Molecular Dynamics Simulations of Oscillatory Couette Flows with Slip Boundary Conditions

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`Movies, preprints @ http://www.egr.msu.edu/~priezjev`

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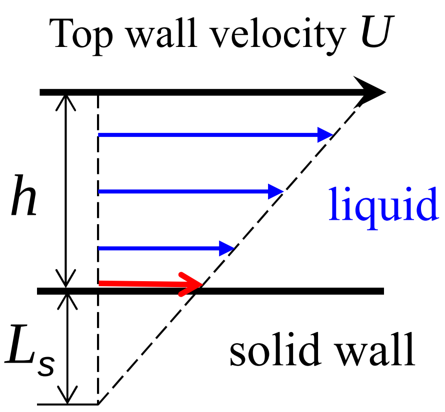
N. V. Priezjev, "Molecular dynamics simulations of oscillatory Couette flows with slip boundary conditions", *Microfluidics and Nanofluidics* **14**, 225 (2013).

N. V. Priezjev, "Fluid structure and boundary slippage in nanoscale liquid films", Chapter 16 in the book "Detection of Pathogens in Water Using Micro and Nano-Technology", IWA (International Water Association) Publishing (2012). ISBN: 9781780401089.

Motivation for investigation of slip phenomena at liquid/solid interfaces

- Navier model states that slip velocity is proportional to the rate of shear. How does it work for time periodic flows?
  Slip length L_s as a function of shear rate in steady flows:

  Thompson and Troian, *Nature* (1997) $L_s(\dot{\gamma}) = L_s^o\,(1-\dot{\gamma}/\dot{\gamma}_c)^{-0.5}$
  Priezjev, *Phys. Rev. E* (2007) Linear & nonlinear dependence



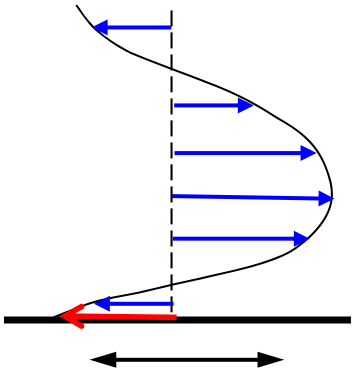
Navier slip condition $V_{slip} = L_s\,\dot{\gamma}$

- Oscillatory flows with slip boundary conditions:

Experimental studies with quartz crystal microbalance:
Ferrante, Kipling, Thompson, *J. Appl. Phys.* (1994)
Ellis and Hayward, *J. Appl. Phys.* (2003)
Willmott and Tallon, *Phys. Rev. E* (2007)

Hydrodynamic predictions for oscillatory Couette flows:
Matthews and Hill, *Microfluid. Nanofluid.* (2009) $u(\omega, z, L_1, L_2)$
Khaled and Vafai, *Int. J. Nonlinear. Mech.* (2004)

Molecular dynamics simulations in the Couette geometry:
Hansen and Ottesen, *Microfluid. Nanofluid.* (2006)
Thalakkottor and Mohseni, arXiv:1207.7090 (2012)
(phase difference between wall and fluid slip velocities leading to a hysteresis loop)



$\alpha\, u_{solid}(t) = u_{fluid}(t)$

Details of molecular dynamics simulations

Lennard-Jones potential: $V_{LJ}(r) = 4\varepsilon \left[\left(\frac{r}{\sigma}\right)^{-12} - \left(\frac{r}{\sigma}\right)^{-6} \right]$

Fluid monomer density: $\rho = 0.81\, \sigma^{-3}$

FCC walls with density $\rho_w = 2.73\, \sigma^{-3}$

Wall-fluid interaction: $\varepsilon_{wf} = \varepsilon$ and $\sigma_{wf} = \sigma$

$$V_{LJ}(r) = 4\, \varepsilon_{wf} \left[\left(\frac{r}{\sigma}\right)^{-12} - \left(\frac{r}{\sigma}\right)^{-6} \right]$$

