Analytical and Numerical Study of Coupled Atomistic-Continuum Methods for Fluids

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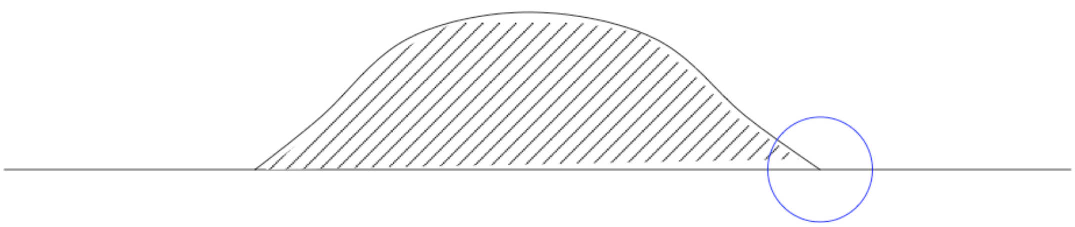
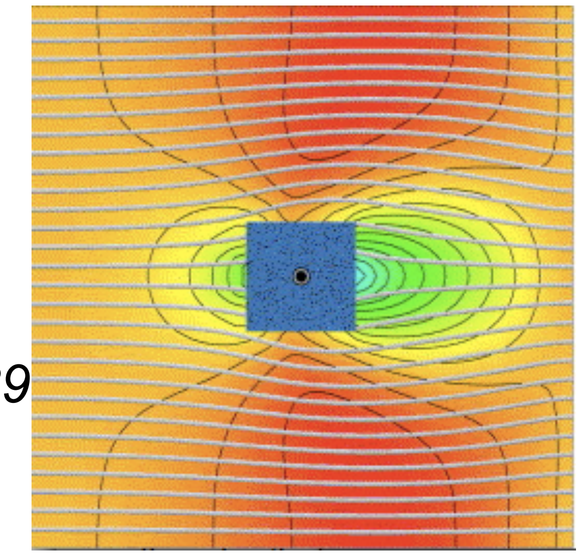
Joint work with Weinan E

Multiscale modeling for two types of problems:

- Complex fluids - *Constitutive modeling*
- Microfluidics - *Atomistic-based boundary condition modeling*



Koplik et al. PRL '88; Thompson & Robbins, PRL '89
Qian et al., PRE '03; Ren & E, PoF '07

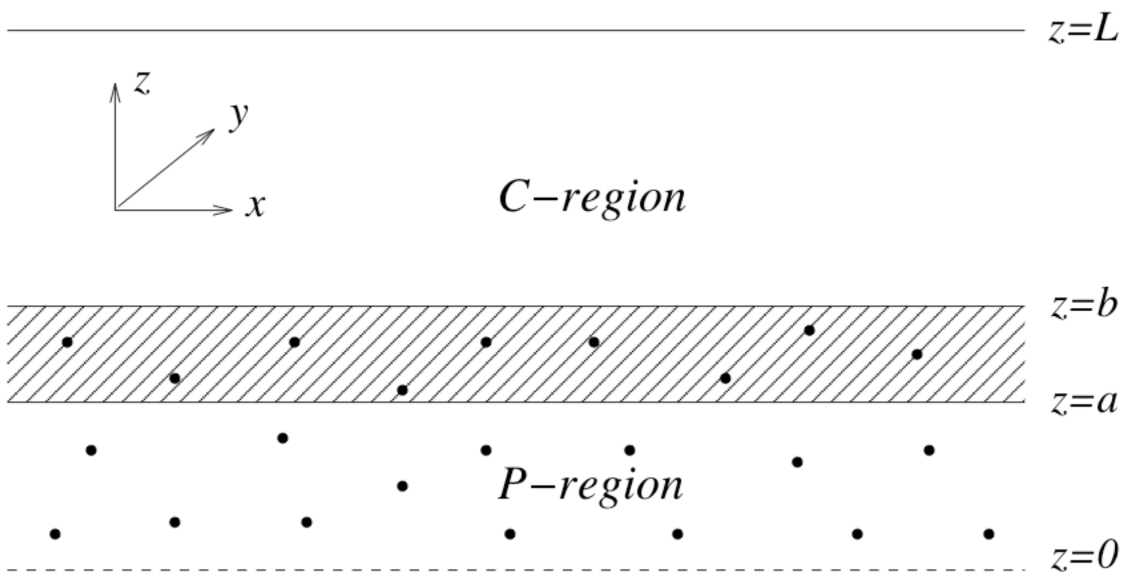


Koumoutsakos, JCP '05

(i) Heterogeneous multiscale method:
Macro solver + missing data from MD

(ii) Domain-decomposition framework

Multiscale method in the domain decomposition framework



C-region : Continuum hydrodynamics

P-region : Molecular dynamics

The two descriptions are coupled through exchanging boundary conditions in the overlapping region after each time interval T_c .

Two fundamental issues:

- What information need to be exchanged between the two descriptions?

  (i) Fields (e.g. velocity):

  (ii) Fluxes of conserved quantities

- How to accurately impose boundary conditions on molecular dynamics?

Existing multiscale methods for dense fluids

- Velocity coupling:

  O'Connel and Thompson 1995

  Hadjiconstantinou and Patera 1997

  Li, Liao and Yip 1999

  Nie, Chen, E and Robbins 2004

  Werder, Walther and Koumoutsakos 2005

- Flux coupling:

  Flekkoy, Wagner and Feder 2000

  Delgado-Buscalioni and Coveney 2003

- Mixed scheme:

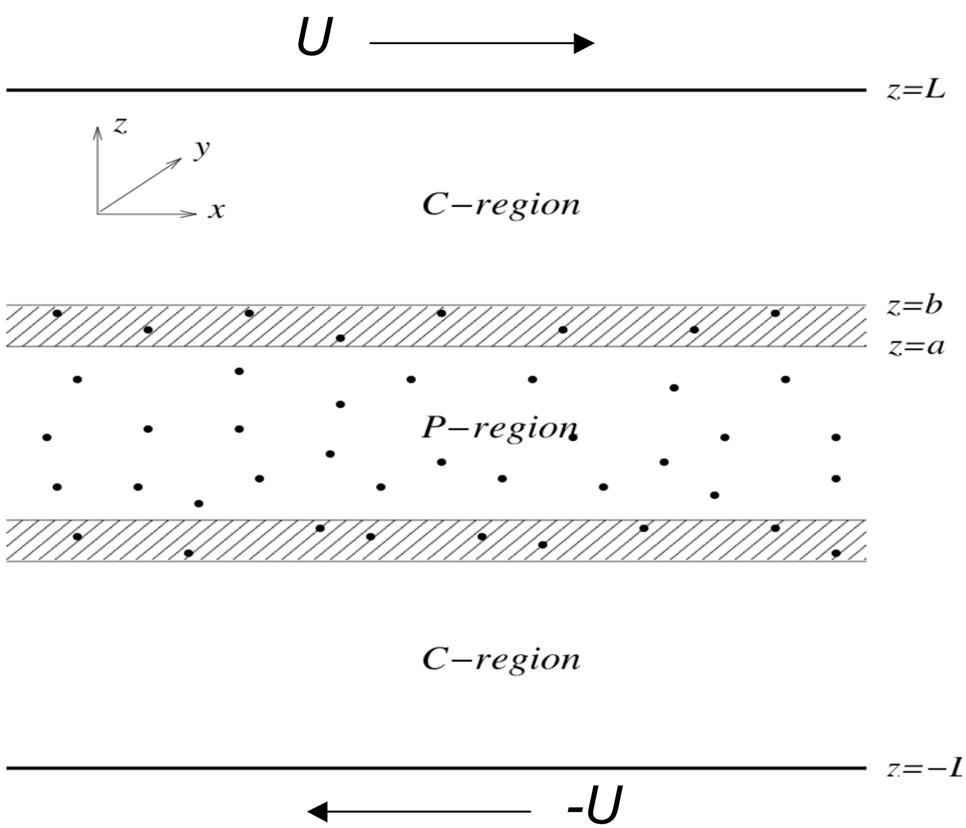
  Ren and E 2005

Present work:

- *Stability and convergence rate of the different coupling schemes; Propagation of statistical errors in the numerical solution.*

- *Error introduced when imposing boundary conditions in MD.*

Problem setup: Lennard-Jones fluid in a channel



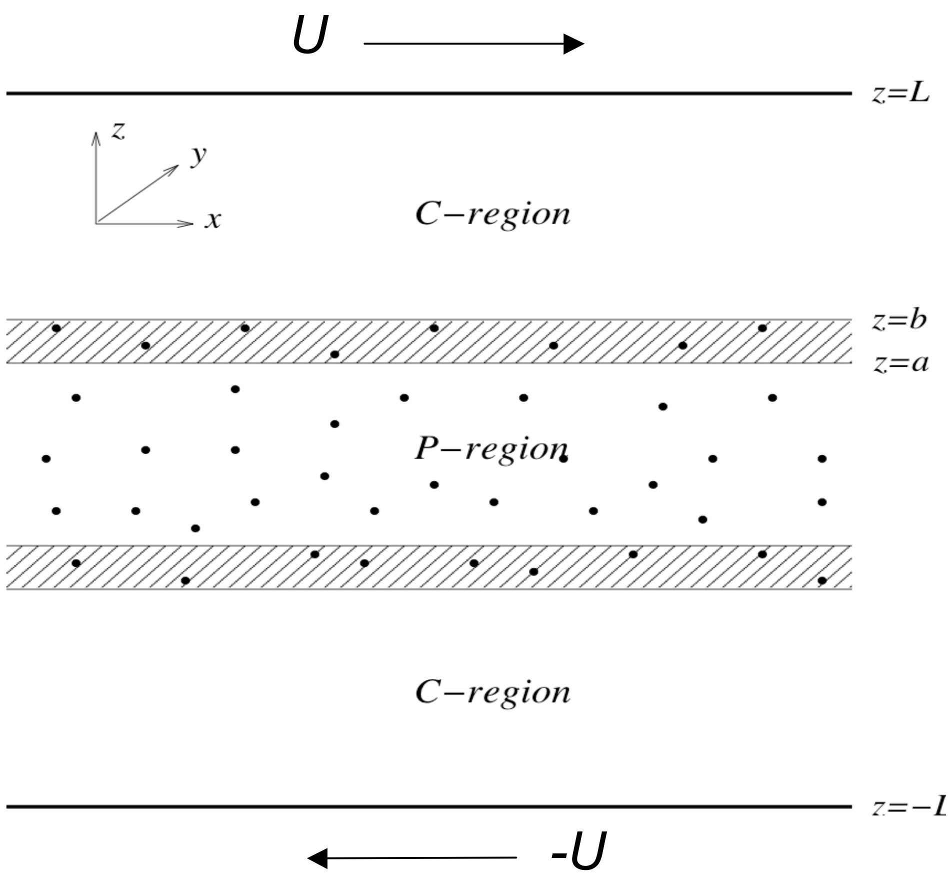
$$\begin{cases} \rho\partial_t u - \partial_z \tau = 0 \\ \tau = \mu \partial_z u \\ u(L,t) = U \end{cases}$$

$$\begin{cases} m_i \ddot{r}_i = F_i \\ F_i = -\sum_{j \neq i} \nabla V(r_{ij}) \end{cases}$$

$$V(r) = 4\varepsilon\left(\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right)$$

