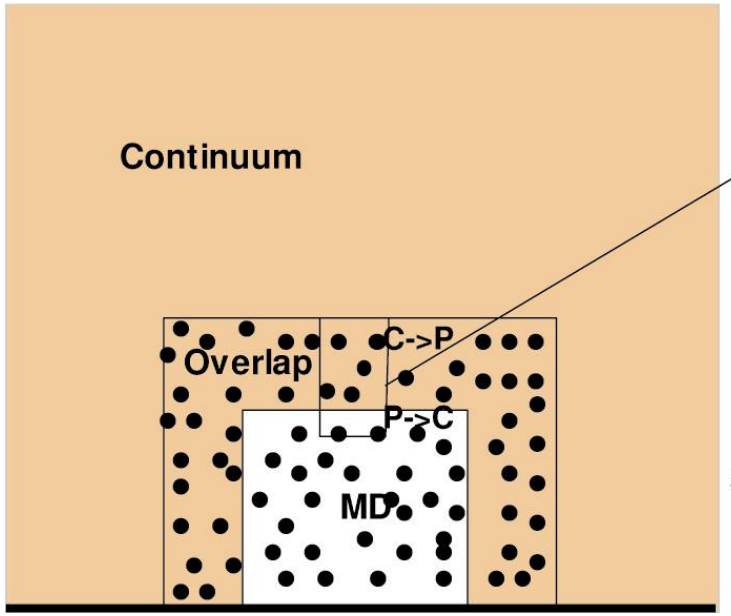
Continuum: Incompressible Navier-Stokes (Projection method)

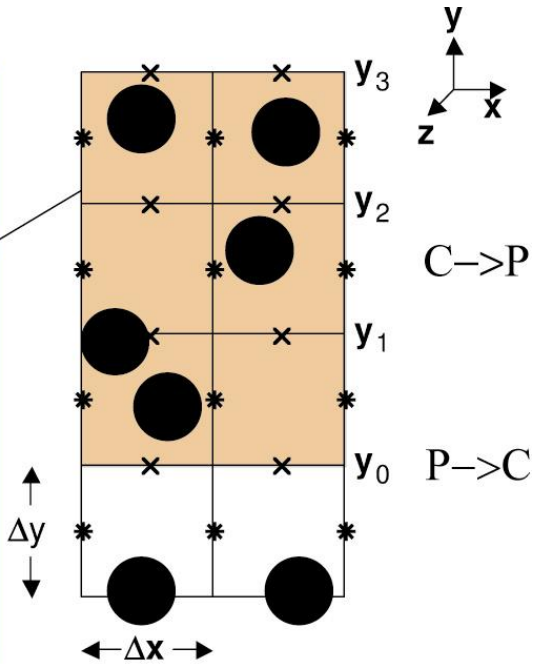
Atomistic: Molecular dynamics of Lennard-Jones atoms, no-slip

Potential: $U(r) = 4\varepsilon((\sigma/r)^{12} - (\sigma/r)^{6}]$; Units ε, σ

MD $\rightarrow$ Continuum $\quad u_J = \frac{1}{N_J}\sum_{i=1}^{N_J} v_i$

Continuum $\rightarrow$ MD $\quad \frac{1}{N_J}\sum_{i=1}^{N_J} v_i = u_J(t) \qquad m\ddot{x}_i = F_i - \frac{1}{N_J}\sum_{k=1}^{N_J} F_k + m\frac{Du_J}{Dt},$





$$F_i = -\frac{\partial}{\partial x}\sum_k V_{ik}^{LJ} \ .$$

Potential confines particles at y_3

Insert/remove number of particles equal to net flux

Equation of Motion for Constrained Particles

The equation of motion for the particle *i:*

$$\ddot{\mathbf{x}}_i = \frac{\mathbf{F}_i}{m} - \frac{1}{N_J m}\sum_{i=1}^{N_J}\mathbf{F}_i + \frac{D\mathbf{u}_J(t)}{Dt}, \quad \mathbf{F}_i = -\frac{\partial}{\partial \mathbf{x}_i}\sum_j \mathrm{V}_{ij}^{\mathrm{LJ}}$$

Finite Difference Scheme for the equation of motion:

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

$$\frac{\mathbf{F}_i}{m} - \frac{1}{N_J m}\sum_{i=1}^{N_J}\mathbf{F}_i - \frac{1}{\Delta t_{MD}}\left(\frac{1}{N_J}\sum_{i=1}^{N_J}\mathbf{v}_i(t) - \mathbf{u}_J(t)\right)$$

$\Delta t_{FD} = 40\Delta t_{MD} \rightarrow$ Staggered time grid

Average MD over Δt_{FD} to fix continuum boundary

Extrapolate continuum to integrate next MD interval

Particle Confinement and Mass Flux

External force *F* for $y_2 \le y \le y_3$

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

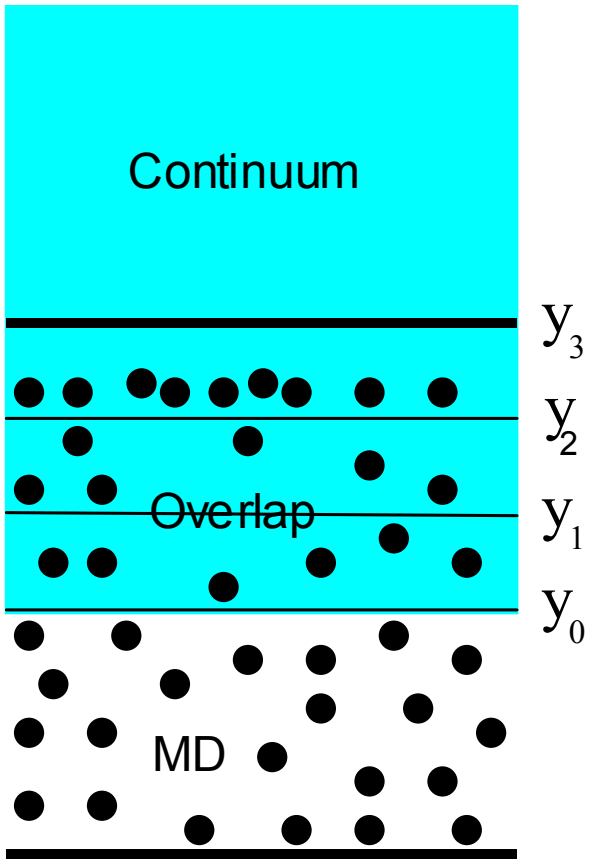
Maintain a mass flux by introducing particles *n(x,t)* near $y = y_2$

$$mn(x,t) = -A\rho u_y(x, y_2, t)\Delta t_{MD}$$

Langevin thermostat for $y_2 < y < y_3$:

$$m\ddot{y}_i = \sum_{j \neq i} \frac{\partial V^{LJ}(r_{ij})}{\partial x_i} - m\Gamma \dot{y}_i + \zeta_i$$

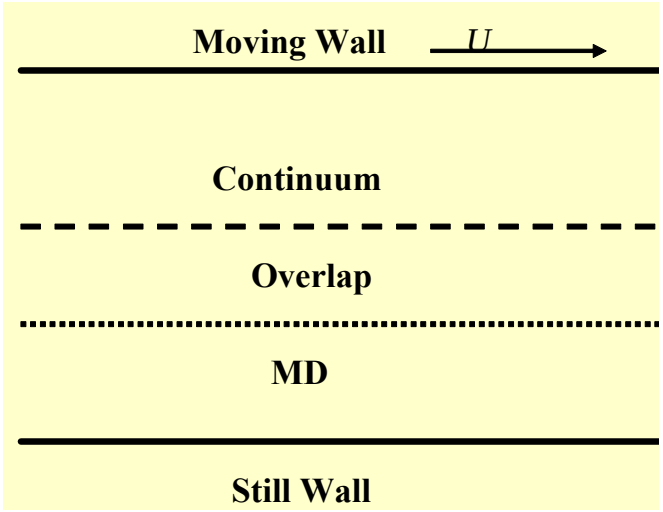
$$\left\langle \zeta_i(t)\zeta_j(t') \right\rangle = \delta_{ij}\delta(t - t')2k_B T\Gamma$$



Werder et al. J. Comp. Phys. 205, 373 (2005)
claim artifacts, but use different implementation

Dynamic Couette Flow

Schematic of simulation

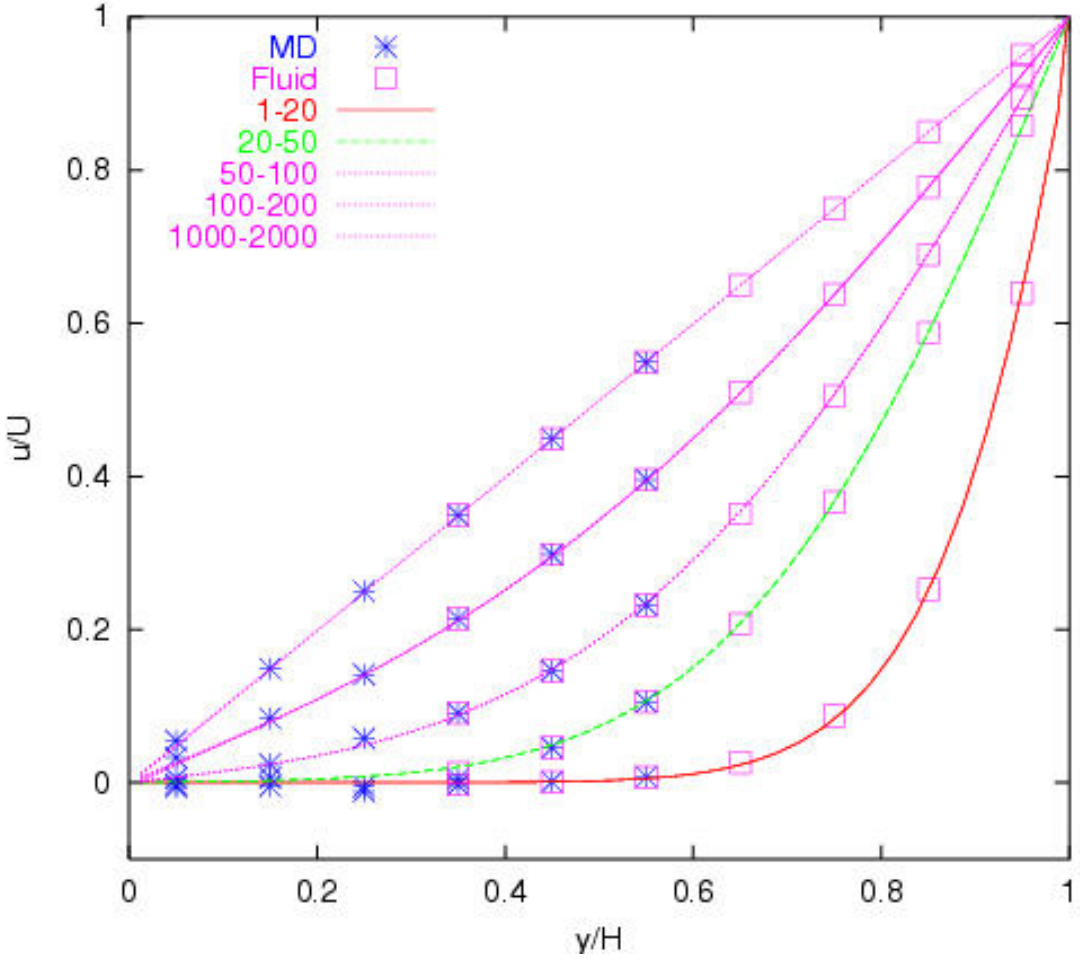


$\Delta t_{FE} = 40 \Delta t_{MD}$

Use 10 realizations of MD, 1 continuum

X. B. Nie, S. Y. Chen, W. N. E and M. O. Robbins, J. Fluid Mech. 2004.

Hybrid solution (symbols) tracks full continuum (lines) as a function of time after motion starts