Oscillation frequency: $\omega\tau = 0.1, 0.01, 0.001,$ and 0.0001

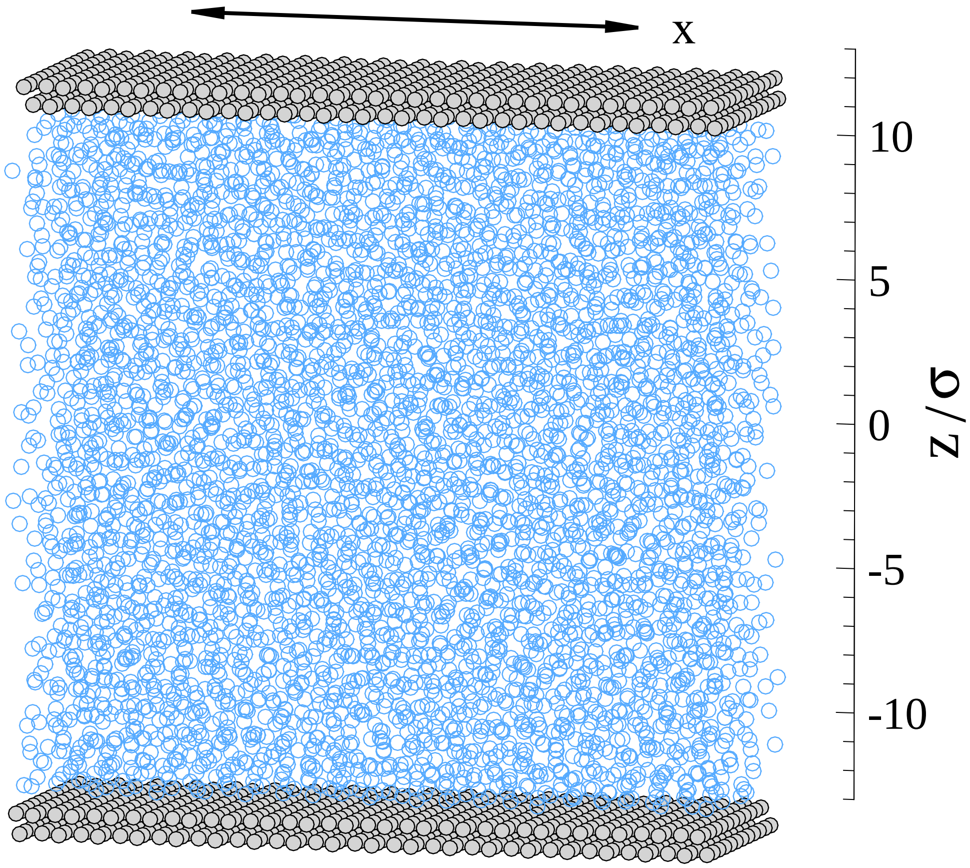
$$m\ddot{y}_i + m\Gamma\dot{y}_i = -\sum_{i \neq j} \frac{\partial V_{ij}}{\partial y_i} + f_i$$

$\Gamma = \tau^{-1}$ friction coefficient

$f_i =$ Gaussian random force

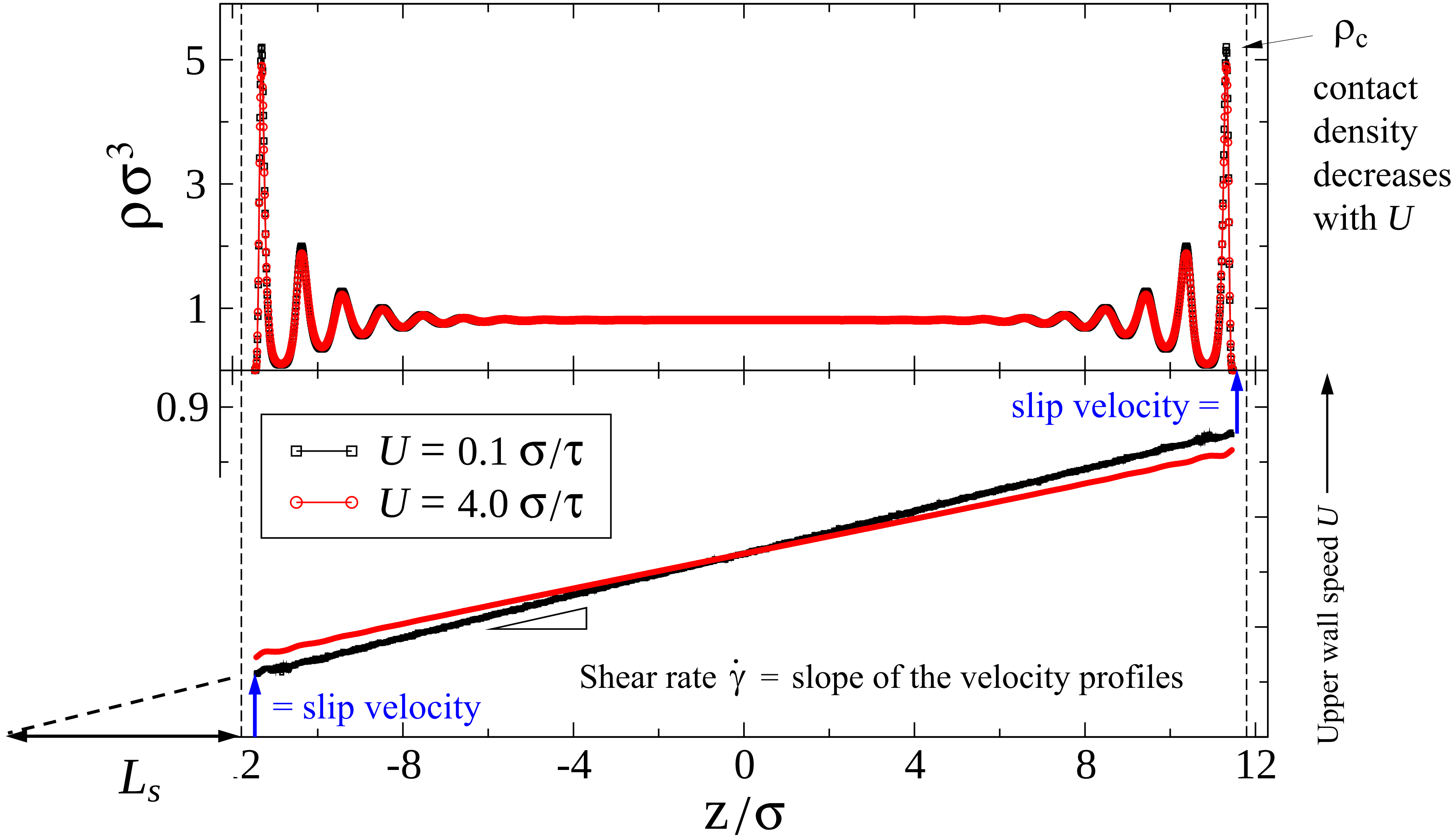
Langevin thermostat: $T = 1.1\varepsilon/k_B$

$$u_x^w(t) = U \sin(\omega t) \qquad T = \frac{2\pi}{\omega}$$



Stationary lower wall (finite slip length)