(i). Static (U=0); *(ii). Impulsively started shear flow*

Four coupling schemes:



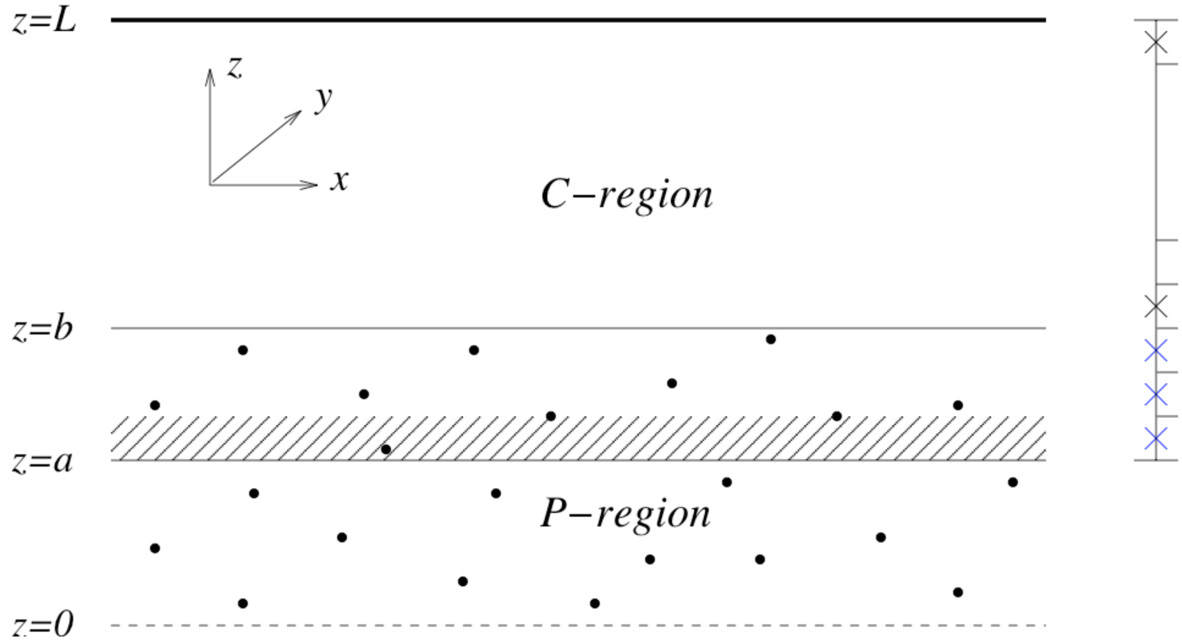
- *Velocity - Velocity*
- *Momentum flux - Velocity*
- *Velocity - Flux*
- *Flux - Flux*

The two models exchange BCs after every time interval T_c.

The rest of the talk:

- Algorithmic details of the multiscale method for the benchmark problems;
- Numerical results;
- Assessment of the error introduced in the imposition of boundary condition in MD.

Solving the continuum model



$$\rho \partial_t u - \partial_z \tau = 0 \longrightarrow \rho \frac{u^{n+1}_{i+1/2} - u^{n+1}_{i-1/2}}{\Delta t} - \frac{\tau^n_{i+1} - \tau^n_i}{h} = 0$$

$$\tau = \mu \partial_z u \longrightarrow \tau_i = \mu \frac{u_{i+1/2} - u_{i-1/2}}{h}$$

$u_{1/2}$ or τ_1 is supplied by MD.

Correspondence of hydrodynamics and molecular dynamics

$$\partial_t m^\omega + \nabla \cdot \tau^\omega(x,t) = 0$$

$$m^\omega(x,t) = \sum_i p_i(t)\delta(r_i(t) - x)$$

$$\tau^\omega(x,t) = \sum_i \frac{1}{m_i}(p_i \otimes p_i)\delta(r_i - x)$$
$$+ \frac{1}{2}\sum_{j\neq i}(r_{ij} \otimes F_{ij}) \int_0^1 \delta\left(\lambda r_i + (1-\lambda)r_j - x\right) d\lambda$$

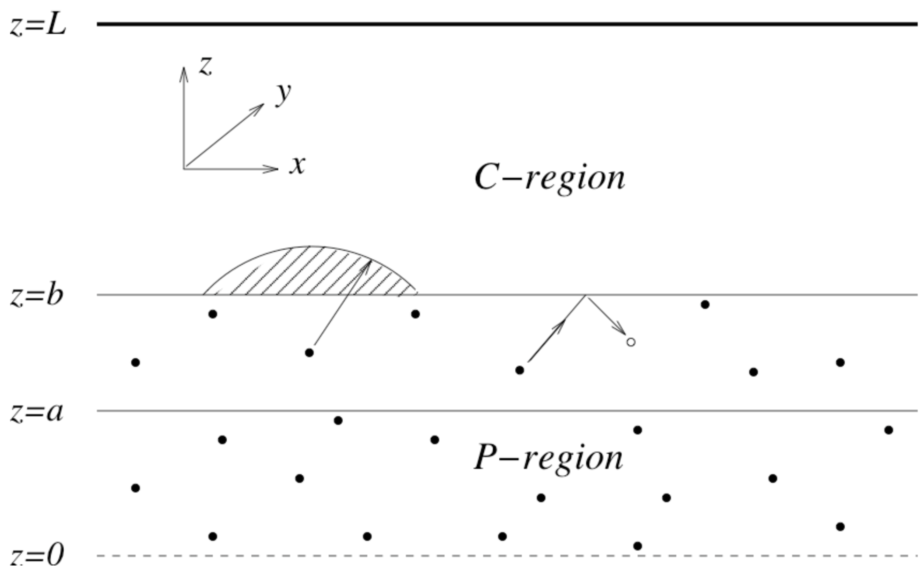
(Irving-Kirkwood 1950)

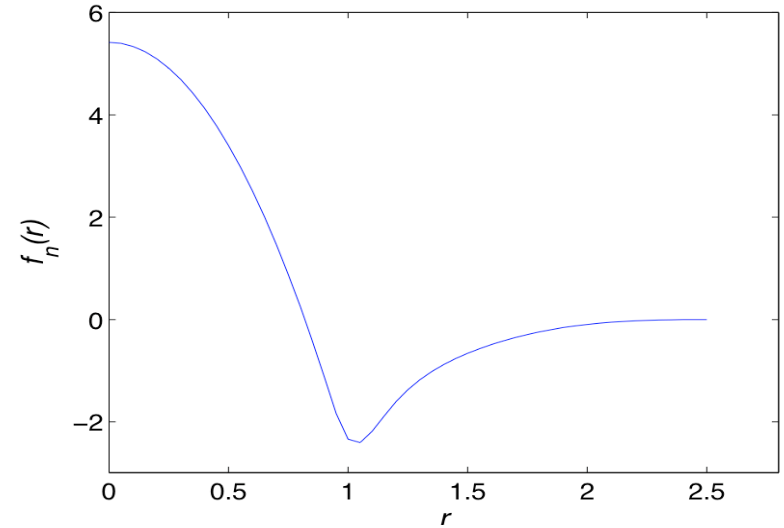
$$\langle m^\omega \rangle \Rightarrow \rho u$$

$$\langle \tau^\omega \rangle \Rightarrow \quad \tau = \rho u \otimes u - \mu(\nabla u + \nabla u^T) + pI$$ *for Newtonian fluids*

Using these formulae to calculate the continuum BCs from MD.