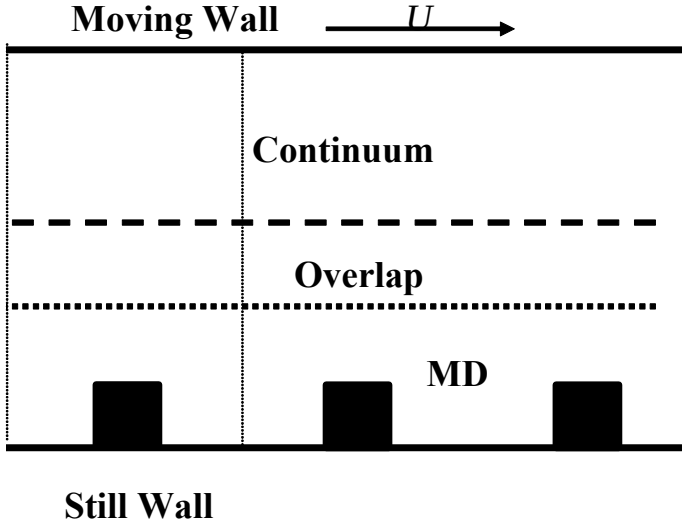


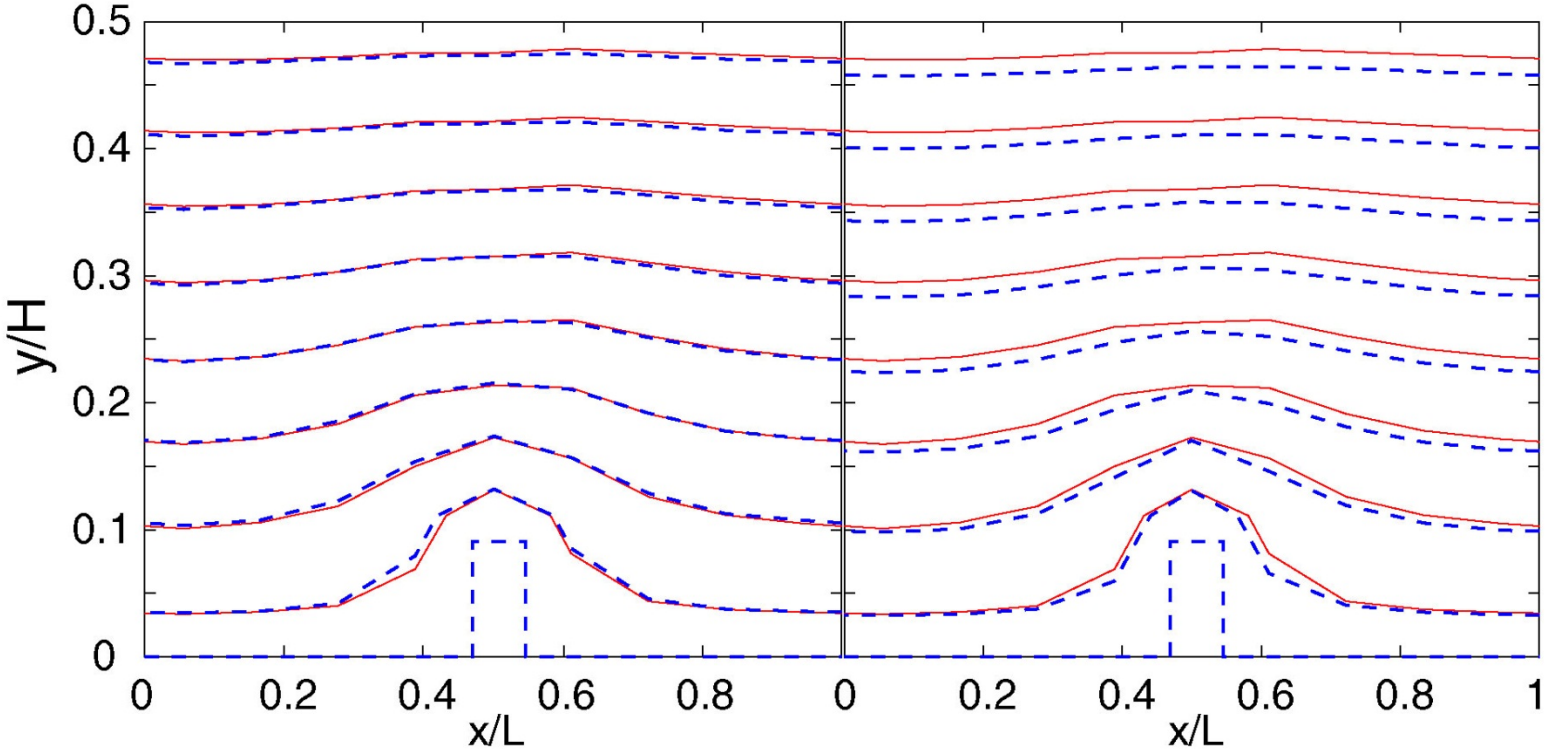
Flow past a rough wall

Streamlines from hybrid ≈ MD

includes flow between regions

Continuum fails because doesn't match complex boundary condition around bump





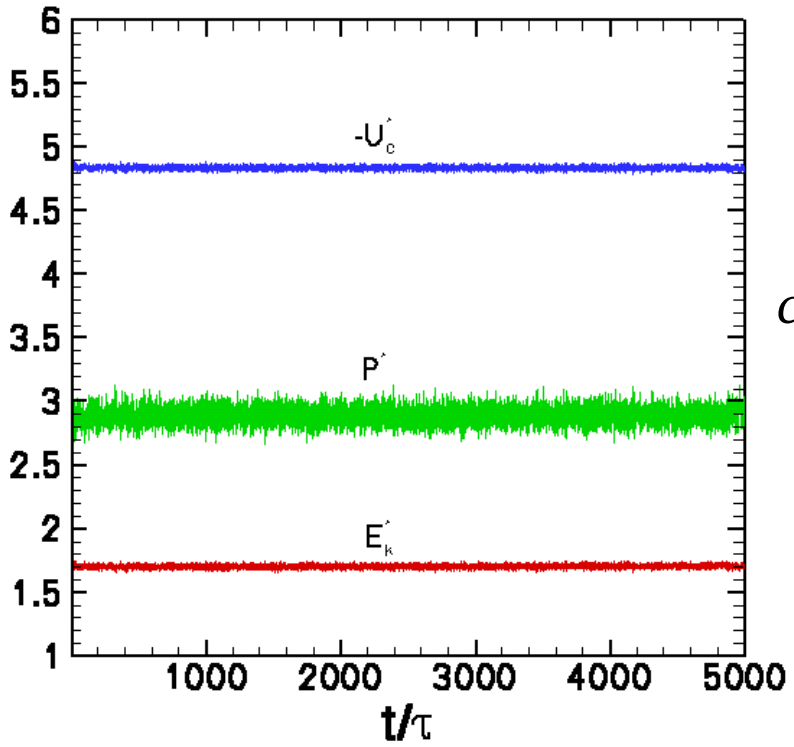
Hybrid vs. MD Hybrid vs. Continuum

Including Heat Flux

$$\nabla \cdot \mathbf{u} = 0$$

$$\rho\left(\partial_t \mathbf{u} + \mathbf{u}\cdot\nabla\mathbf{u}\right) = -\nabla p + \mu\nabla^2\mathbf{u}$$

$$\rho c_V\left(\frac{\partial T}{\partial t} + \vec{u}\cdot\nabla T\right) = \lambda\nabla^2 T + \mu\left[2\left(\frac{\partial u_x}{\partial x}\right)^2 + 2\left(\frac{\partial u_y}{\partial y}\right)^2 + \left(\frac{\partial u_x}{\partial y} + \frac{\partial u_y}{\partial x}\right)^2\right]$$



Heat capacity c_V, for incompressible fluid

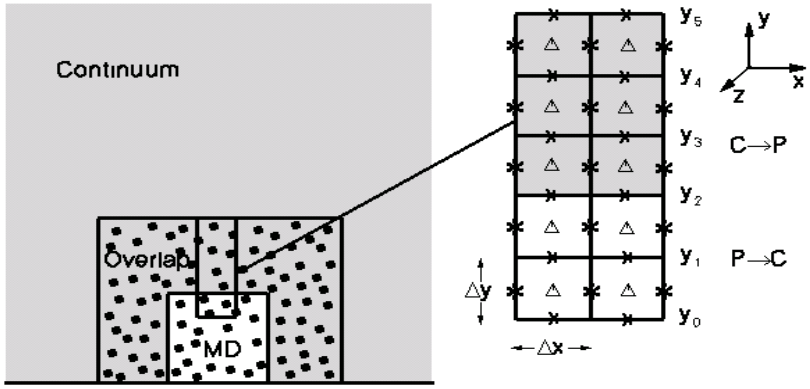
$$c_V = \frac{3k_B}{2m}\left[1 - \frac{2}{3N(k_B T)^2}\left\langle\left(\delta E_k\right)^2\right\rangle\right]^{-1} = 2.43\frac{k_B}{m}$$

Coupling Scheme: Momentum and Energy

MD→Continuum :

$$\frac{1}{N_J}\sum_i \mathbf{v}_i = \mathbf{u}_{J,MD}(t)$$

$$\rightarrow \quad \frac{1}{N_J - 1}\sum_i \frac{1}{2} m(\mathbf{v}_i - \mathbf{u}_{J,MD})^2 = T_{J,MD}(t)$$



Continuum→MD (Constraint Dynamics and velocity rescaling):

$$\begin{cases} \dfrac{1}{N_J}\sum_i \mathbf{v}_i = \mathbf{u}_{J,C}(t) & \ddot{\mathbf{x}}_i = \dfrac{D\mathbf{u}_{J,C}(t)}{Dt} + \varsigma_i & \sum_i \varsigma_i = 0 \\ \varsigma_i = \dfrac{\mathbf{F}_i}{m} - \dfrac{1}{N_J m}\sum_{i=1}^{N_J} \mathbf{F}_i & \mathbf{F}_i = -\dfrac{\partial}{\partial x_i}\sum_{j\neq i} V^{LJ}(r_{ij}) & \\ \ddot{\mathbf{x}}_i = \dfrac{\mathbf{F}_i}{m} - \dfrac{1}{N_J m}\sum_{i=1}^{N_J} \mathbf{F}_i + \dfrac{D\mathbf{u}_{J,C}(t)}{Dt} & & \end{cases}$$

X. Nie et al. *JFM* ***500***, *55-64 (2004)*

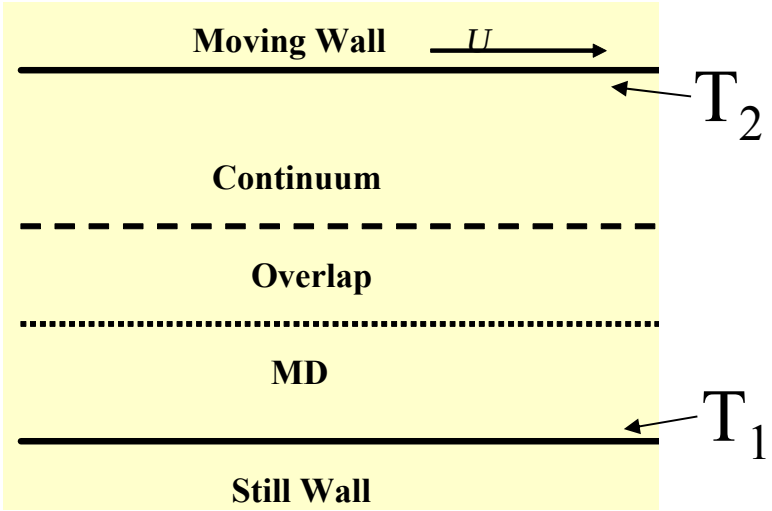
$$\rightarrow \quad \mathbf{v}_i - \mathbf{u}_{J,MD} = \sqrt{\frac{T_{J,C}}{T_{J,MD}}} \times (\mathbf{v}_i - \mathbf{u}_{J,MD})$$

J. Liu, S. Chen, X. Nie, and M. O. Robbins, J Comp. Phys. (2007)

Mass flux across the interface :

$$n' = -A\rho u_y \Delta t_{FD} / m$$

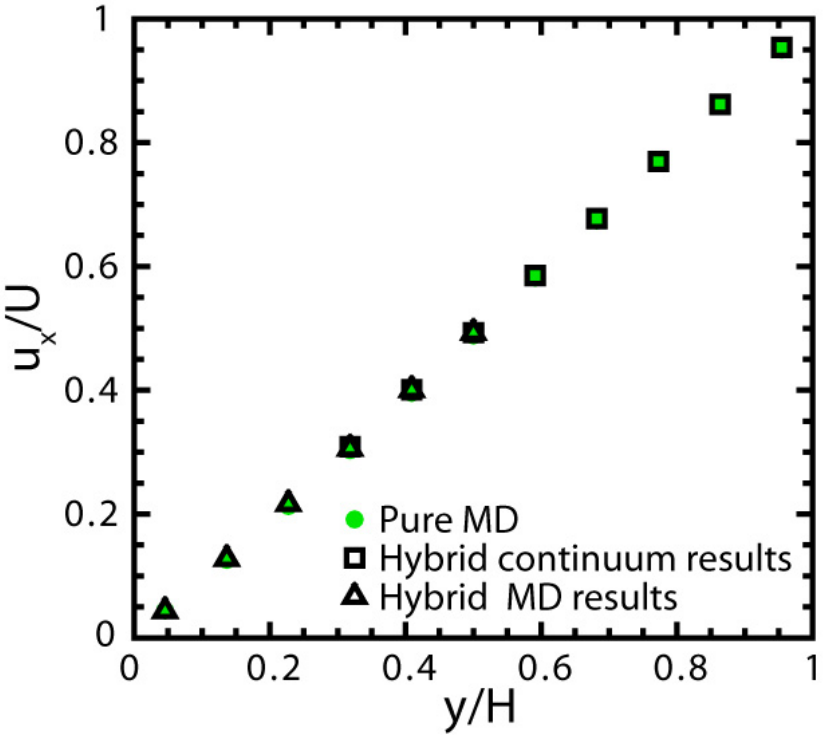
Temperature in Steady State Couette Flow