Part I: Velocity and density profiles in steady-state shear flows



ρ_c

contact
density
decreases
with *U*

slip velocity =

= slip velocity

Shear rate $\dot{\gamma}$ = slope of the velocity profiles

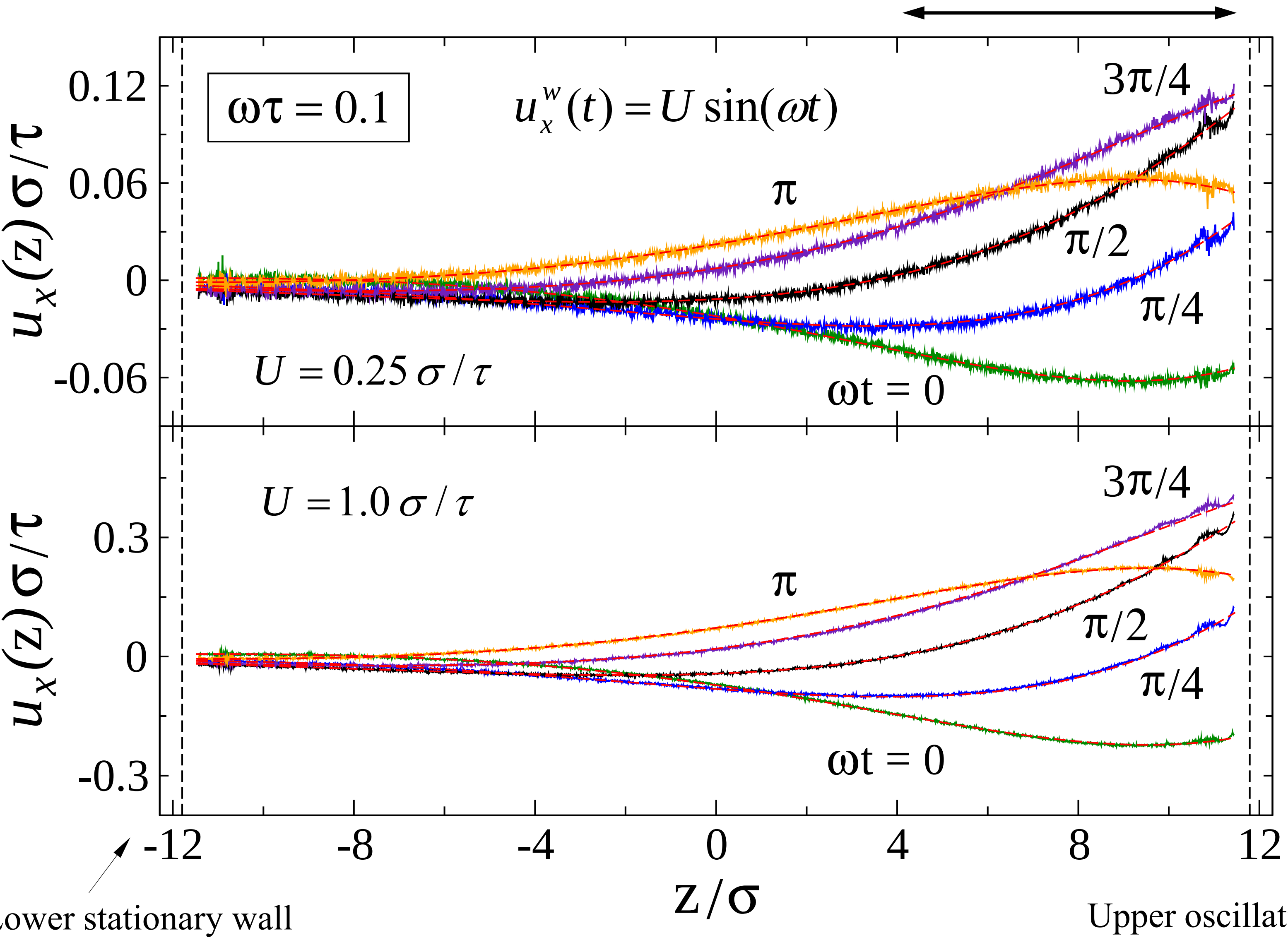
Upper wall speed *U*

L_s

N.V. Priezjev, Phys. Rev. E **75**, 051605 (2007).

The slip length increases almost linearly with shear rate.