Boundary conditions for MD:
Reflection BC + Boundary force

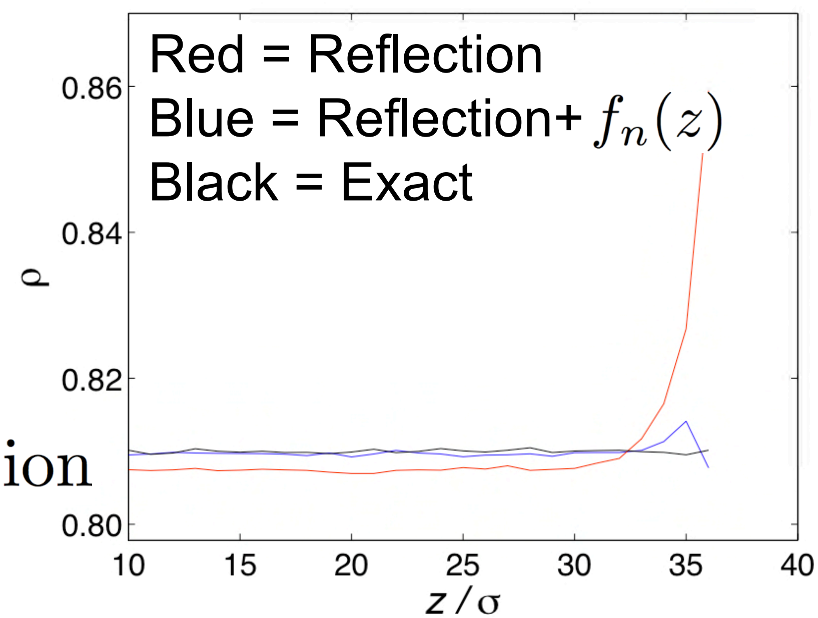




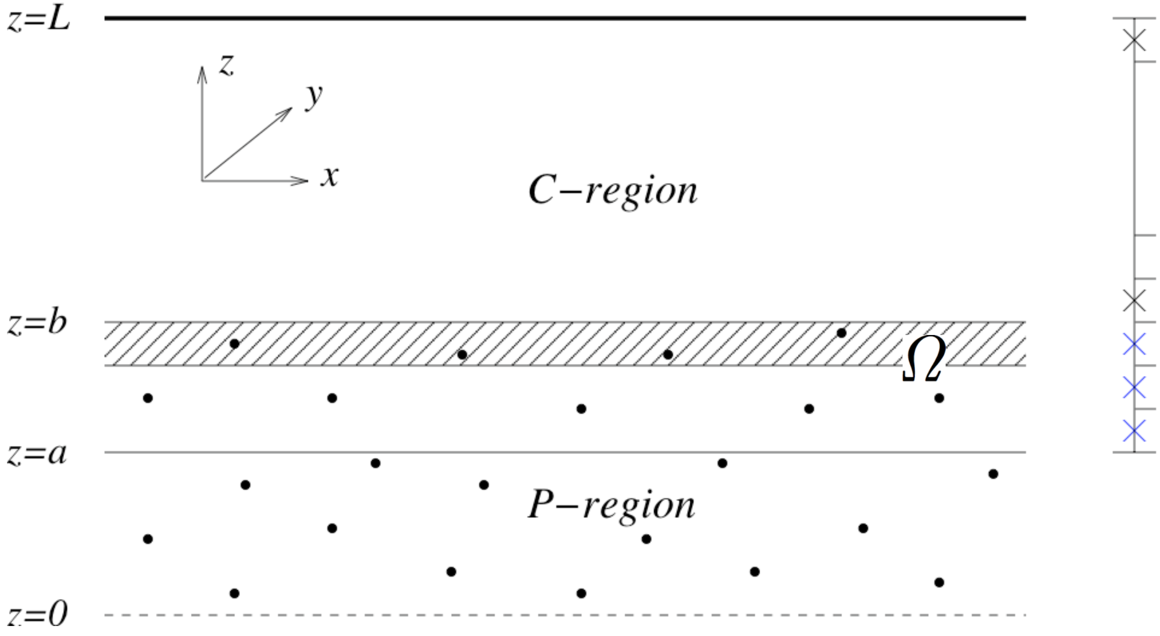
Mean boundary force:

$$F_n(r_w) = \rho \int_{z \geq r_w} \frac{\partial V}{\partial z} g(r)\, dr$$

$$g(r) = \text{radial distribution function}$$



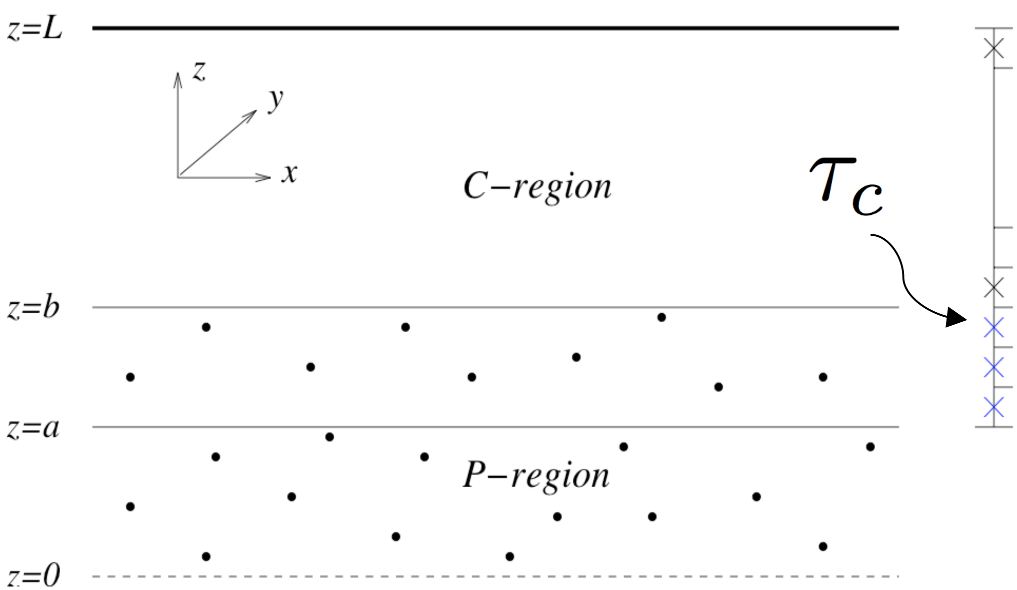
Matching with continuum - Imposing velocity BC on MD

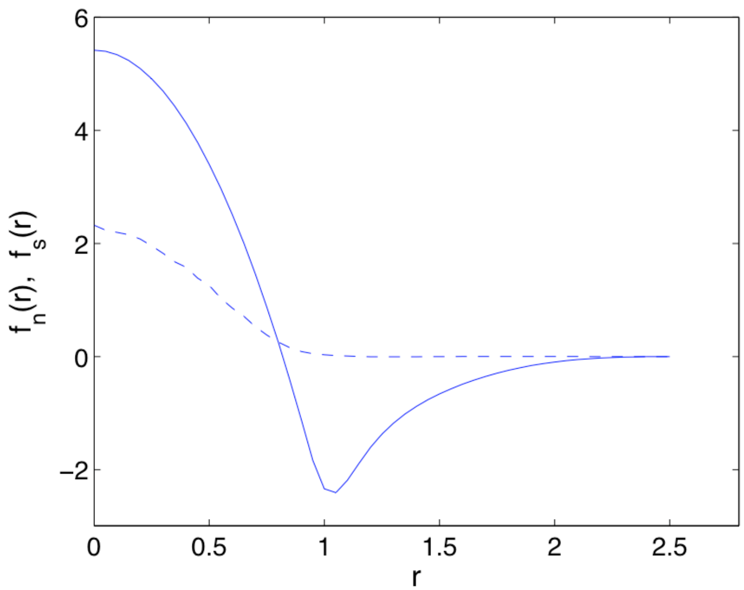


$$m_i \dot{v}_i = F_i + f(t), \quad \text{for } r_i \in \Omega$$

$$f(t): \quad N_\Omega^{-1} \sum_{r_i \in \Omega} v_i = u_c$$

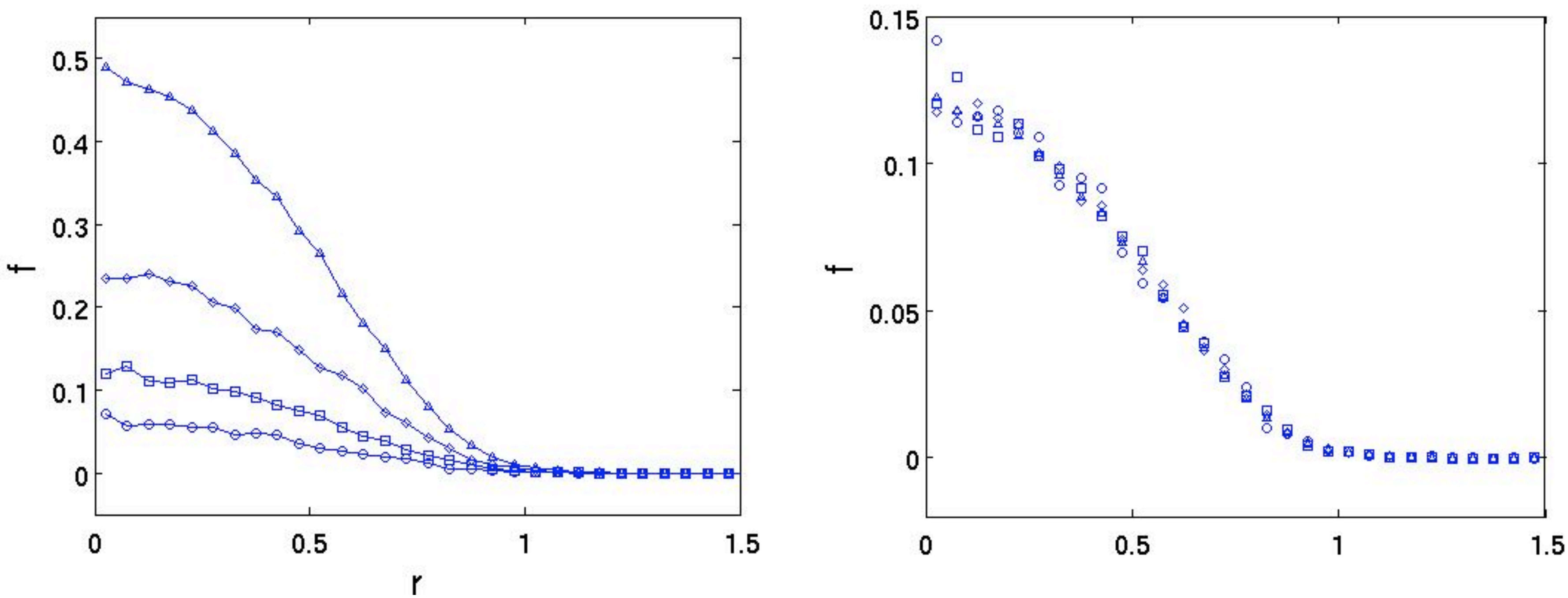
Matching with continuum: Imposing shear stress on MD





Particle with distance r_w to the boundary experiences a shear force $\tau_c f_s(r_w)$.

Microscopic profile of shear stress



Left: Shear stress profile at various shear rates;
Right: Shear stress profile rescaled by the shear rate.