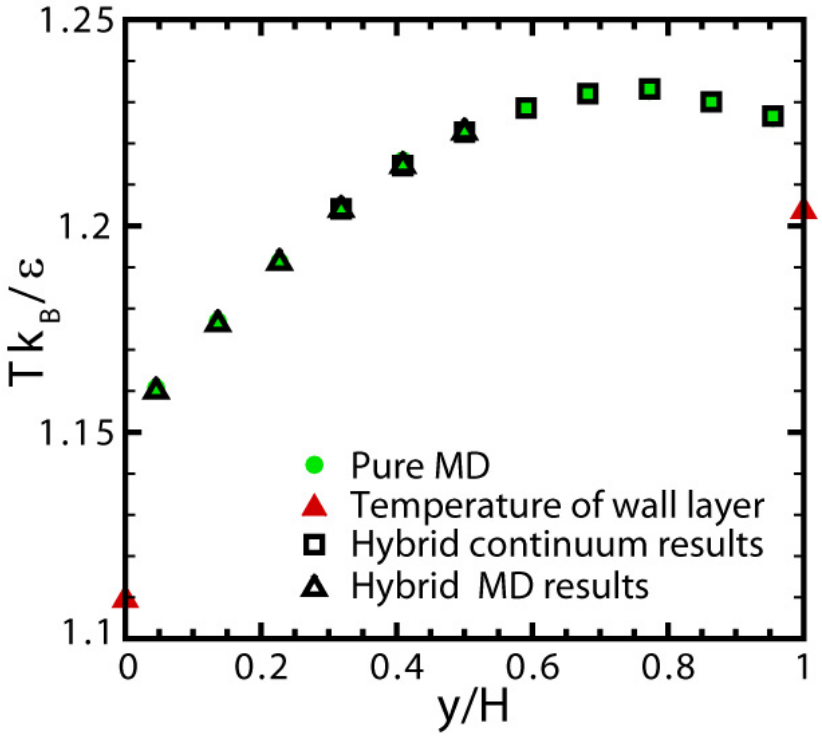


At boundaries of overlap region:
rms MD veloc. ⇔ continuum T

Hybrid solution tracks pure MD

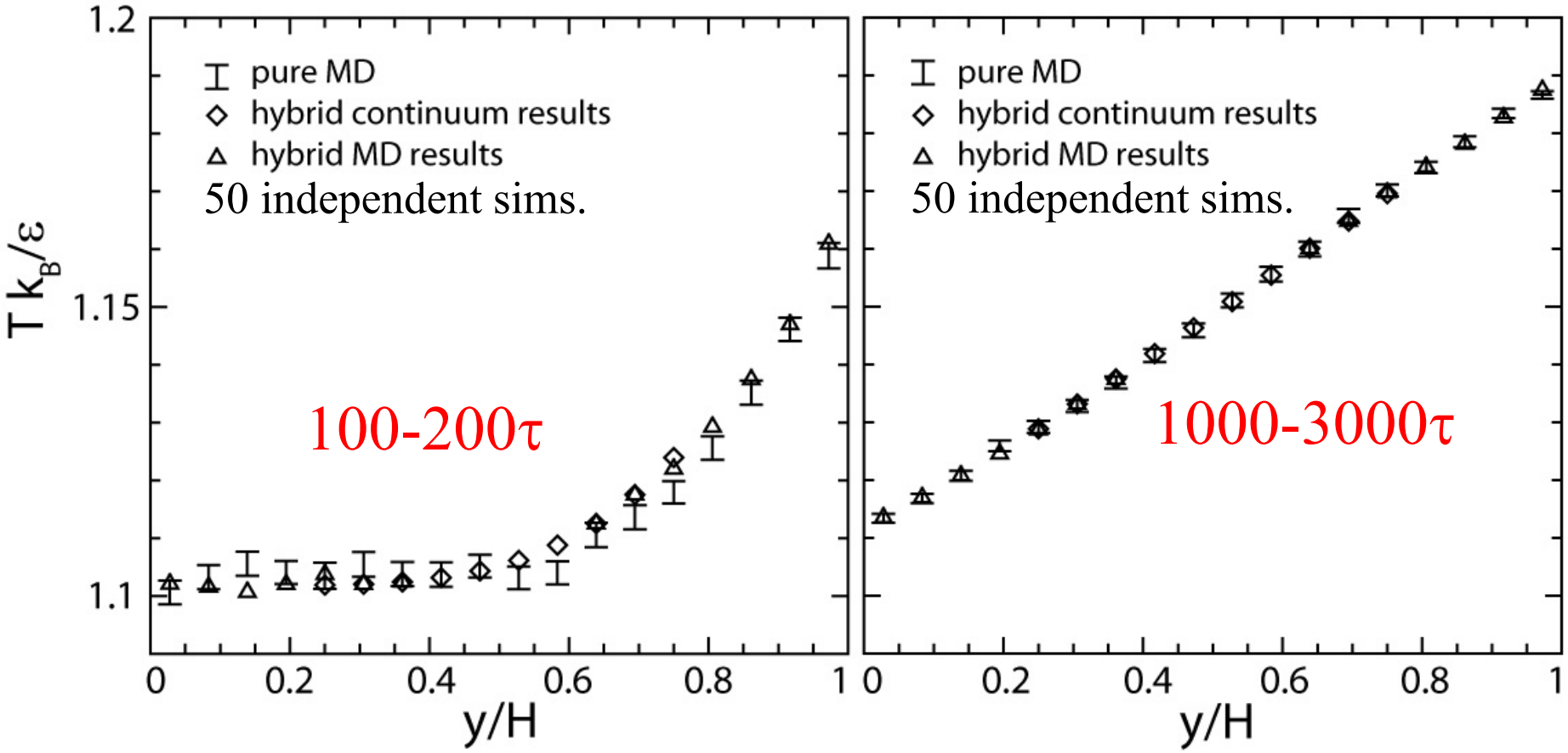
Reproduces behavior in fluid and Kapitza resistance at solid-fluid interface





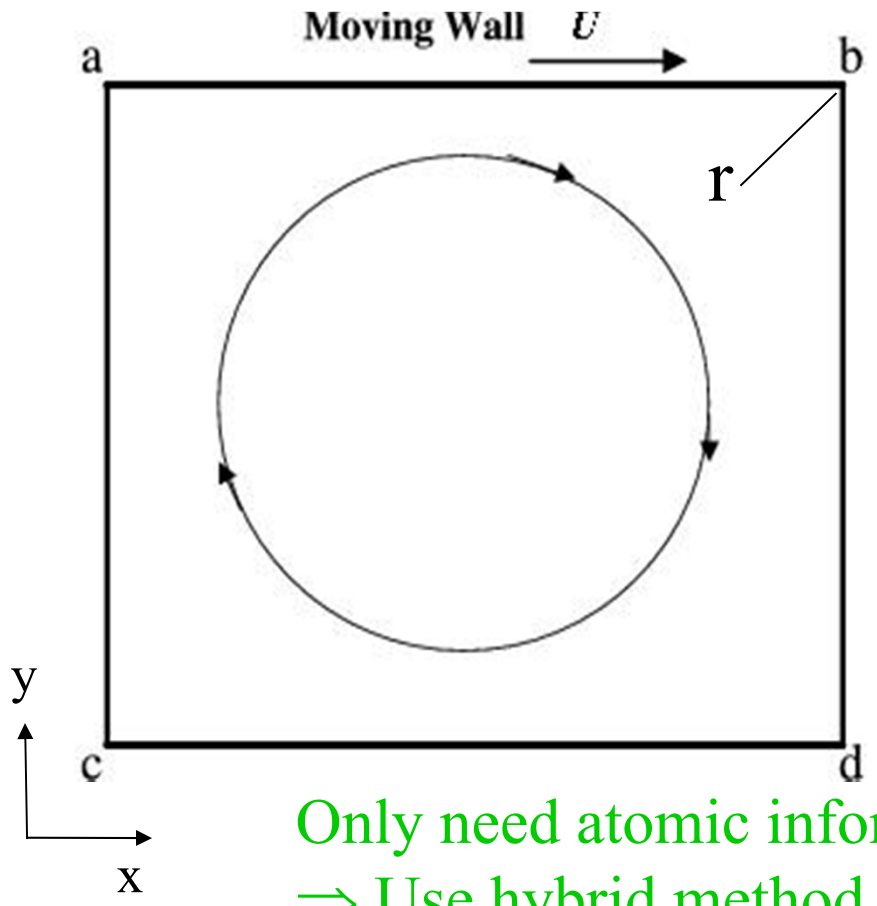
Unsteady Temperature Profiles

Increase T of top wall to 1.2 at t=0 follow evolution of T
Hybrid agrees with pure MD
Hybrid has smaller statistical fluctuations since thermal noise only in MD region. Ave. before coupling to cont.



Singular Cavity Flow

Continuum approach: Navier-Stokes + no-slip boundary condition (bc)
Usually phenomenological no-slip bc has little effect at large scales



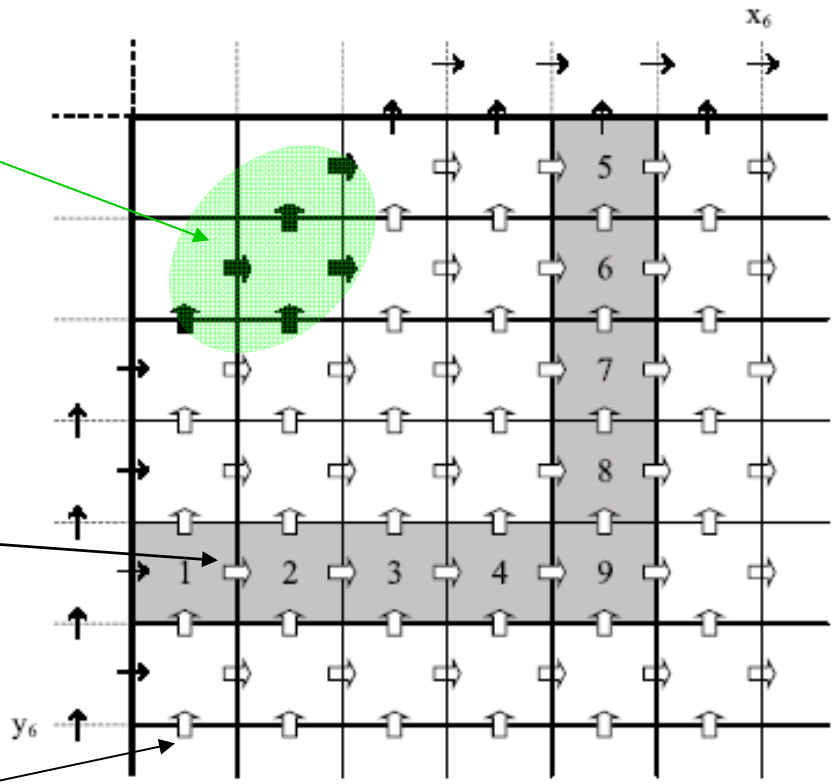
Corner flow ⇒Molecular scale influences macroscopic forces

No-slip boundary condition is discontinuous at corners a, b
⇒Stress diverges as 1/r
⇒Log divergence in total force on wall

Only need atomic information near corners
⇒ Use hybrid method that treats bulk with continuum Navier-Stokes equations, corners with MD

Coupling in Overlap Region

MD ⇒ Navier Stokes
Mean atomic velocity gives boundary condition to NS eqs.



Continuum ⇒ MD

1) Average tangential MD velocity in shadowed bins forced to NS value:

$$\ddot{x}_i = \frac{F_i}{m} - \frac{1}{mN_J}\sum_{j=1}^{N_J} F_j + \frac{Du_J}{Dt}, F_j = -\frac{\partial}{\partial x}\sum_k V_{jk}^{LJ}$$

2) Normal MD velocity constrained by matching mass flux at boundary

Have tested:
Agrees with pure MD calculations.
Independent of continuum grid 1, 3 and 6σ and specific set of constrained velocities (within MD noise)

X.B. Nie, S.Y. Chen and M. R. Robbins, Physics of Fluids **16**, 3579 2004.

Treating Large Range of Length Scales

Problem: Size of atomistic region independent of system size L

BUT time to equilibrate NS flow field grows with L**.**

Explicit dynamics approach limited to L~0.1μm.

Solution: Multigrid and time approach

Integrate to steady state at each scale with optimum time step.

Iterate between scales till self-consistent (~10 times).

Result: Size limited only by onset of non-steady, turbulent flow

Show results for 0.3mm cavities.