Part II: Velocity profiles in oscillatory flows: phase and frequency



Lower stationary wall

Upper oscillating wall

Stokes layer:

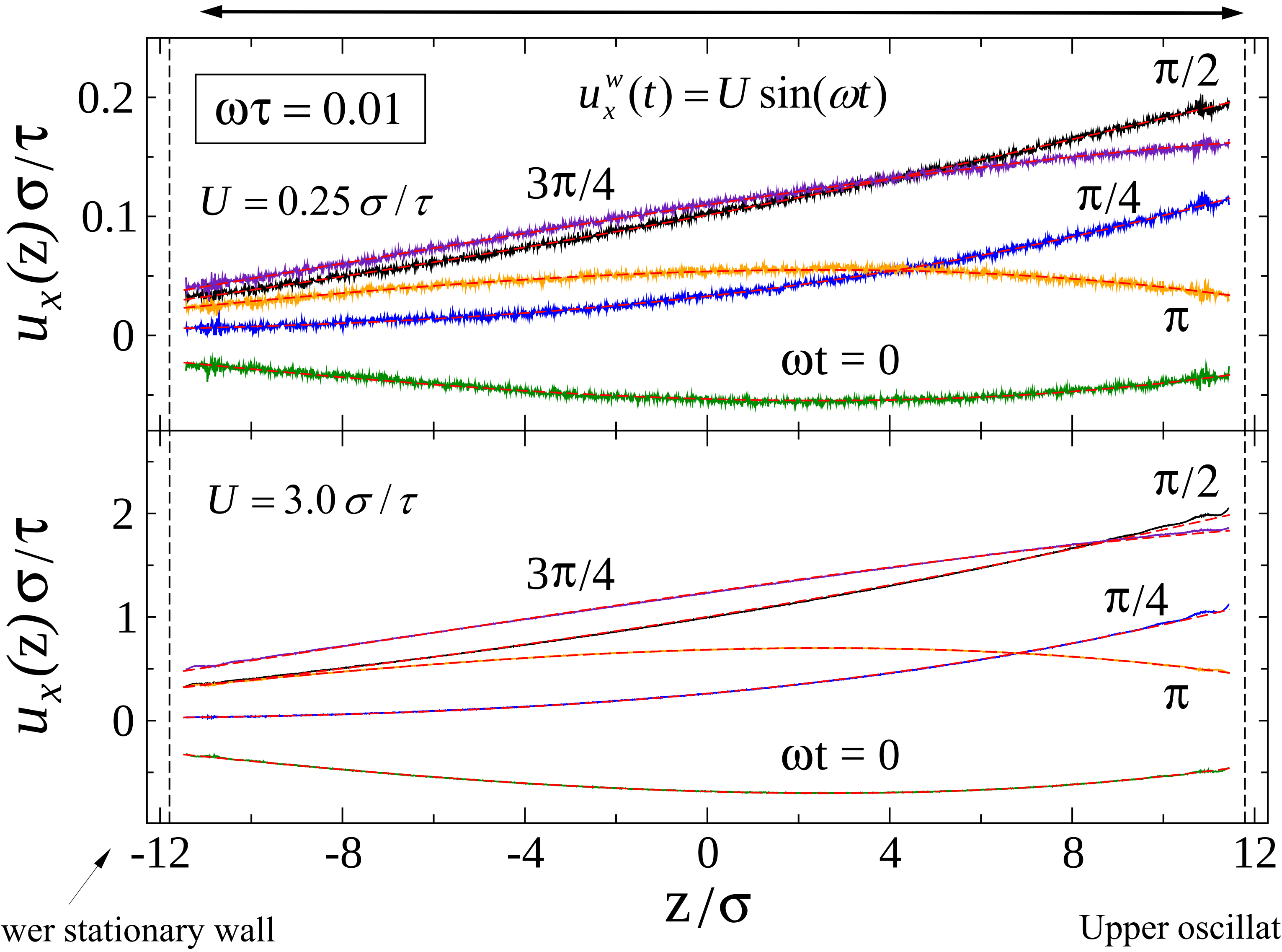
$$\delta = \sqrt{\frac{2\mu}{\rho\omega}}$$

$\delta = 7.3\,\sigma$

$h = 24\,\sigma$

Dashed red lines: best fit to continuum solution with L_1, L_2

Part II: Velocity profiles in oscillatory flows: phase and frequency



Lower stationary wall

Upper oscillating wall

Stokes layer:

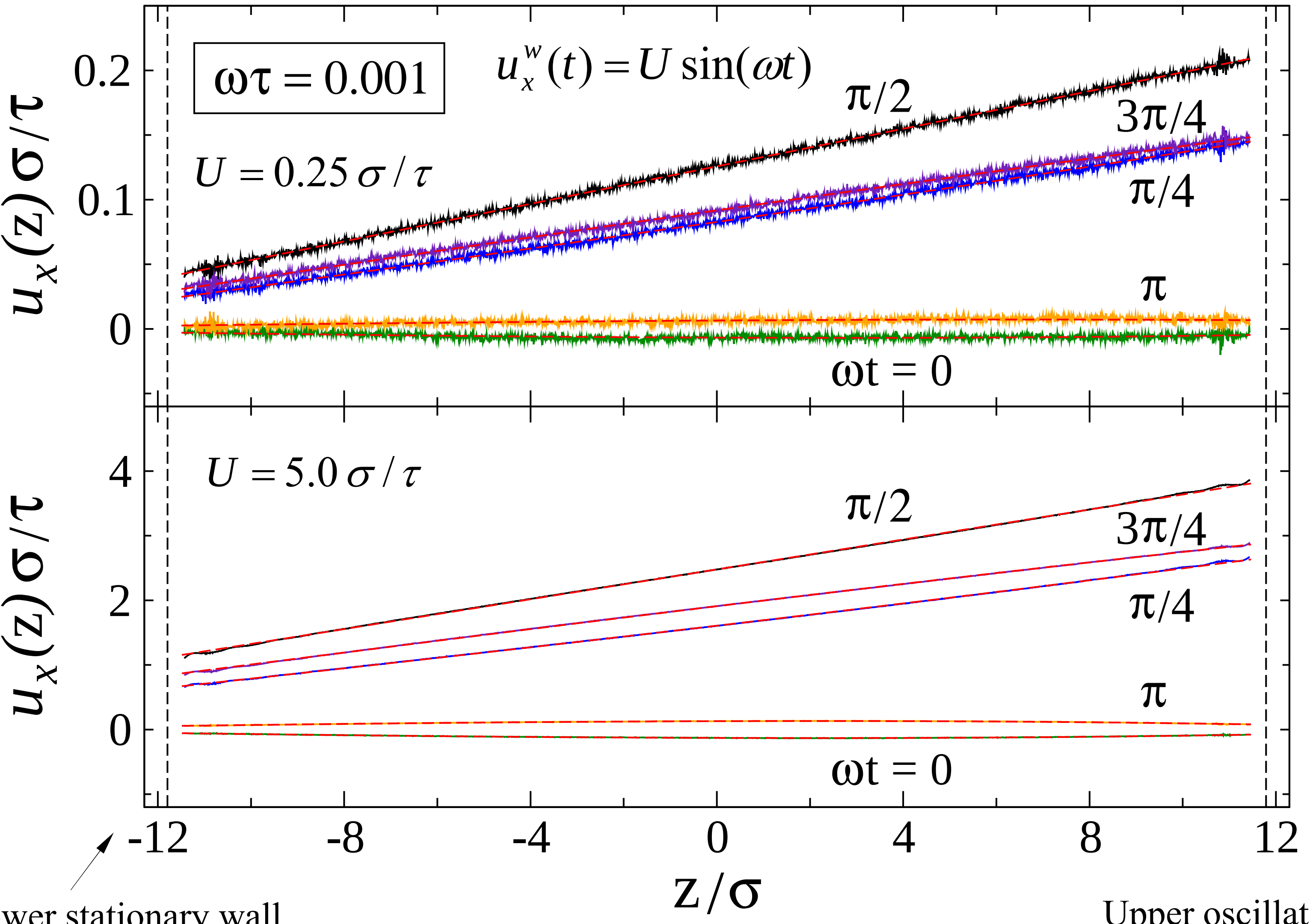
$$\delta = \sqrt{\frac{2\mu}{\rho\omega}}$$

$\delta = 23\,\sigma$

$h = 24\,\sigma$

Dashed red lines: best fit to continuum solution with L_1, L_2

Part II: Velocity profiles in oscillatory flows: phase and frequency



Stokes layer:

$$\delta = \sqrt{\frac{2\mu}{\rho\omega}}$$

$\delta = 73\,\sigma$

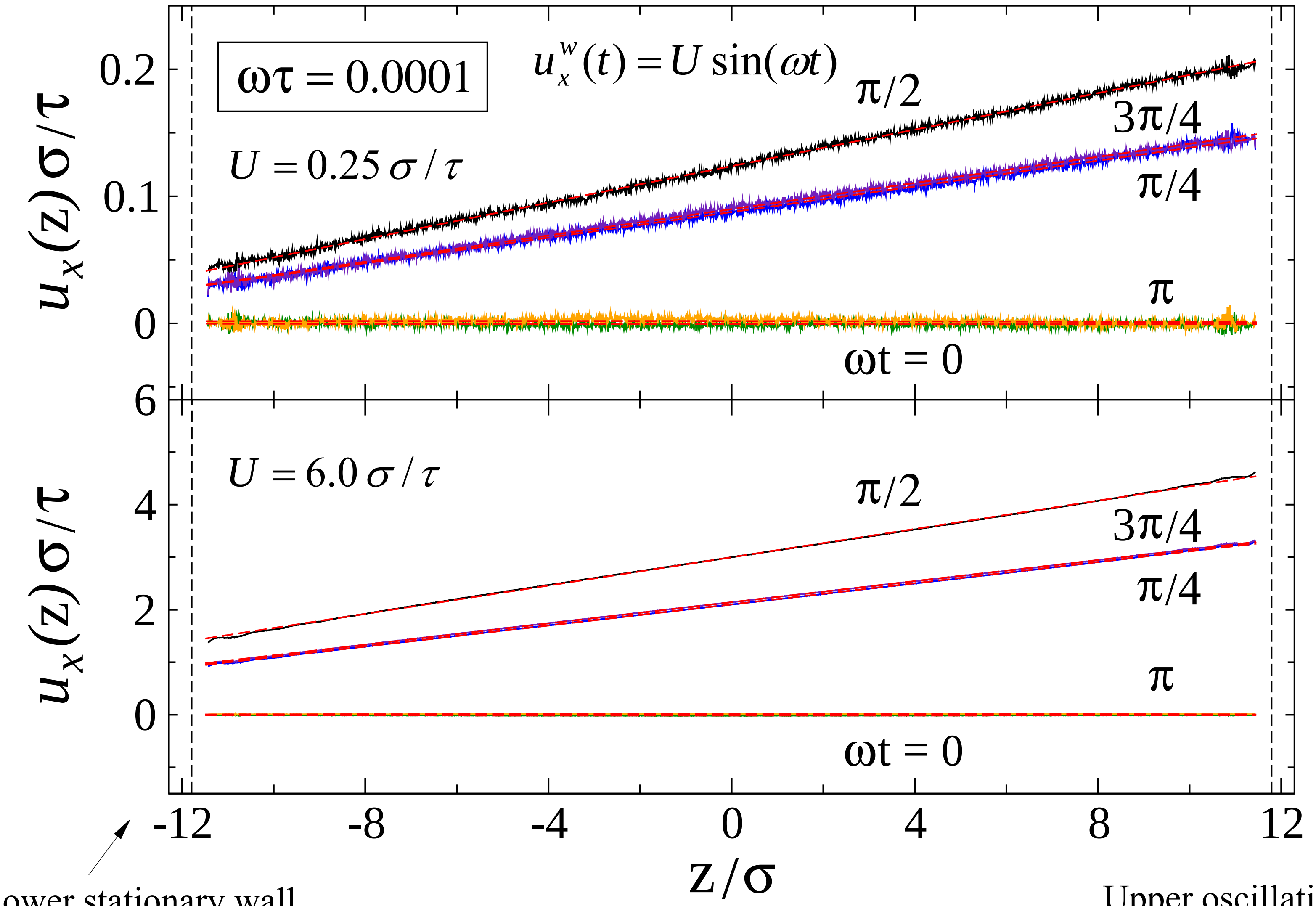
$h = 24\,\sigma$

Dashed red lines: best fit to continuum solution with L_1, L_2

Lower stationary wall

Upper oscillating wall

Part II: Velocity profiles in oscillatory flows: phase and frequency



Lower stationary wall

Upper oscillating wall

Stokes layer:

$$\delta = \sqrt{\frac{2\mu}{\rho\omega}}$$

$$\delta = 230\,\sigma$$

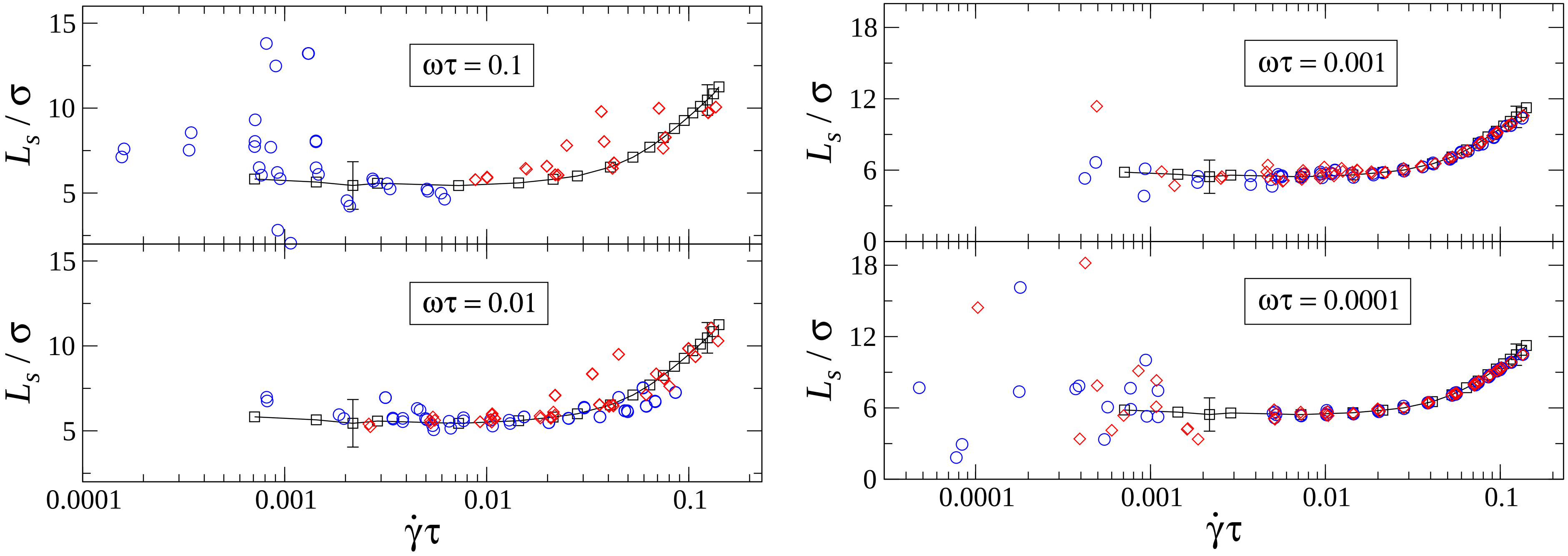
$$h = 24\,\sigma$$

Dashed red lines: best fit to continuum solution with L_1, L_2

Quasi-steady flows and the velocity profiles are nearly linear throughout the channel.