Summary of the multiscale method

- Continuum solver: Finite difference in space + forward Euler's method in time

- Molecular dynamics:

(1) Velocity Verlet, Langevin dynamics to control temperature;

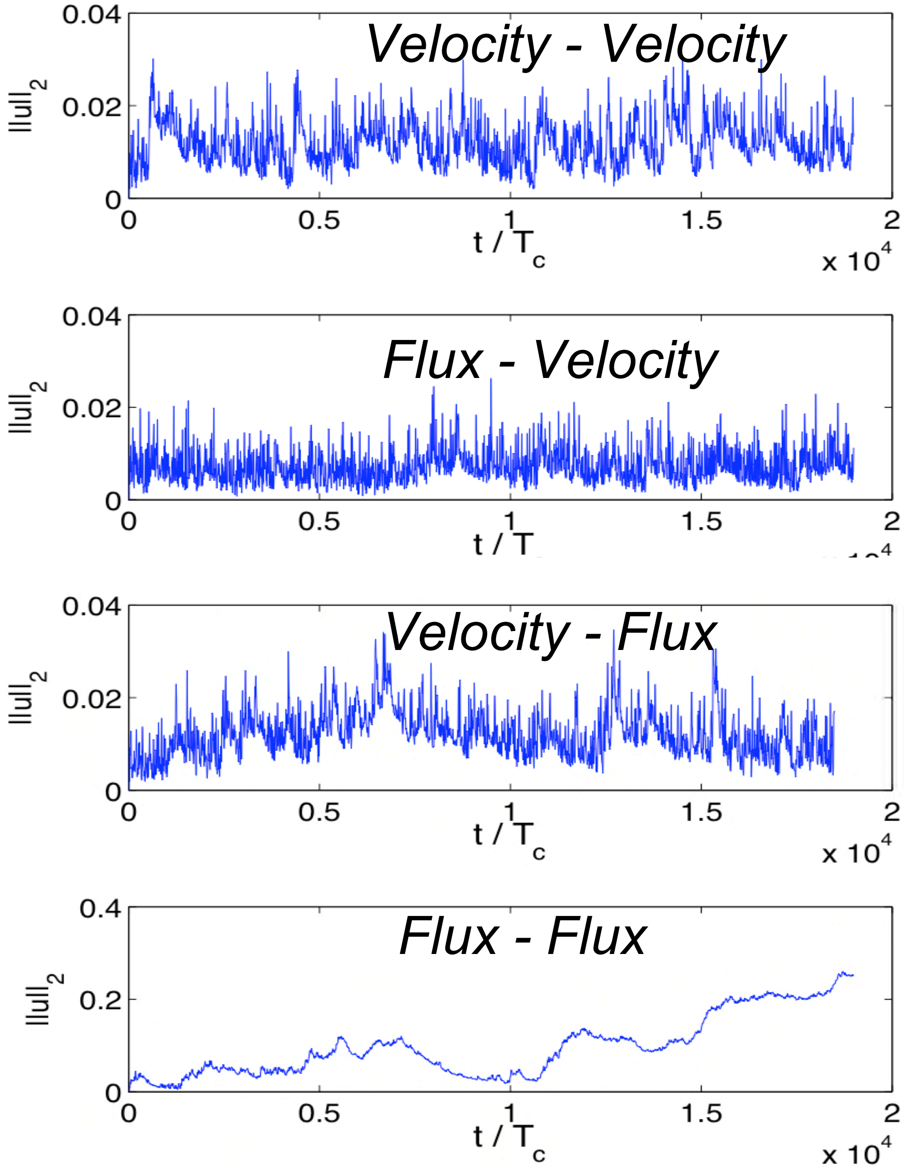
(2) Refection BC + Boundary force;

(3) Projection method to match the velocity;

(4) Distribute the shear stress based on an universal profile.

Numerical result for the static problem:

$$T_c = \Delta t$$

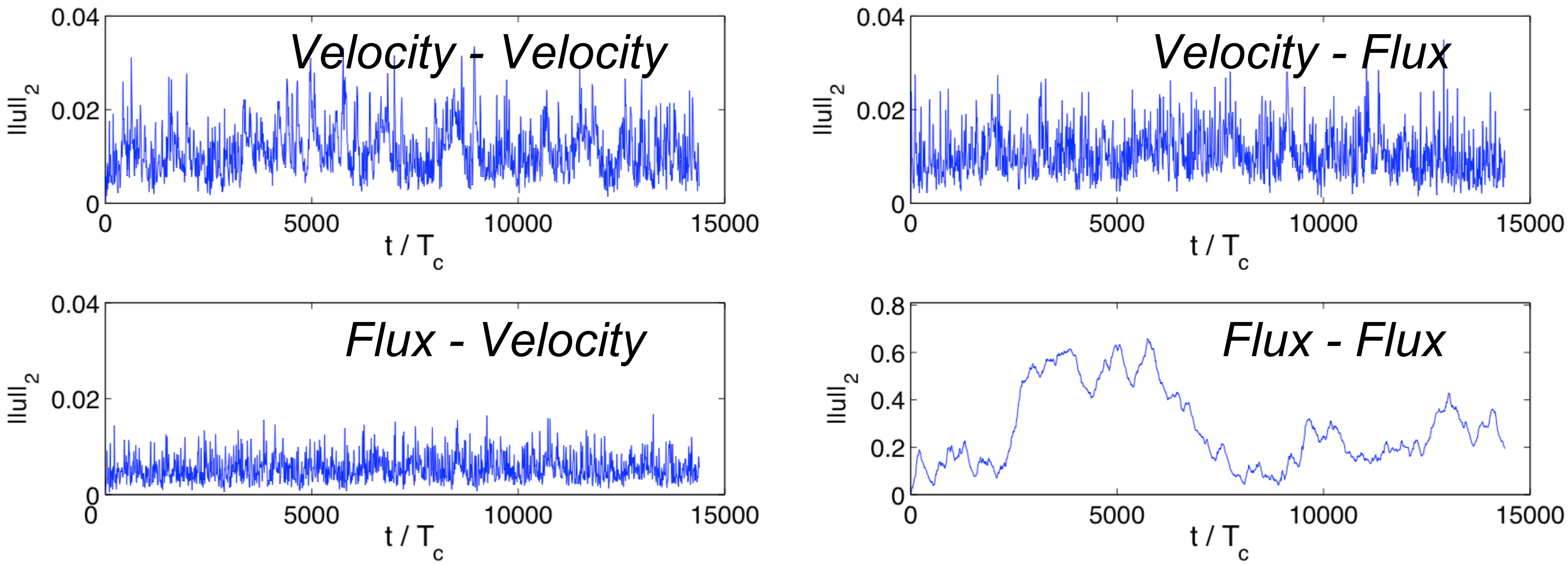


(i). Errors are due to statistical errors in the measured boundary condition (velocity,or shear stress) from MD.

(ii). Errors are bounded in *VV, FV, VF* schemes, while accumulate in the *FF* scheme.

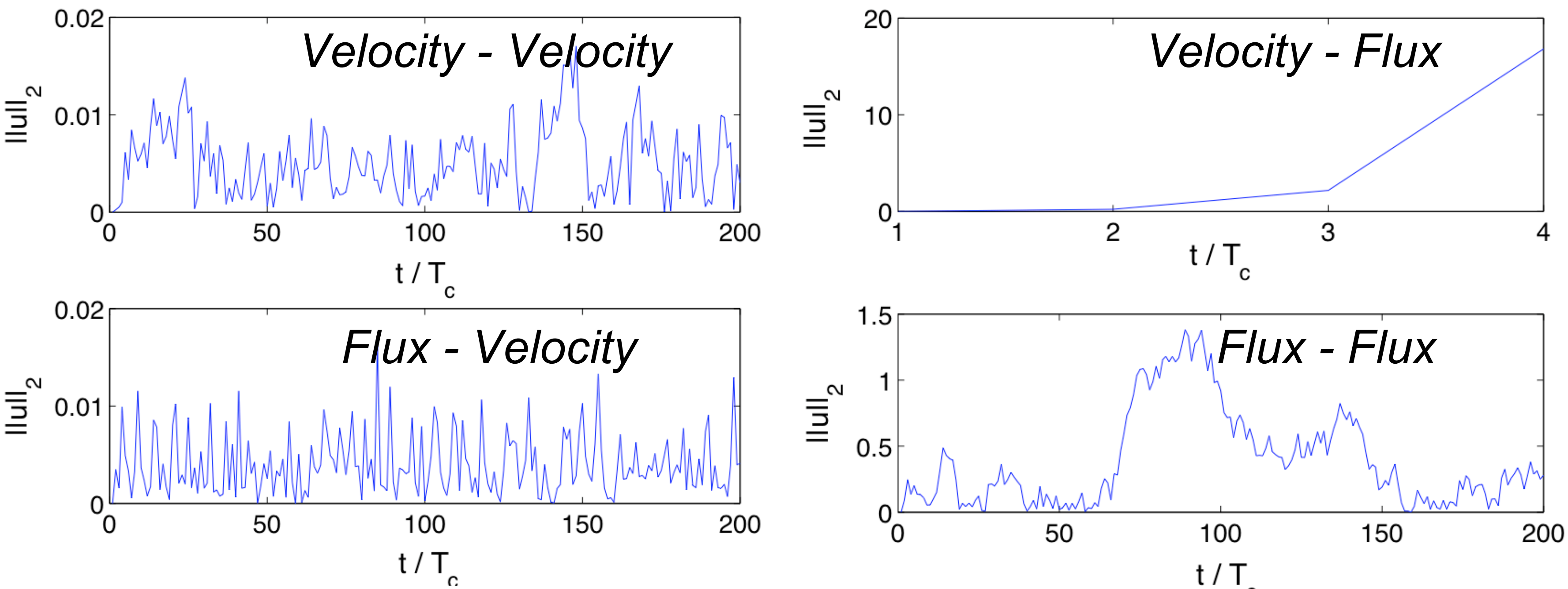
Numerical result for the static problem:

$$T_c = 10\Delta t$$



Numerical result for the static problem:

$$T_c = 1.67 \times 10^3$$



Analysis of the problem for “$T_c = +\infty$”

Velocity - Velocity coupling scheme:

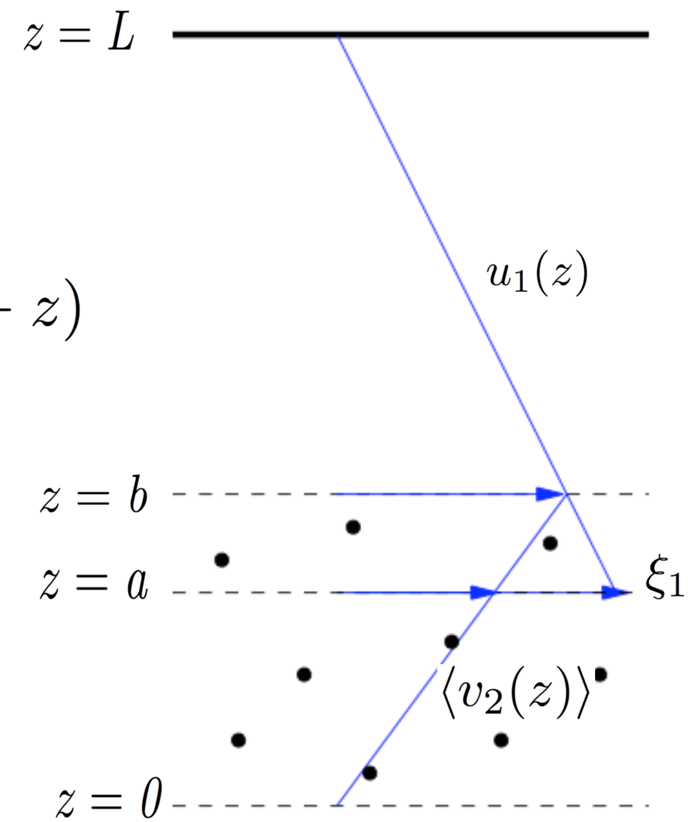
$$u_1(z) = \frac{L-z}{L-a}\xi_1$$

$$u_2(z) = \left(\frac{a(L-b)}{b(L-a)^2}\xi_1 + \frac{1}{L-a}\xi_2\right)(L-z)$$

$$u_n(z) = \left(\sum_{i=1}^{n} k_{vv}^{n-i}\xi_i\right)\frac{L-z}{L-a}$$

$$k_{vv} = \frac{a(L-b)}{b(L-a)} \approx 1 - c/b$$

--- *Amplification factor*



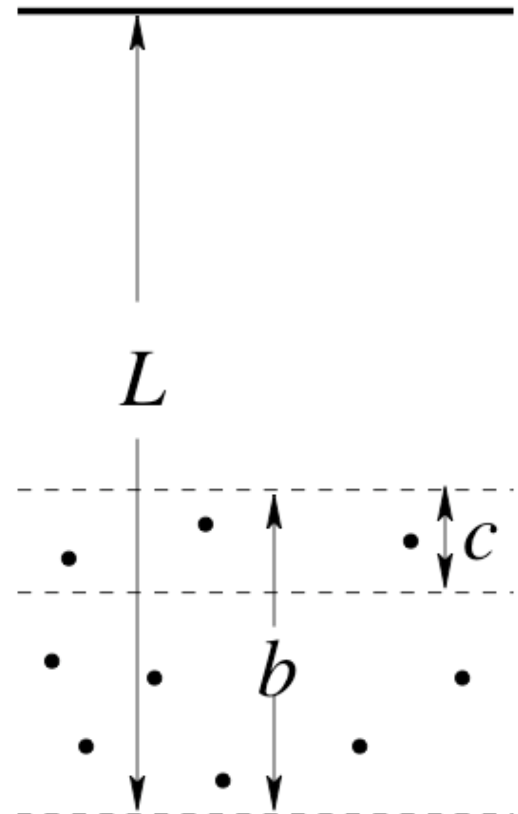
$$\langle \|u_n\|_2 \rangle \le \left(\frac{1}{3(1-k_{vv}^2)}\right)^{1/2}\sigma_v$$

where $\sigma_v^2 = \langle \xi_i^2 \rangle$

Analysis of the problem for "$T_c = +\infty$"

The numerical solution has the following form:

$$u_n(z) = \left(\sum_{i=1}^{n} k^{n-i}\xi_i\right) g(z)$$



$$k_{vv} = \frac{a(L-b)}{b(L-a)} \approx 1 - c/b \qquad |k_{vv}| < 1$$

$$k_{fv} = \frac{a}{a-L} \approx -a/L \qquad |k_{fv}| \ll 1$$

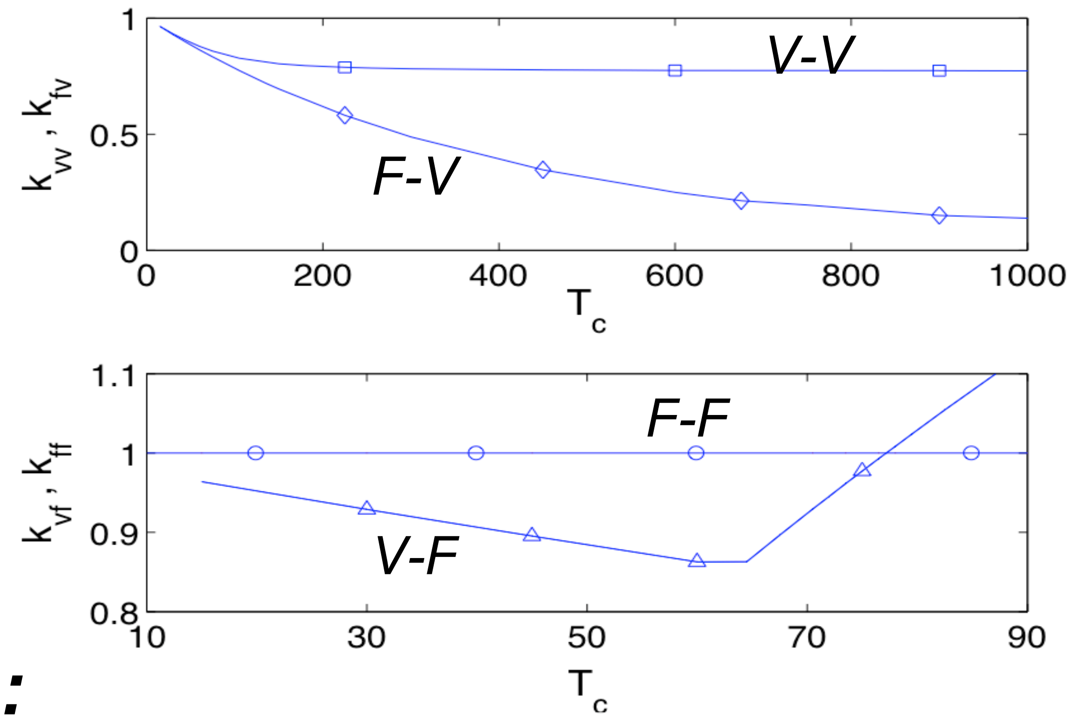
$$k_{vf} = \frac{b-L}{b} \approx -L/b \qquad |k_{vf}| \gg 1$$

$$k_{ff} = 1 \qquad |k_{ff}| = 1$$

$$g_{vv}(z) = g_{fv}(z) = (L-z)/(L-a)$$

$$g_{vf}(z) = g_{ff}(z) = z - L$$

Analysis of the problem for finite T_c



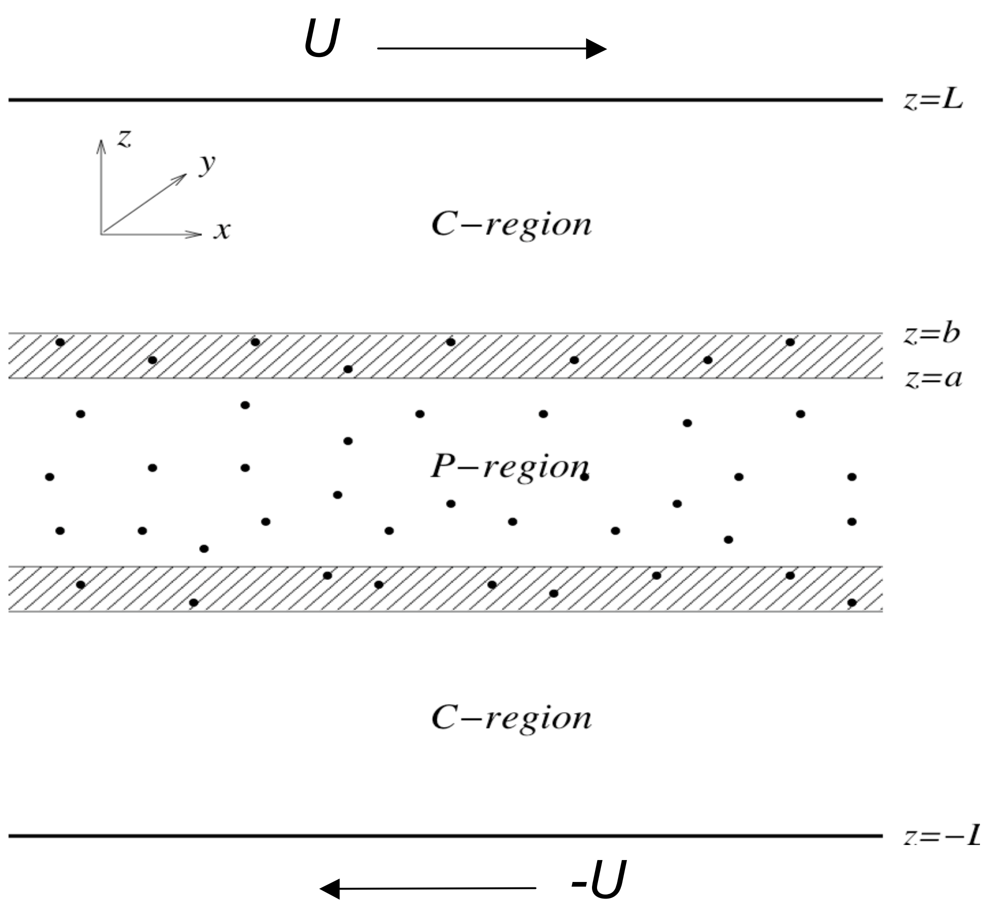
Conclusions:

(i). The VV and FV schemes are stable;

(ii). Velocity-Flux is stable when $T_c < T^*$, and unstable when $T_c > T^*$

(iii). Flux-Flux scheme is weakly unstable.