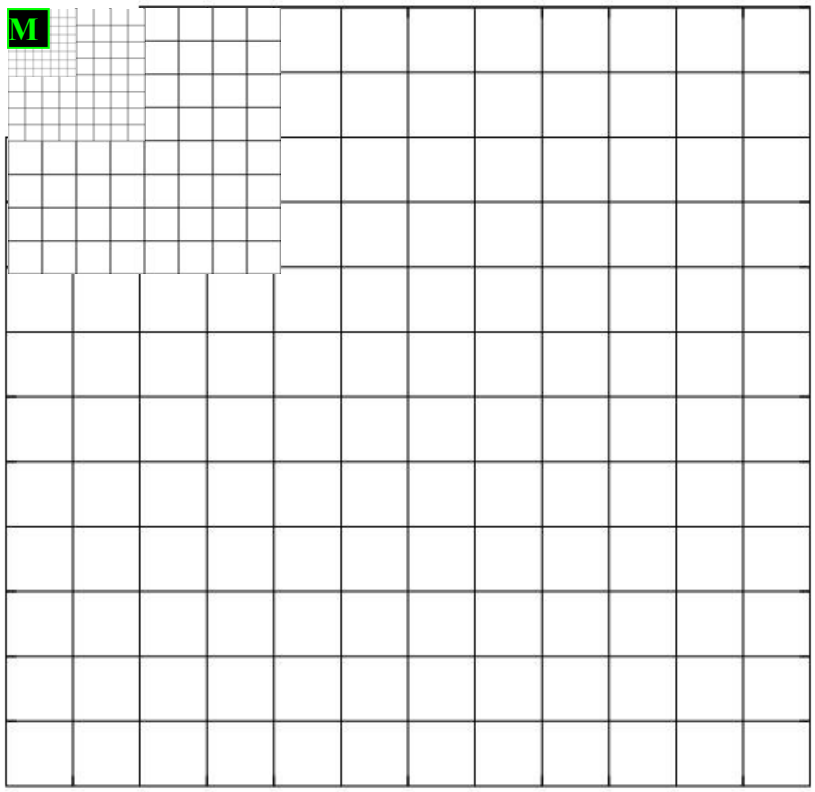
> 10 orders of magnitude faster than fully atomistic

~ 20 minutes per iteration

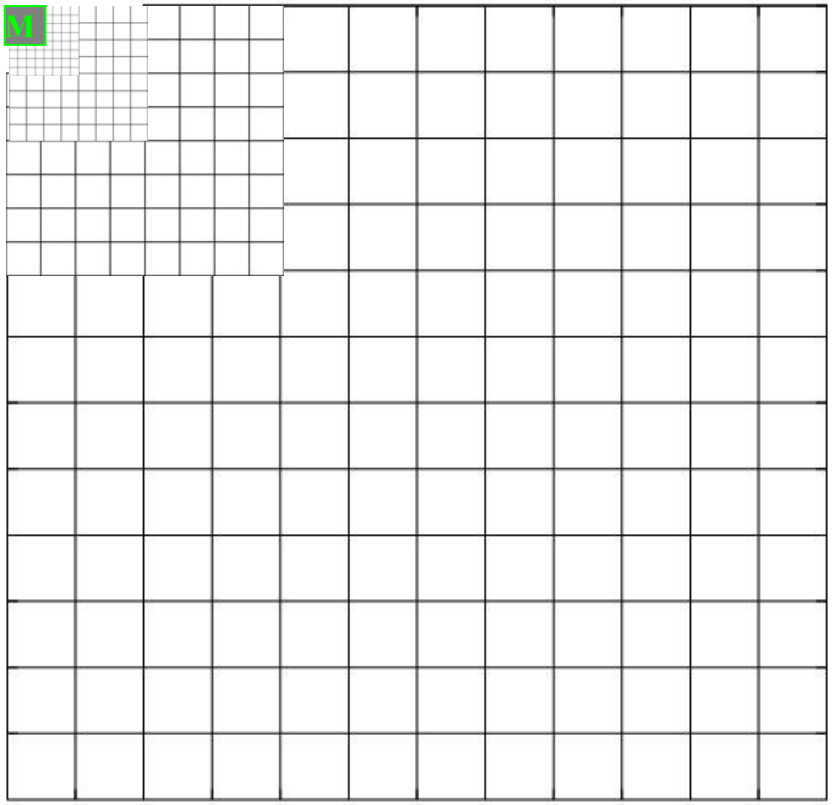
Use average over 16 MD representations to accelerate

Schematic of Local Refinement

Coarse ->Fine: Prolongation.

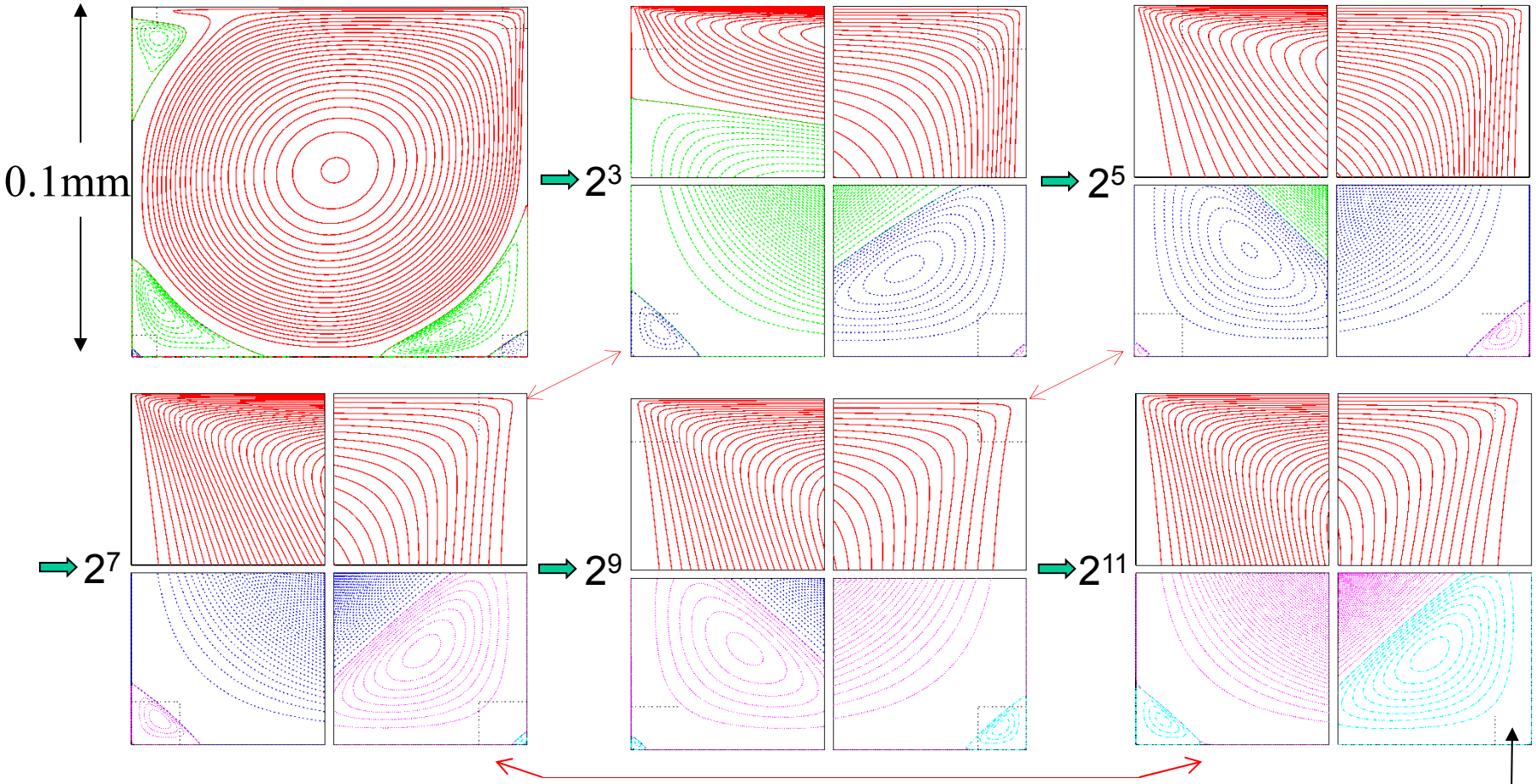


Fine->Coarse: Restriction.



Flow at each scale reaches steady state at its own characteristic time (Phys. Rev. Lett. **96** 134501 (2006))

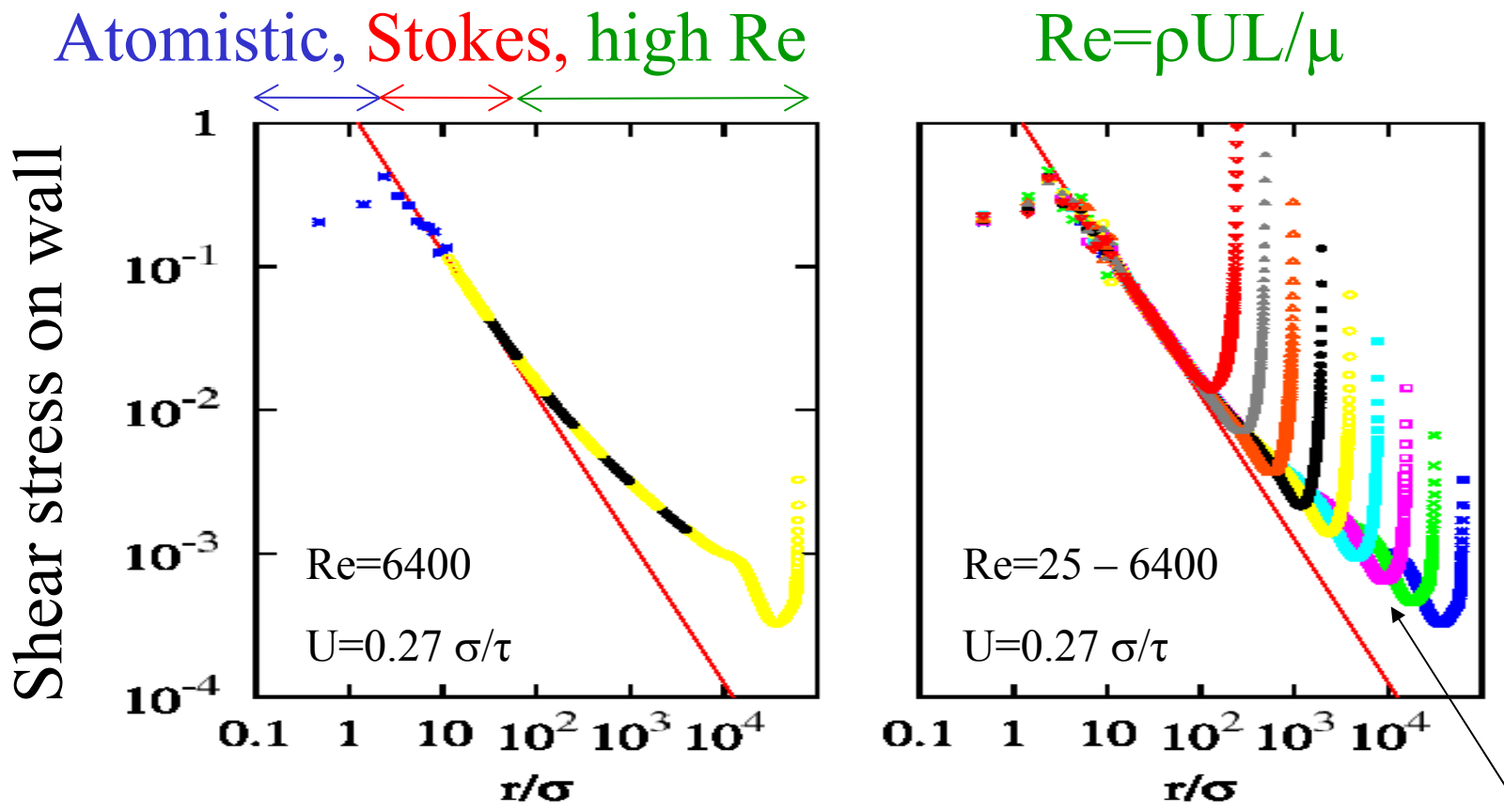
Multiscale Solution for Re=6400 ($U=0.068\sigma/\tau$)



- Ten grid levels, largest 256x256, others 64x64, smallest mesh 0.95σ
- Dashed lines: the regions expanded in successive plots. Final plot → MD region
- Stokes equations→ bottom corners self-similar under mag. by ~16 (red arrows) This scaling is cut off by atomic structure.
- Computational time saving more than 10^{10} over fully atomistic.

Stress along the moving wall

Three regions contribute to force F:



Breakdown of Stokes for r<S – atomistic or r>$R_I \equiv \mu/\rho U$ – inertial

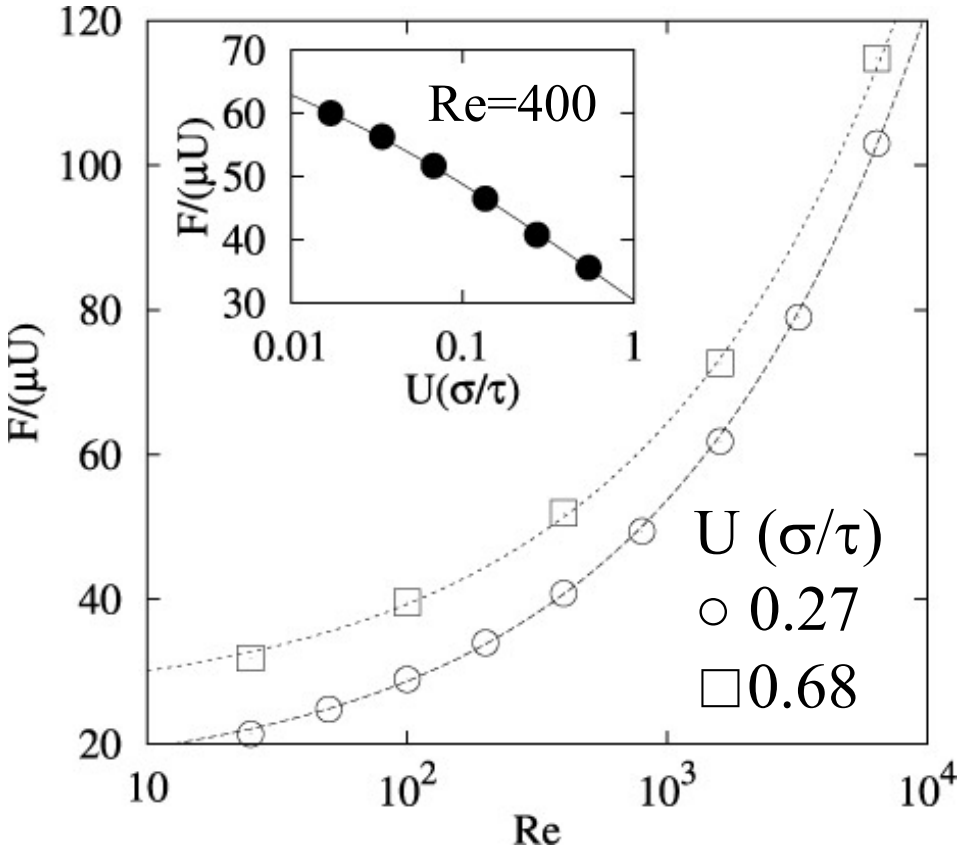
Little change for r < R_I as increase Re by increasing L

Large r contribution gives change in F for fixed U, atomic props.