Steady-state vs. oscillatory flows: slip length L_s as a function of shear rate

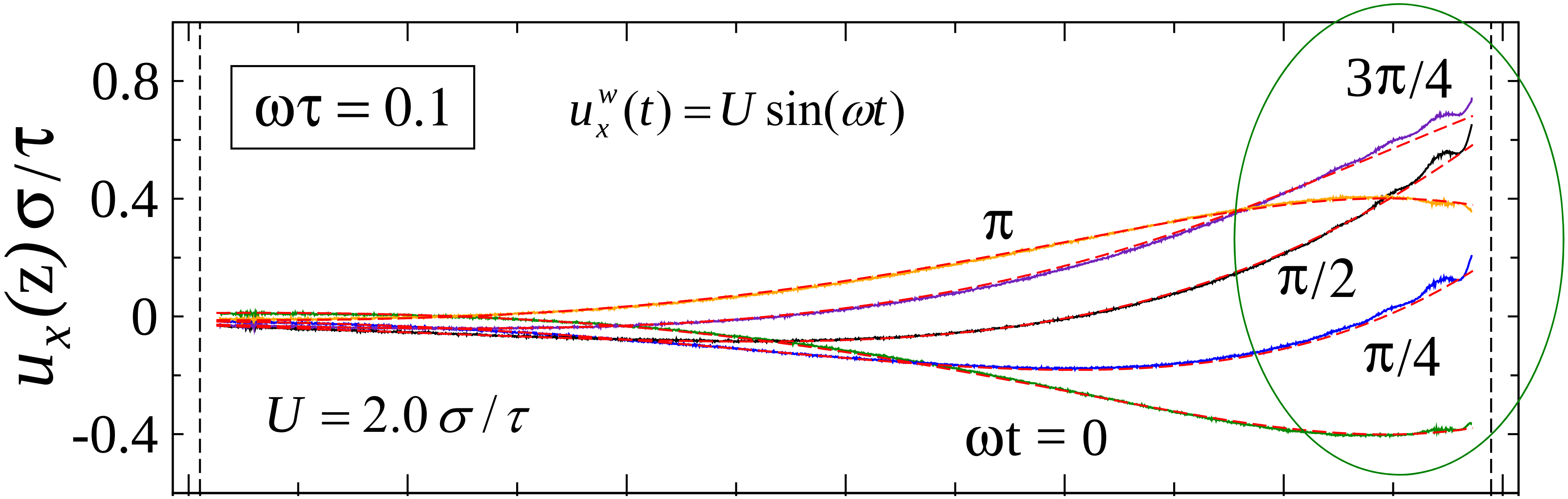
Black squares (□) = steady-state



Blue circles (○) = L_s at the stationary lower wall Red diamonds (◊) = L_s at the oscillatory upper wall

The shear rate dependence of the slip length obtained in steady-state shear flows is recovered when the slip length in oscillatory flows is plotted as a function of the local shear rate magnitude. *Discrepancy at high frequencies and amplitudes.* Scattered data at small *U*.

Slip length vs. shear rate ⇨ friction coefficient vs. slip velocity



- The estimate of shear rate and L_s directly from the MD velocity profiles is not precise because of the <u>nonlinearity of the velocity profiles near interfaces</u> and the ambiguity in choosing the size of the fitting region.

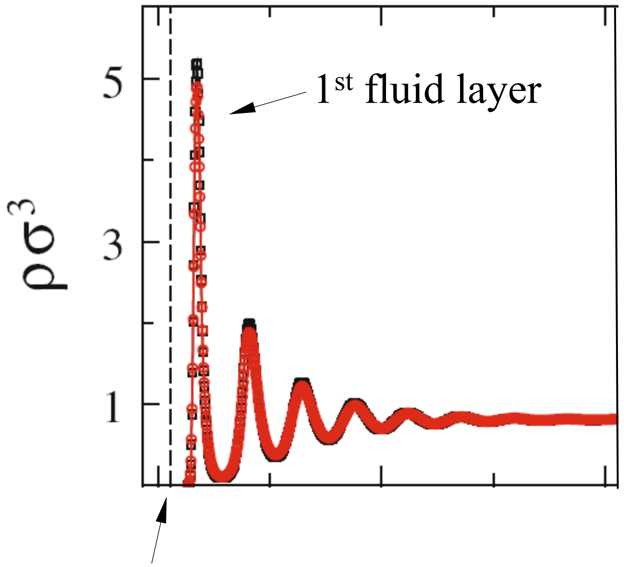
- Instead, one can compute the <u>friction coefficient as a function of slip velocity</u>:

$$\sigma_{xz}(\omega t) = k(u_s)\,u_s(\omega t)$$

- The friction coefficient at the liquid-solid interface *k(u*$_s$*)* obtained in steady shear flows agrees very well with the friction coefficient in oscillatory flows. Fluid structure?

Analysis of the fluid structure in the first layer near the solid wall

Fluid density profiles near the solid wall:



1st fluid layer

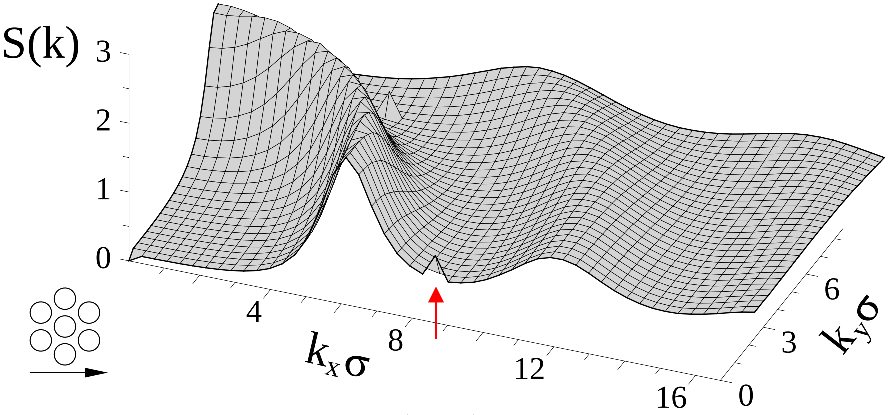
Liquid-solid interface

ρ_c = contact density (max first fluid peak)

The amplitude of density oscillations ρ_c is reduced at higher slip velocities u_s (by about 10%).