A dynamic problem: Impulsively started shear flow



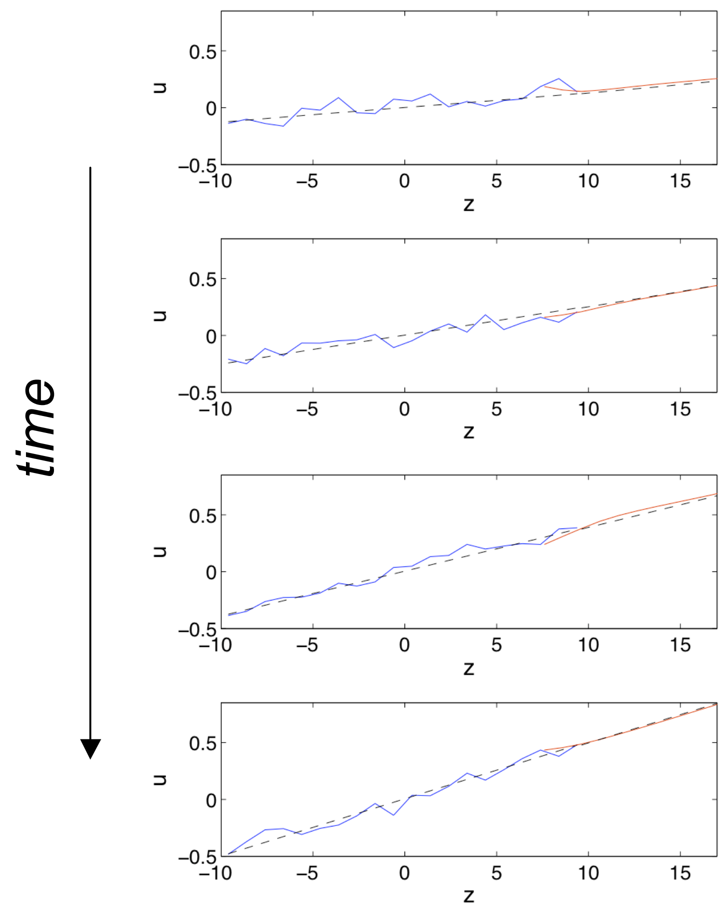
$$\rho \partial_t u - \partial_z \tau = 0$$

$$\tau = \mu \partial_z u$$

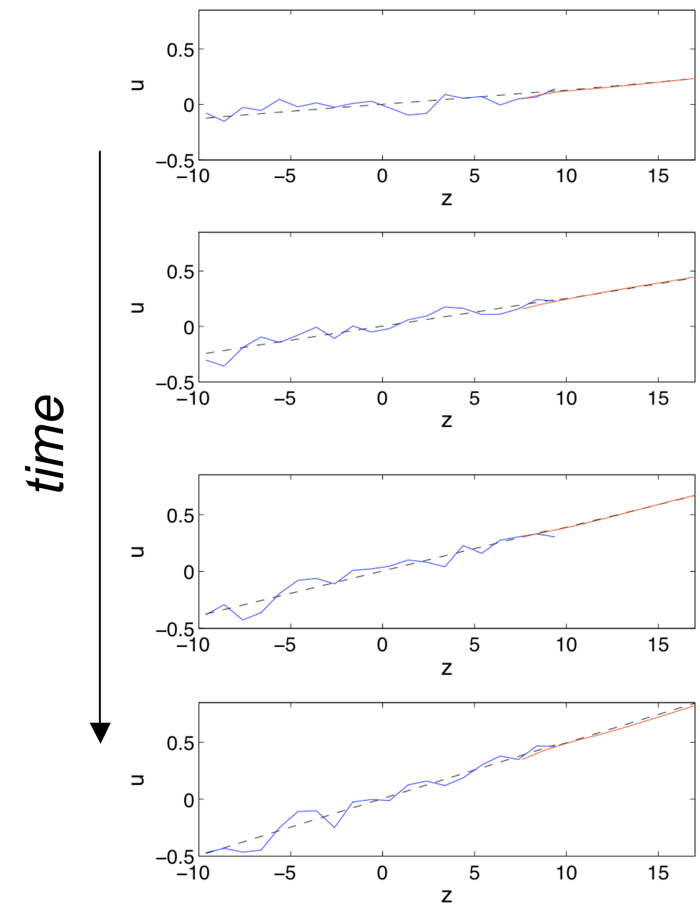
$$u(L, t) = U$$

$$u(x, 0) = 0$$

Numerical results: $T_c = \Delta t$

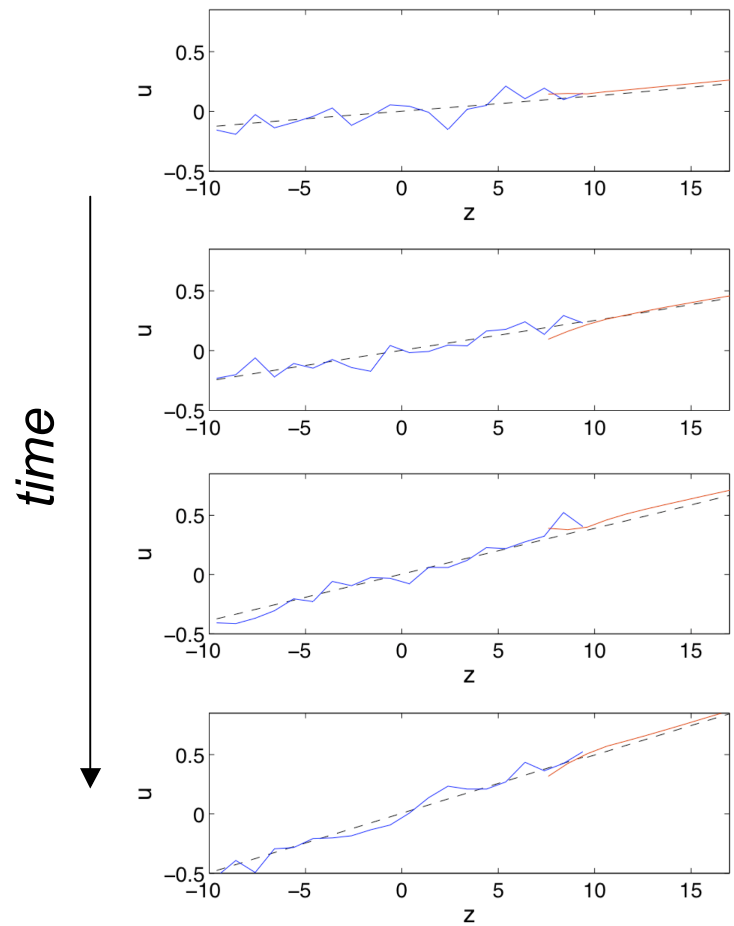


Velocity-Velocity

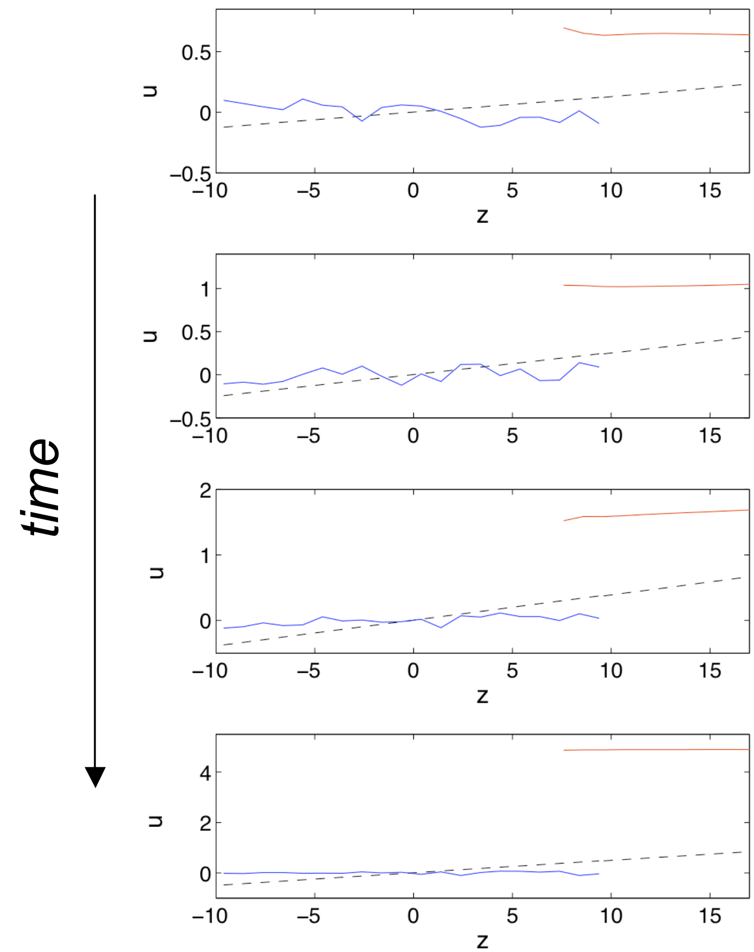


Flux-Velocity

Numerical results: $T_c = \Delta t$

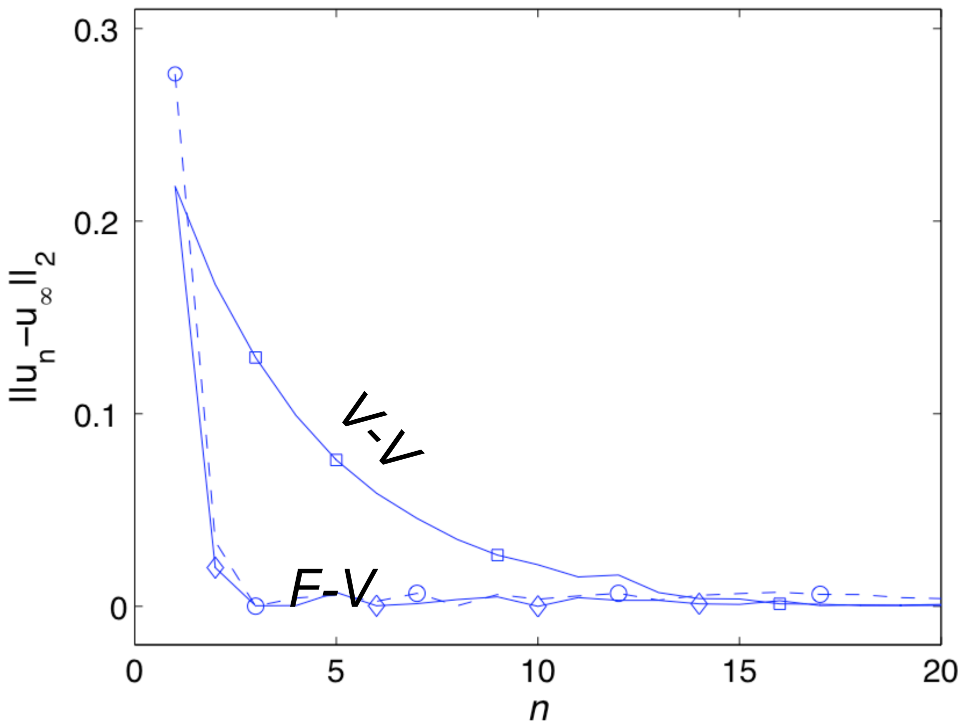


Velocity-Flux



Flux-Flux

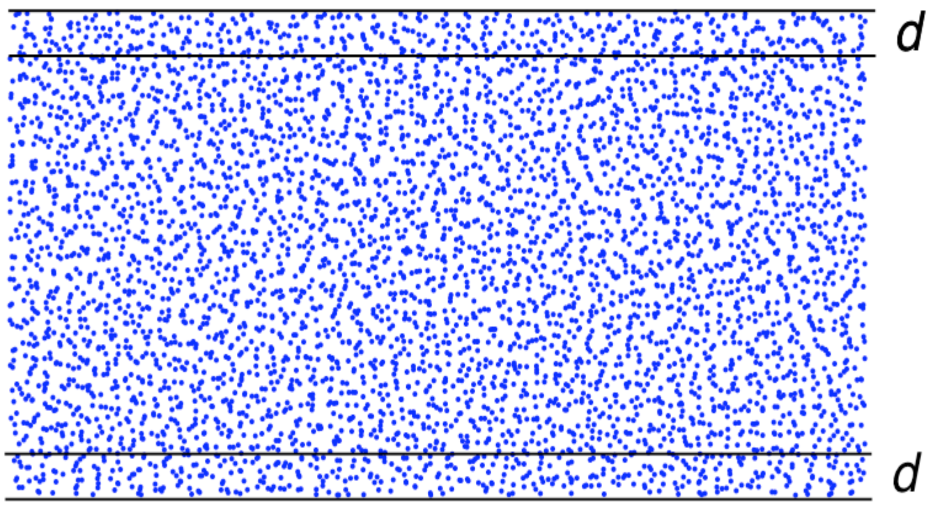
Steady state calculation: Comparison of convergence rate