Total Force on the Moving Wall

Re - only parameter in continuum theory

Find strong variation with U at fixed Re, atomic model



$$\frac{F}{\mu U} = f_S + f_{Stokes} + f_{\mathrm{Re}}$$

$r<S$ $S<r<R_I$ $R_I<r$

$$f_S = 4.3$$

$$f_{Stokes} = \frac{8\pi}{\pi^2 - 4}\ln(R_I / S)$$

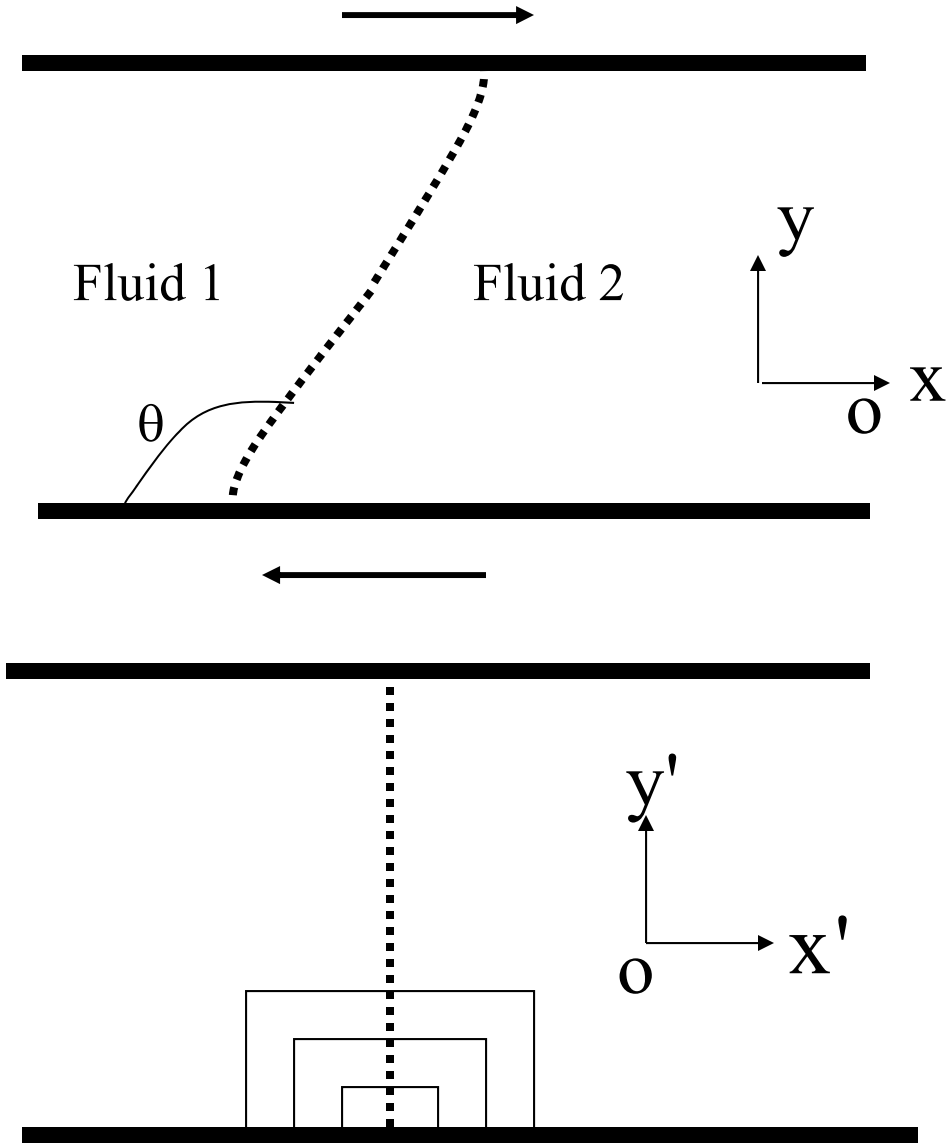
$$f_{\mathrm{Re}} = 3.85 + 1.98\mathrm{Re}^{0.434}$$

f_S given by assumption that stress saturates at S

$S= 0.3+ 7Ut_{LJ}$; f_{Re} is phenomenological fit

Similar Singularity at Moving Contact-Line

AND must solve for interface shape self-consistently



Transformation:

Interface : $x_s = f(t, y_s)$

Transformation :

$x' = x - f(t, y)$

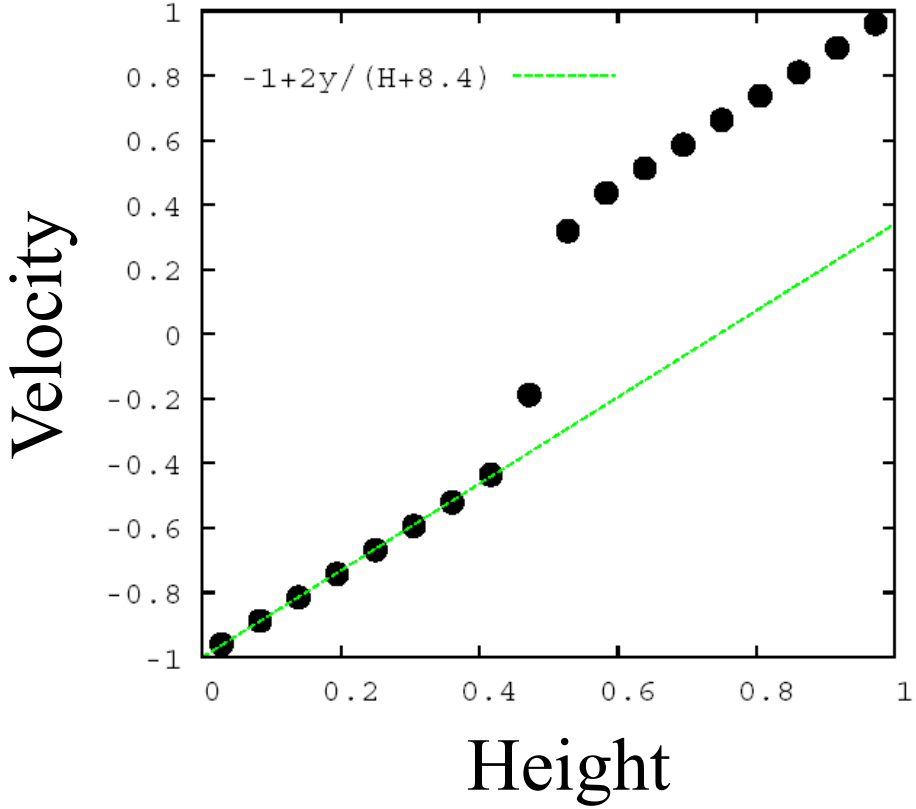
$y' = y$

Find Slip at Fluid-Fluid Interface

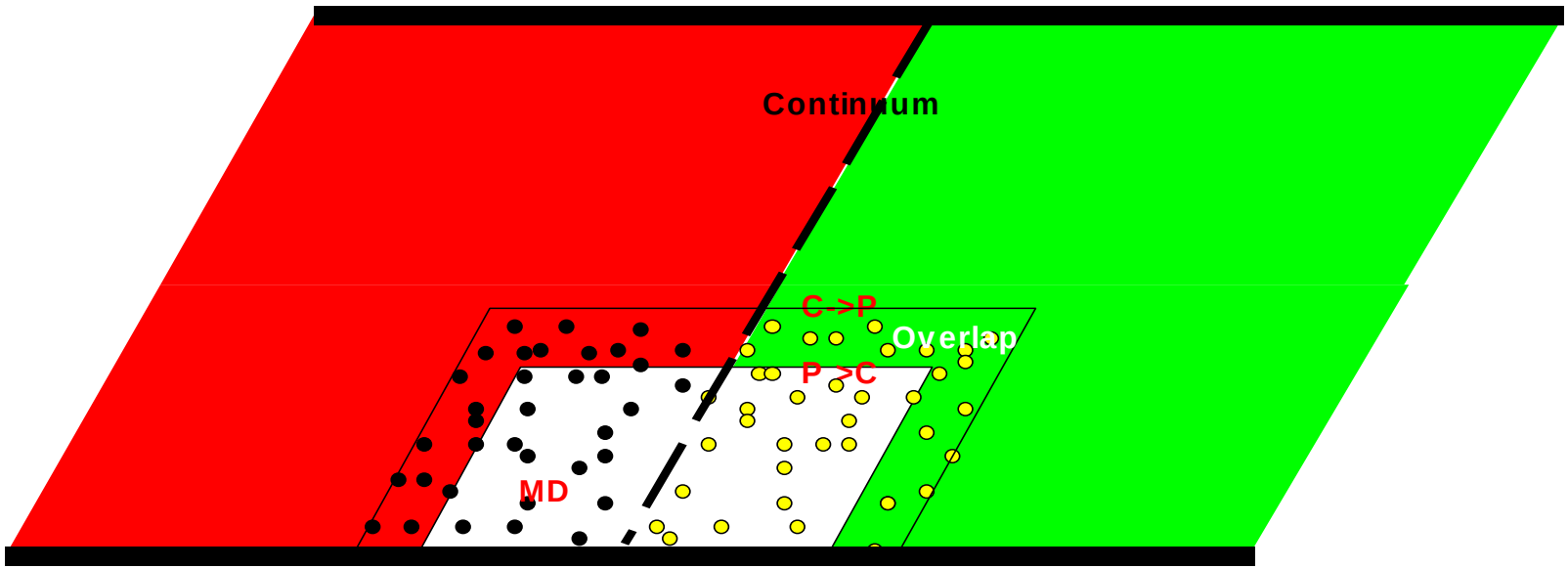
Choose wall-fluid coupling so no-slip far from contact line

BUT slip at fluid-fluid interface

Must build this into continuum model



Hybrid Scheme for Two Phase Flow: P->C



P->C:

1. Average particle velocity to give continuum u
2. Determine the interface direction in the overlap from MD and constrain continuum interface

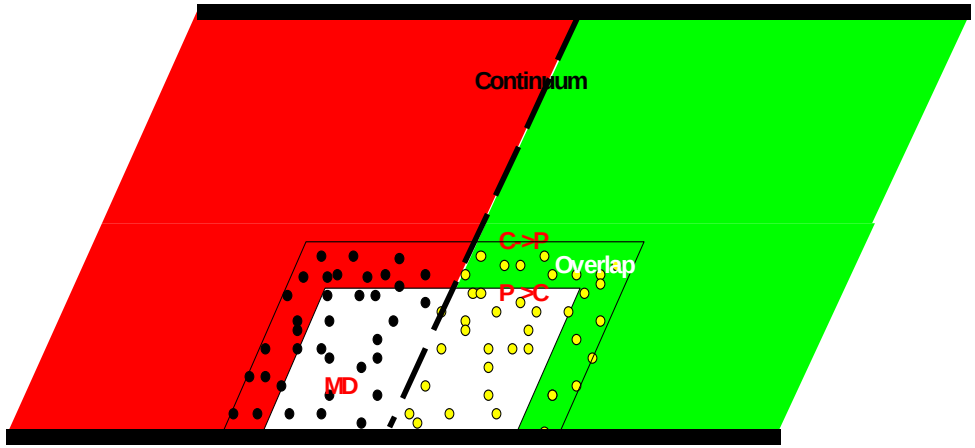
Hybrid Scheme for Two Phase Flow: C->P

C->P:

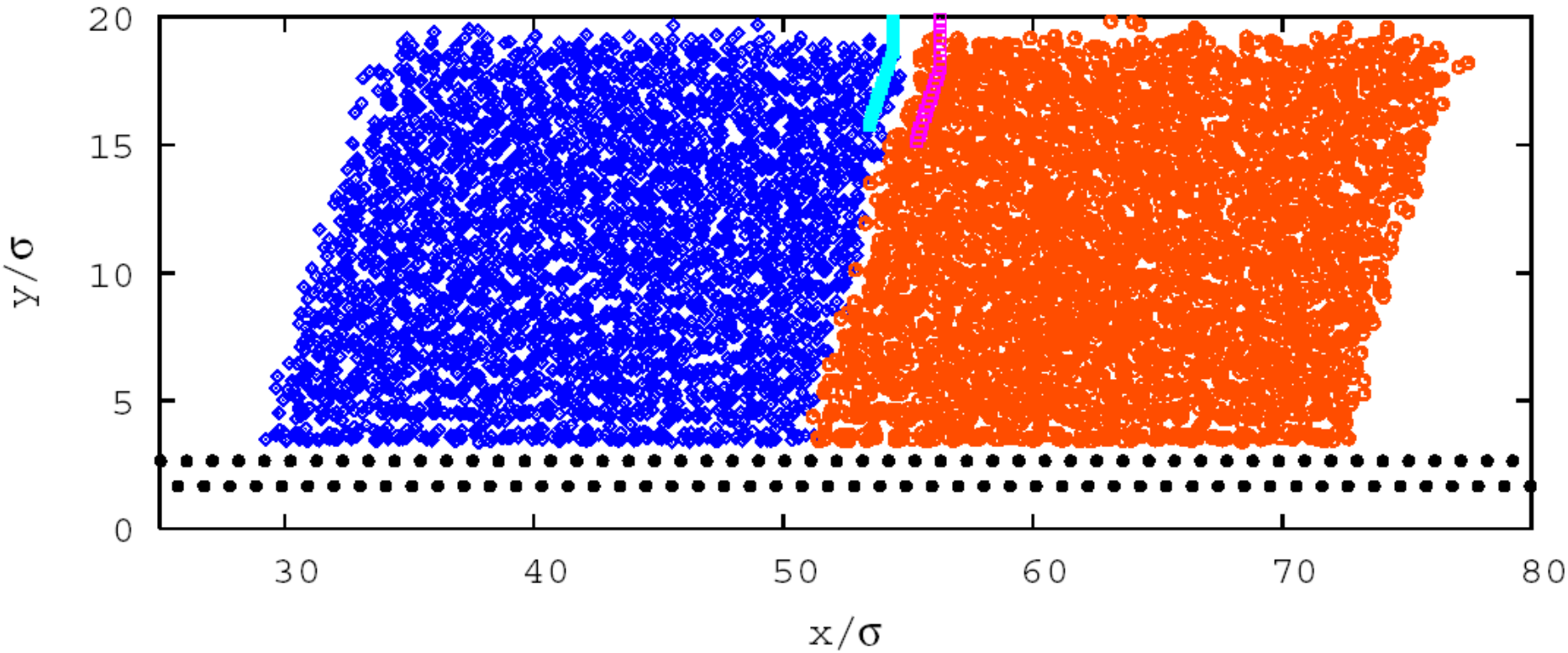
1) Constrain velocities and mass flux as above

2) Force the interface to follow continuum interface equation by putting a membrane in the overlap region.