Structure factor in the first fluid layer:

$$S(\mathbf{k}) = \frac{1}{N_l}\left|\sum e^{i\,\mathbf{k}\cdot\mathbf{r}_j}\right|^2$$



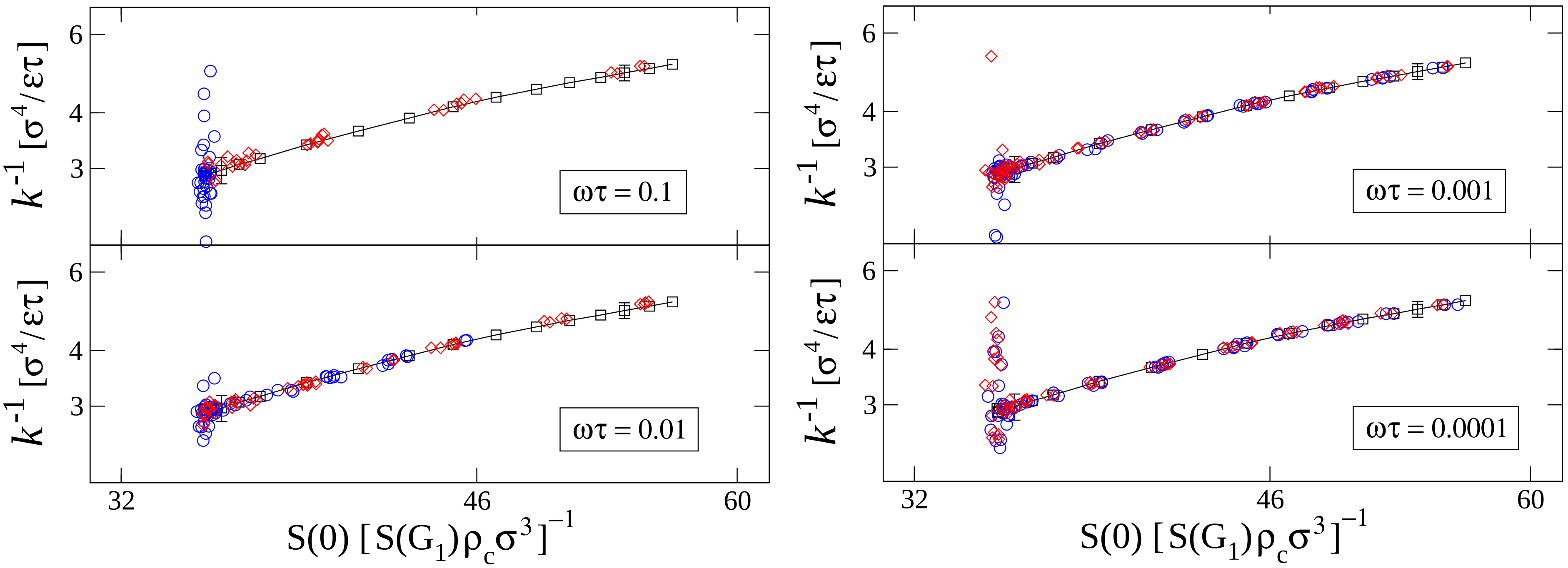
$S(G_1)$

Sharp peaks in the structure factor (due to periodic surface potential) are reduced at higher slip velocities u_s

N.V. Priezjev, *Phys. Rev. E* **82**, 051603 (2010)

Steady-state and oscillatory flows: friction coefficient vs. fluid structure

Black squares (□) = steady-state



Blue circles (○) = L_s at the stationary lower wall   Red diamonds (◊) = L_s at the oscillatory upper wall

- The friction coefficient and induced fluid structure decrease at higher slip velocities.
- For both types of flows, the friction coefficient at the liquid-solid interface correlates well with the structure of the first fluid layer near the solid wall.

Important conclusions

- Steady-state shear flow: The slip length increases almost linearly with shear rate for sufficiently strong wall-fluid interactions and incommensurate structures of the liquid and solid phases at the interface. N.V. Priezjev, Phys. Rev. E **75**, 051605 (2007).

- Time-periodic oscillatory flows: velocity profiles in oscillatory flows are well described by the continuum solution with the slip length that depends on the local shear rate.

- Interestingly, the rate dependence of the slip length obtained in steady shear flows is recovered when the slip length in oscillatory flows is plotted as a function of the local shear rate magnitude.

- For both types of flows, the friction coefficient at the liquid-solid interface correlates well with the structure of the first fluid layer near the solid wall.

N. V. Priezjev, "Molecular dynamics simulations of oscillatory Couette flows with slip boundary conditions", *Microfluidics and Nanofluidics* **14**, 225 (2013).