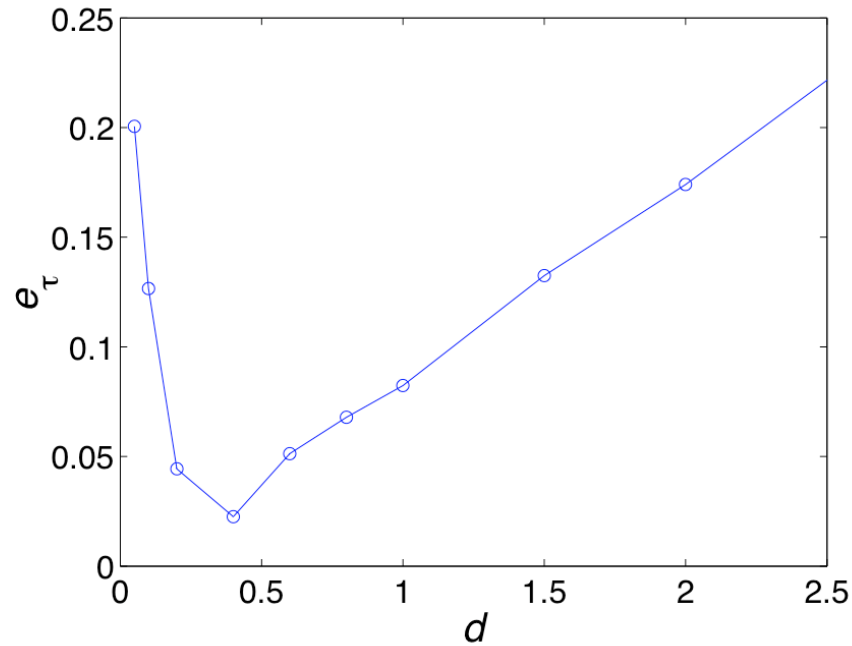


$$k_{vv} = 1 - \frac{\text{overlapping region}}{\text{particle region}} = 0.7 \qquad T_c = 8000\Delta t$$

$$k_{fv} = \frac{\text{size of p-region}}{\text{system size}} = 0.08$$

Assessment of the error from the imposition of velocity BC in MD



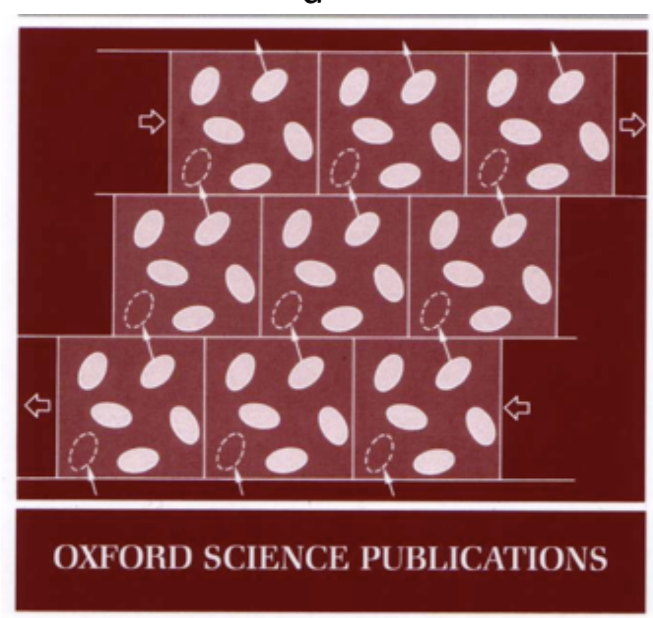


$$e_\tau \quad = \text{Error of stress}$$

$$= |\tau(d) - \tilde{\tau}| / |\tilde{\tau}|$$

$$\tilde{\tau} = \text{exact shear stress}$$

from MD using Lees-Edwards BC



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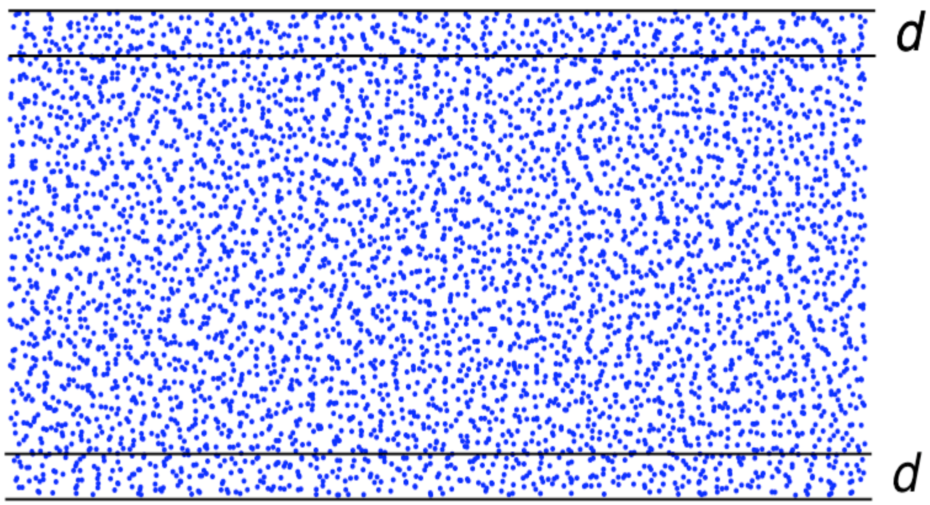

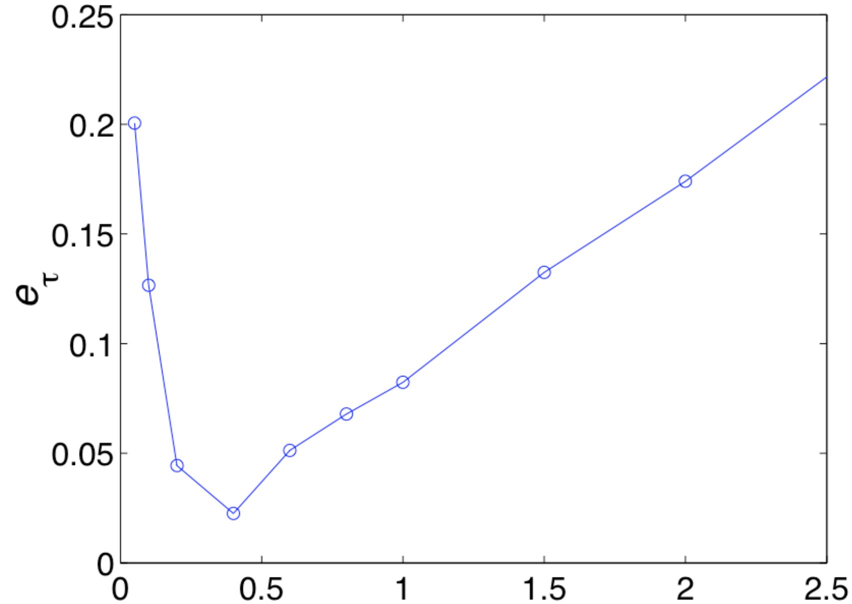

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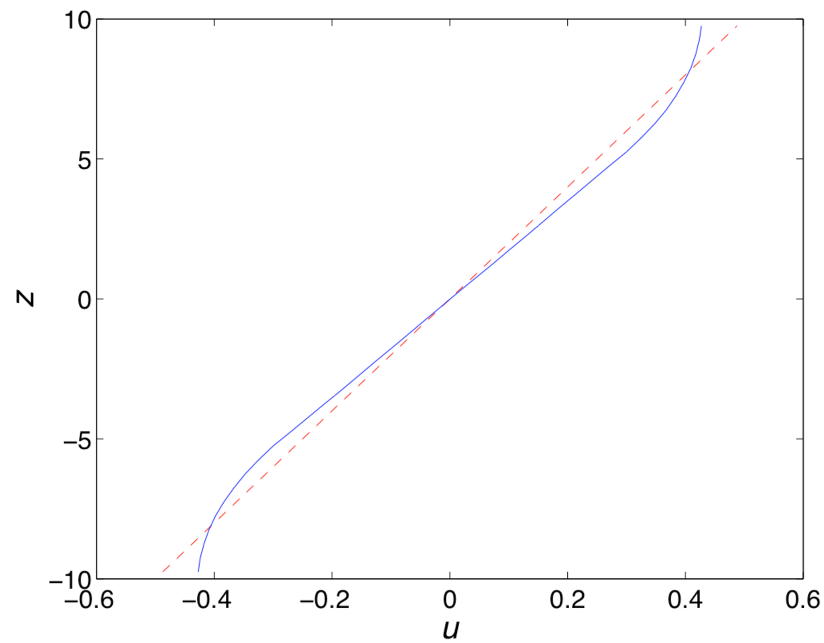
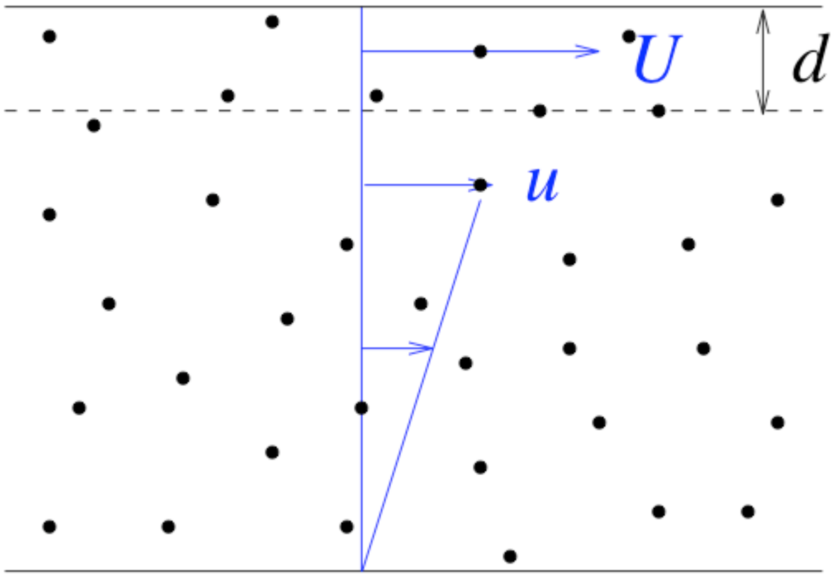