3) Solve flow for given boundary and iterate until self-consistent

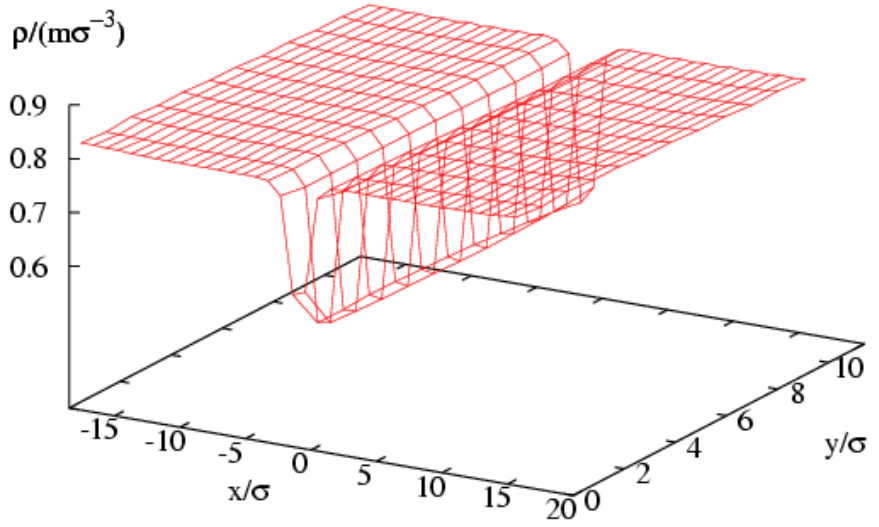


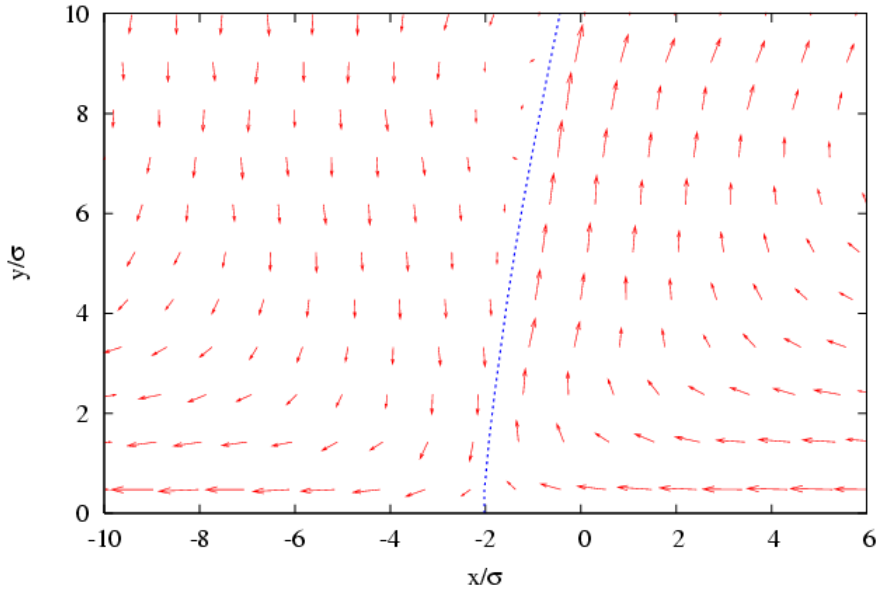
Procedure to reach steady state in MD

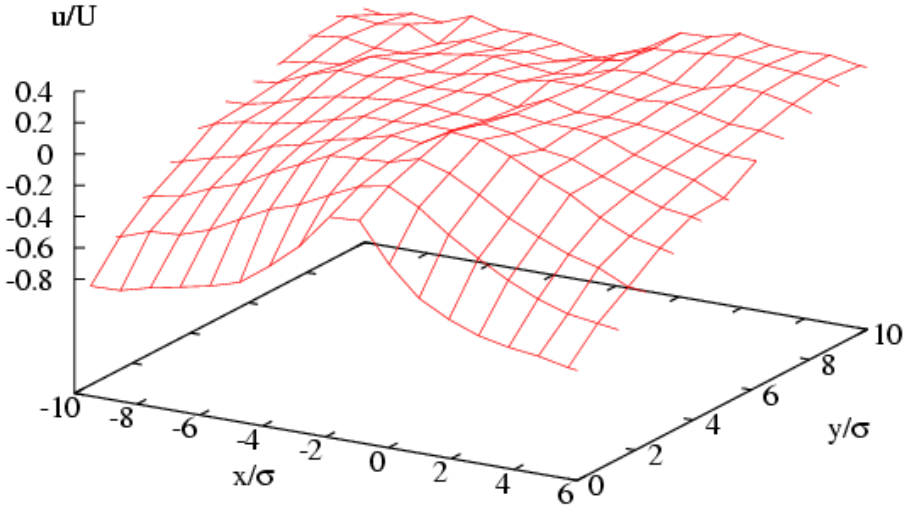


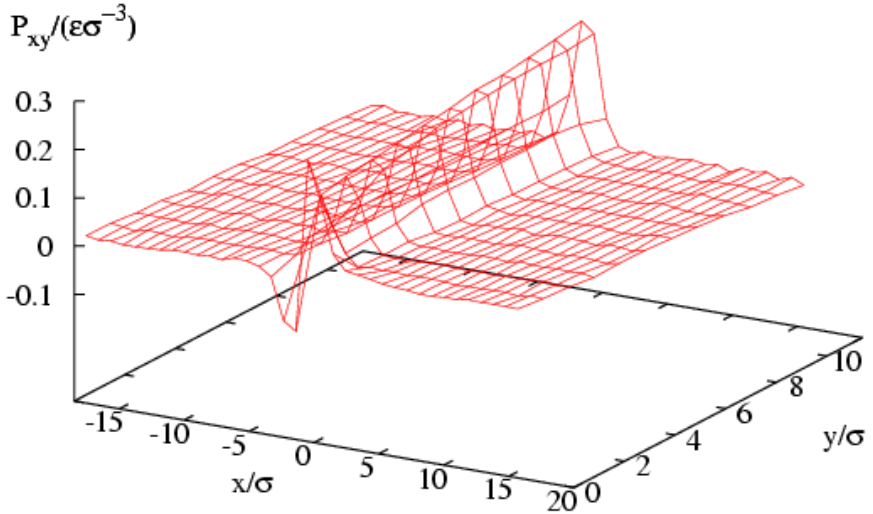
- Fix the boundary shape to let the system reach steady state.
- Correct the boundary shape according to the new interface and then repeat the last step until the boundary and the interface shapes are consistent.