Assessment of the error for $\mathbf{d < r_c}$



$$\mu_d (U - u)/l = \mu_\infty u/L$$

$$u = \frac{\tilde{\mu}_d}{\tilde{\mu}_d + \tilde{l}} U$$

$$e_\tau = \left| \frac{u}{U} - 1 \right| = \frac{\tilde{l}}{\tilde{l} + \tilde{\mu}_d}$$

$\mu_d = \mu_\infty$:= viscosity in bulk when $d > r_c$

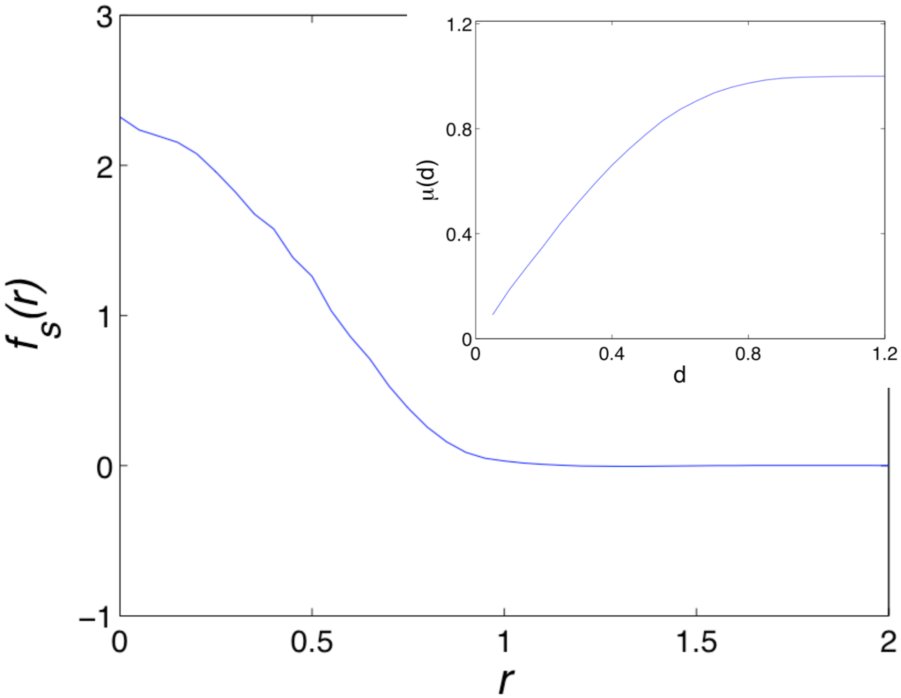
$\mu_d < \mu_\infty$ when $d < r_c$

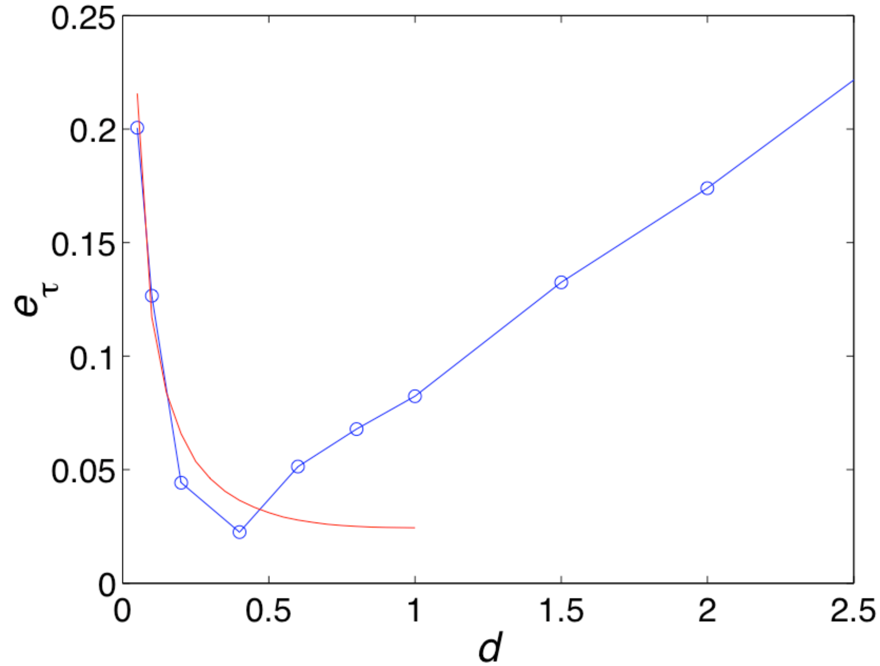
$l = O(1\sigma)$ $\quad L =$ system size

$\tilde{\mu}_d = \mu_d / \mu_\infty$ $\quad \tilde{l} = l/L$

Error of the stress: Analysis vs. Numerics

$$\tilde{\mu}_d = \frac{\int_0^d f_s(z)\,dz}{\int_0^\infty f_s(z)\,dz}$$





Red curve: $e_\tau = \frac{\tilde{l}}{\tilde{l}+\tilde{\mu}_d}$

Blue curve: Numerics

Summary:

(1). Stability of different coupling schemes.
Schemes based on flux coupling is weakly unstable. Flux-velocity scheme performs the best.

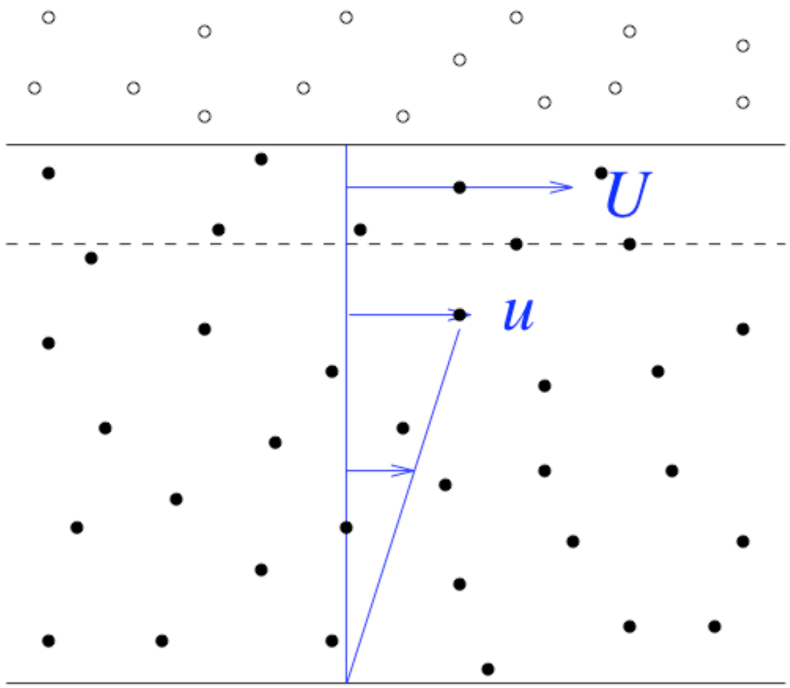
(2). Error introduced when imposing velocity boundary condition in MD.

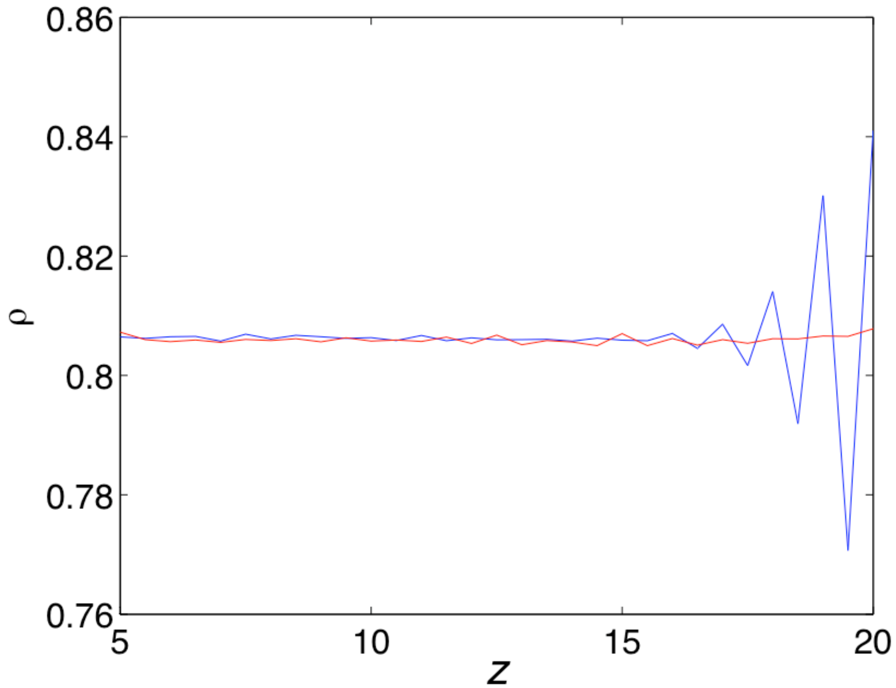
Ongoing work:

Boundary conditions for non-equilibrium MD;

Incorporating fluctuations in the BC of MD;
Coupling fluctuating hydrodynamic with molecular dynamics.

Improved numerical scheme: Using ghost particles





- *Less disturbance to fluid structure*
- *Mass reservoir for 2d velocity field*

References:

- Analytical and Numerical study of coupled atomistic-continuum methods for fluids*, preprint*

- Boundary conditions for the moving contact line problem, *Physics of Fluids, **19**, 022101 (2007)*

- Heterogeneous multiscale method for the modeling of complex fluids and microfluidics, *J. Comp. Phys.* ***204,*** *1 (2005)*