Typical Results Near A Contact-line

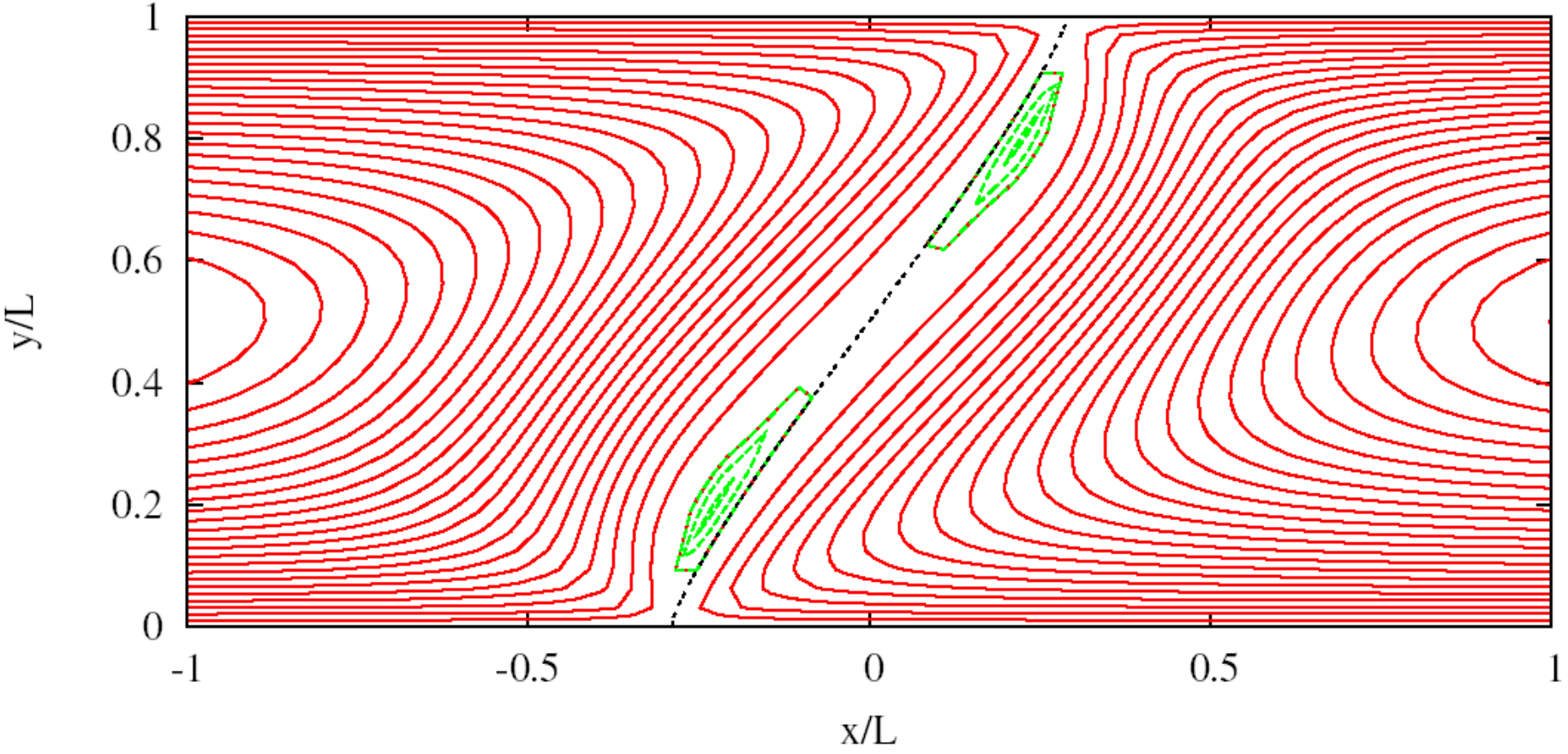




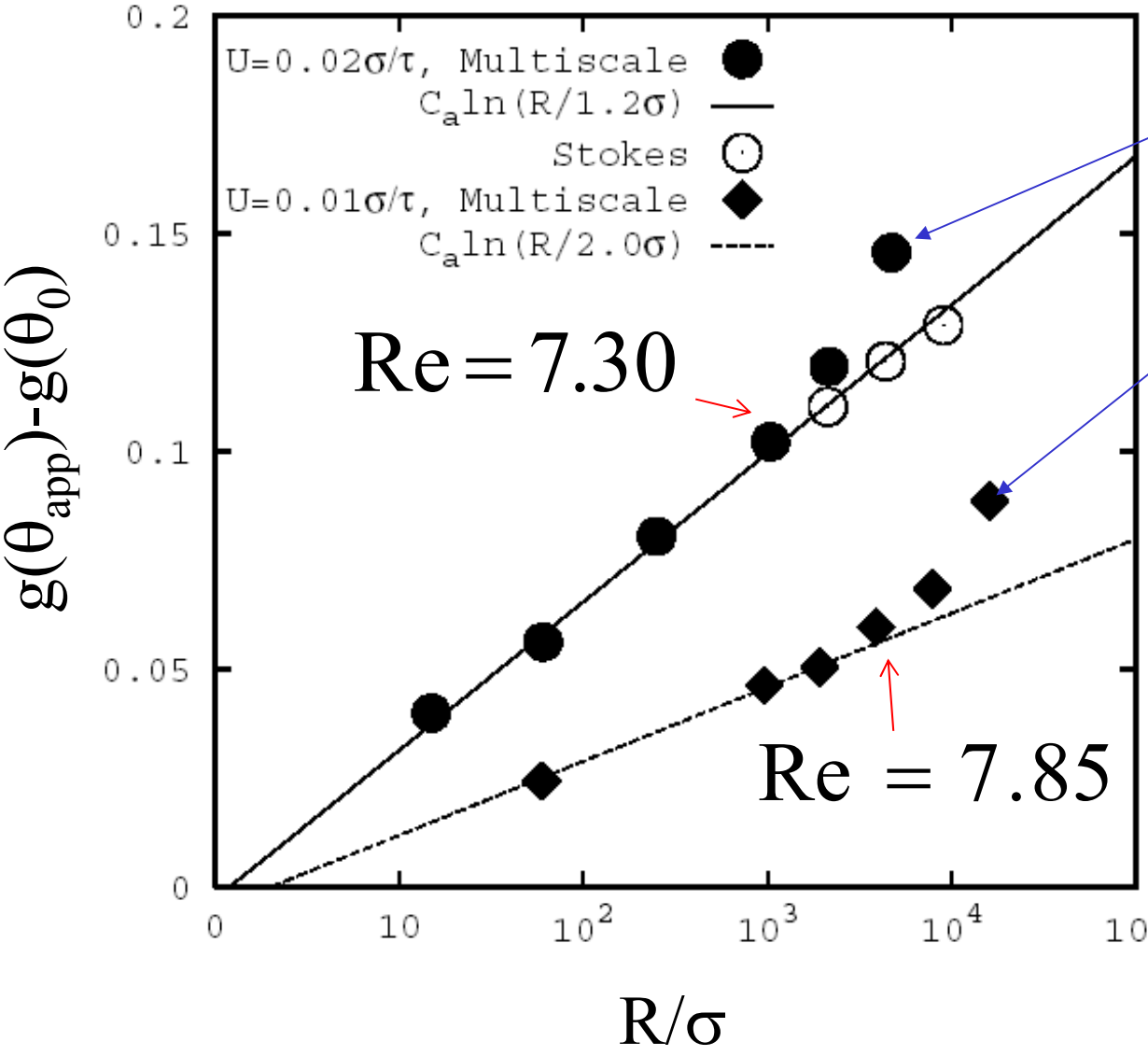




Typical Results of the Whole Flow Field



Deviation from Cox Solution



We = 0.448

We = 0.525

Weber # We $= \dfrac{\rho R U^2}{\sigma}$

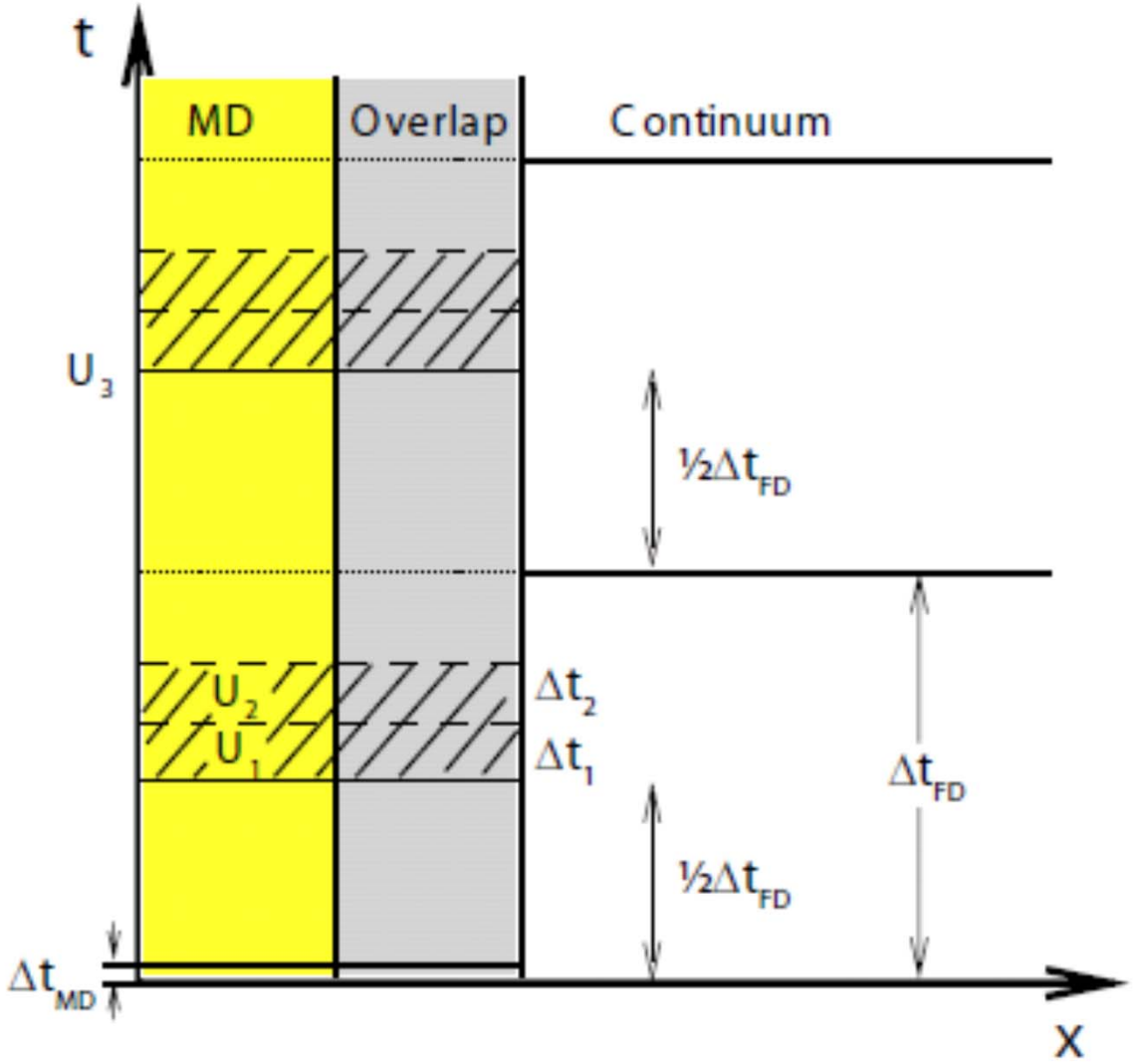
Reynolds # Re $= \dfrac{\rho R U}{\mu}$

Time Extrapolation Scheme

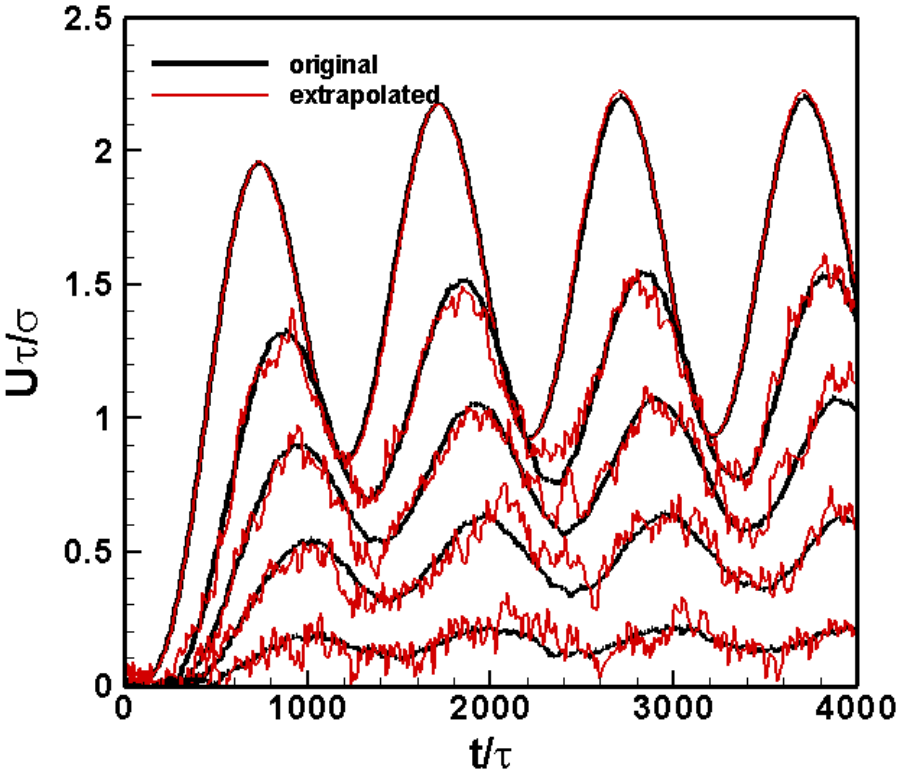
Need different approach for dynamic problems

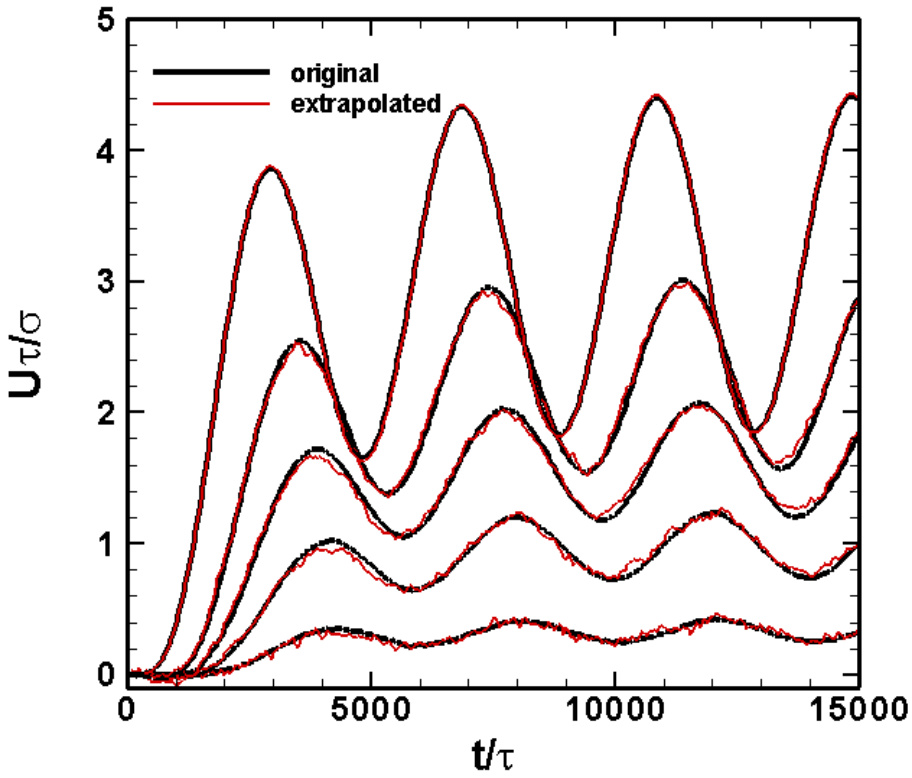
MD for short Δt then extrapolate to continuum time step

Problem: Extrapolate signal AND noise



Couette flow driven by oscillating wall





$\Delta x=\Delta y=15.6\sigma$, $\Delta t_{FD}=10\tau$,

$\Delta t_1=\Delta t_2=0.5\ \tau$

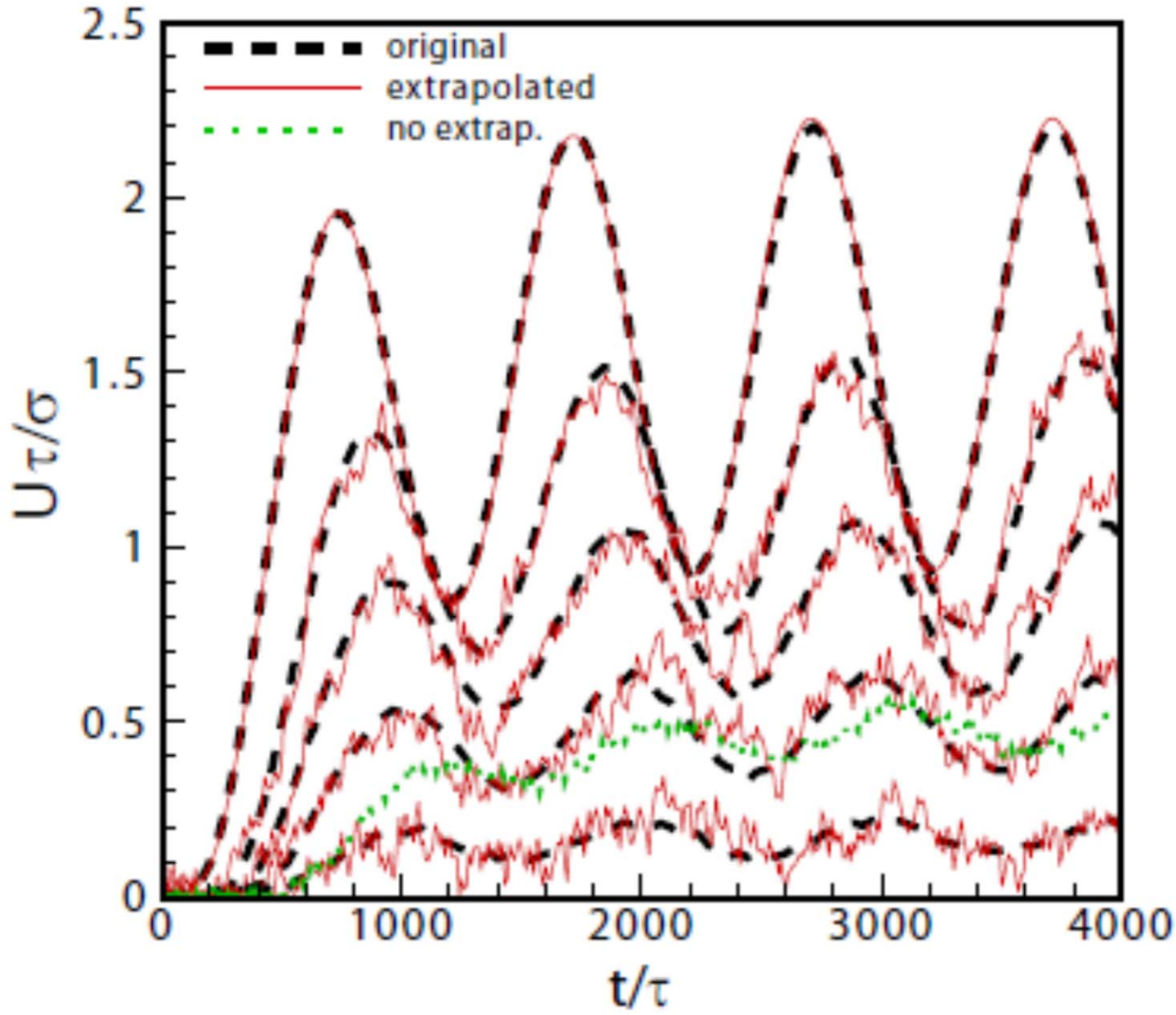
Ten-fold extrapolation in time

$\Delta x=\Delta y=31.3\sigma$, $\Delta t_{FD}=50\tau$,

$\Delta t_1=\Delta t_2=2.5\ \tau$

Comm. In Comp. Phys. **4**, 1279 (2008)

See Delay If No Time Extrapolation



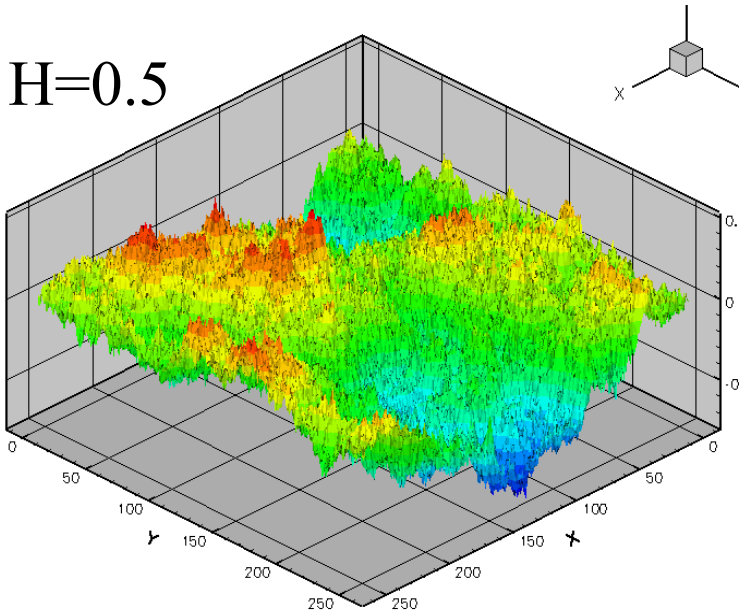
Weinan E, W. Ren, and E. Vanden-Eijnden, and Yamamoto and collaborators have considered non-extrapolated case.
OK if large time scale separation

Multi-scale modeling of contacts between self-affine surfaces

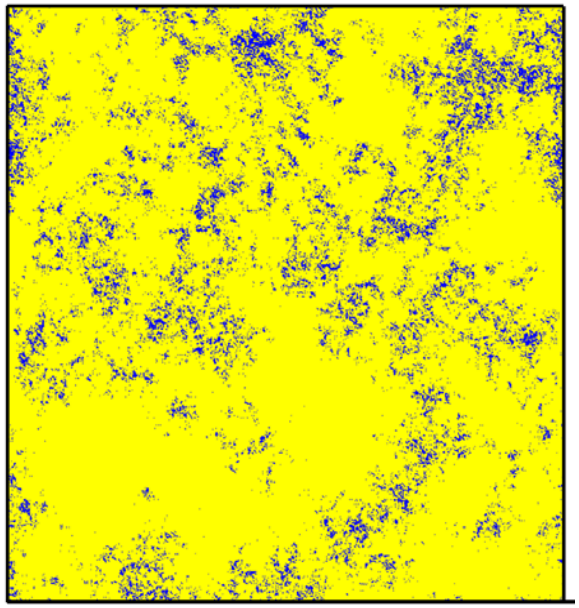
Contact geometry and stresses central to friction & adhesion

Real surfaces often rough on many scales → self-affine - $\delta h \sim l^H$

Surfaces steeper at smaller scales, fractal contact regions,
most connected regions of contact at resolution of calculation
⇒Not clear continuum mechanics applies

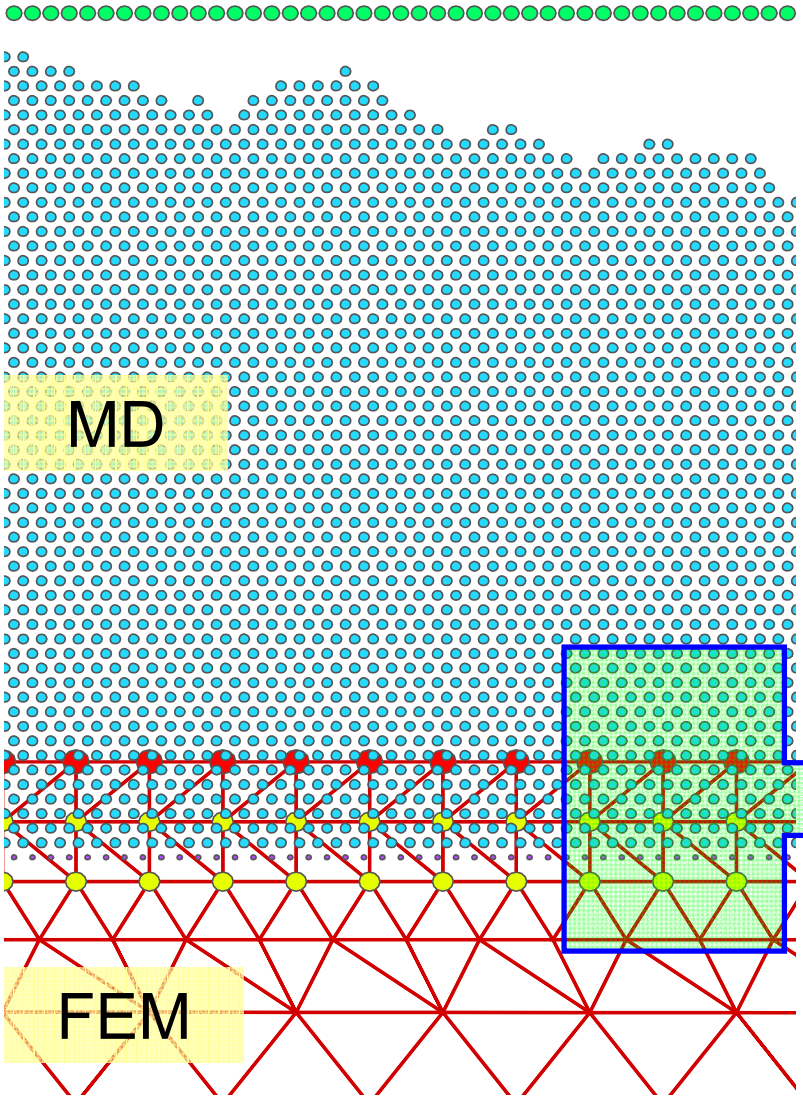


Self-affine surface

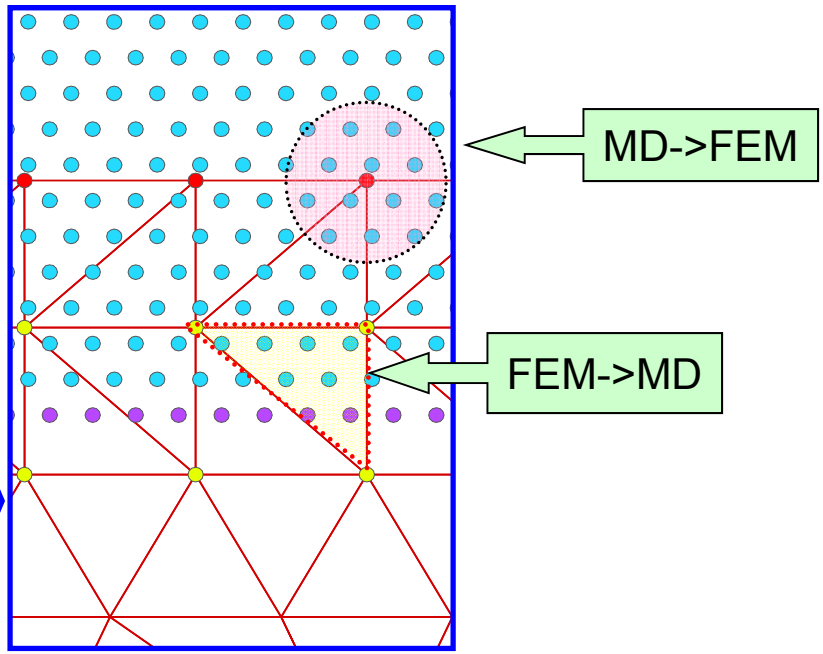


Contact (blue) of self-affine surface

Hybrid model for 2d self-affine surfaces
Easily treat volumes with ~10^8 atoms



At edge of overlap region MD and FEM displacements provide BC's for each other



overlap

Discrete Greens Function Approach

Lennard-Jones (LJ) interactions

Discrete atoms near surface

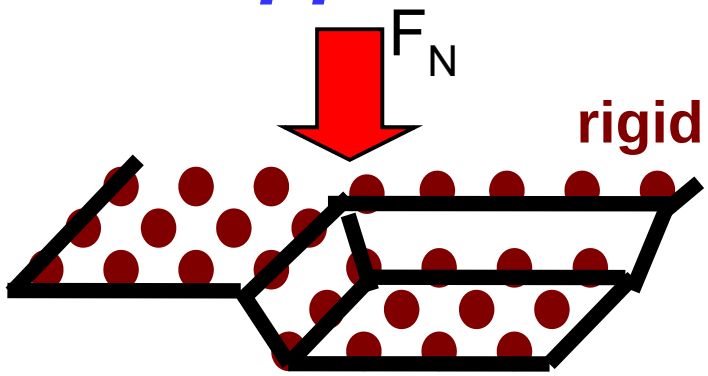
Green's function for multilayer

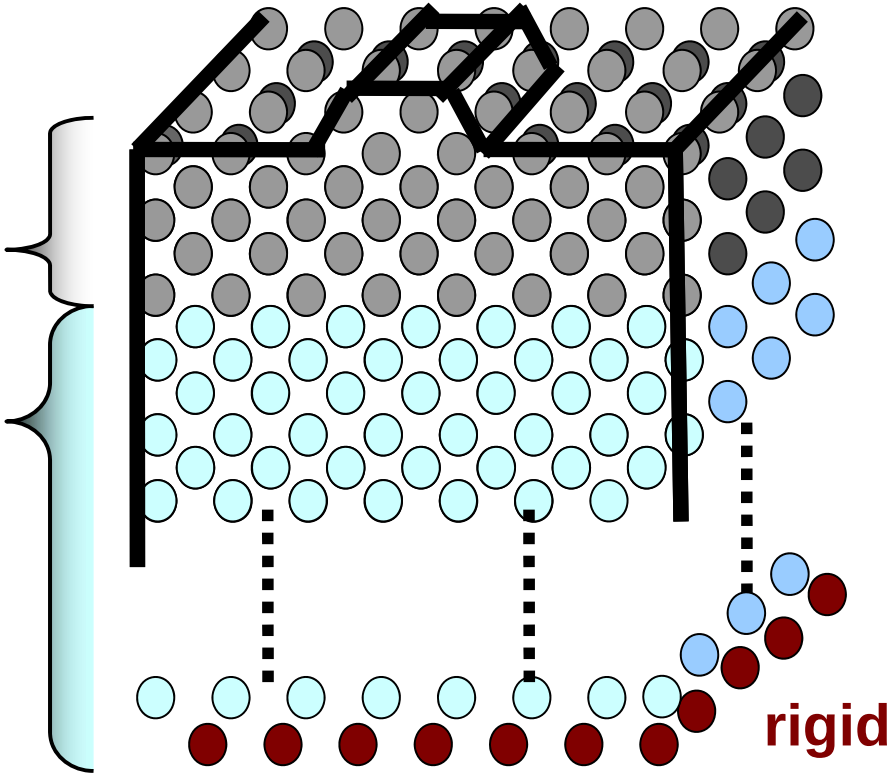
interactions for substrate

Energy minimization, T=0

Systems up to 10^{12} atoms

Simulate up to 10^{8} at surface





Simulate bulk: Greens function atoms