Development of a Lattice Boltzmann-Based Oldroyd-B Model for Simulating Viscoelastic Fluids

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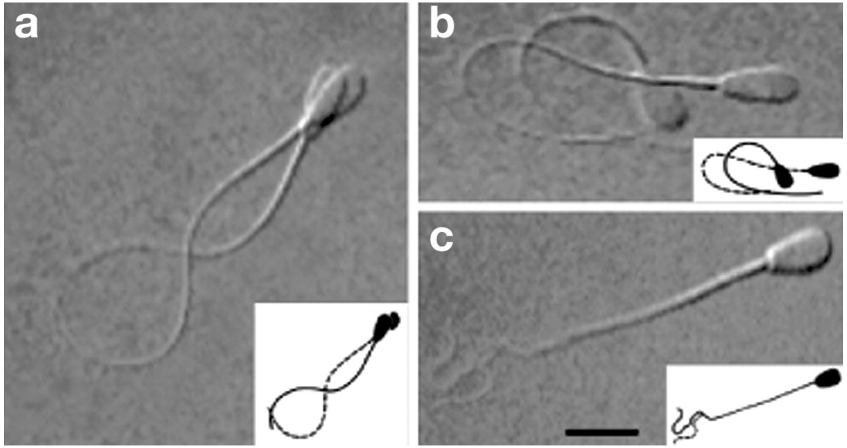
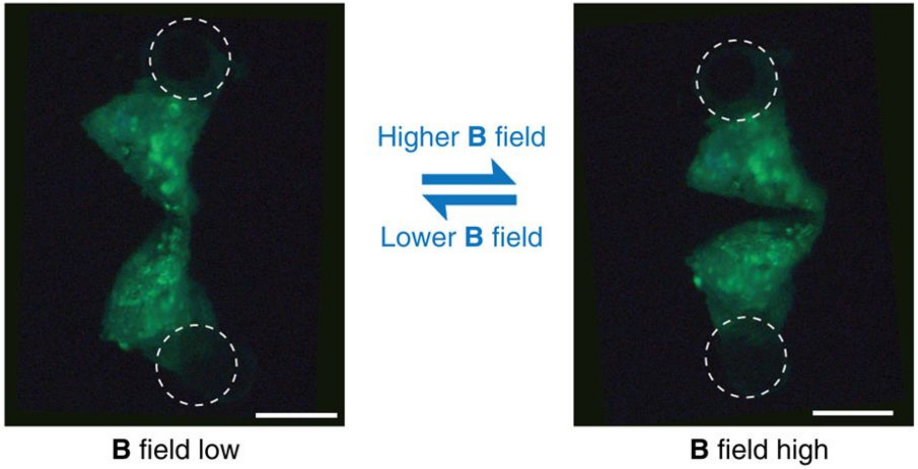
Swimmers in Complex Fluid

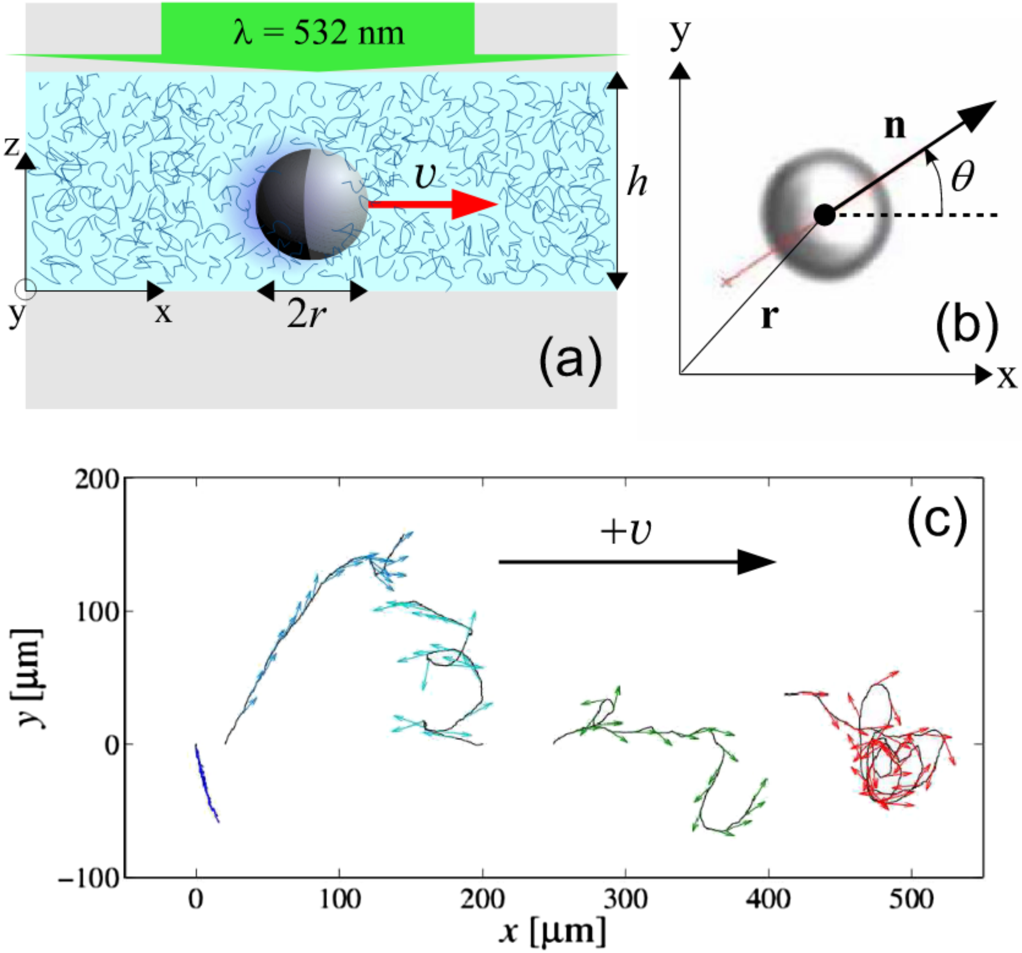


L. Fauci, R. Dillon *Annu. Rev. Fluid. Mech.* (2006)

T. Qiu et al. *Nature Communications* (2014)



Our Inspiration



J. Gomez-Solano et al. *PRL* (2016)

Continuum Model

- Navier-Stokes Equations

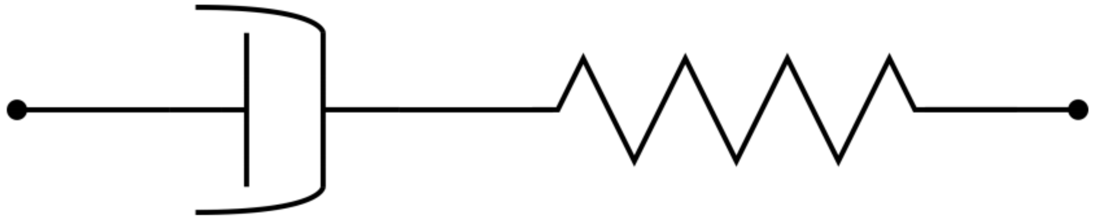
$$\rho \frac{D}{Dt} = \nabla \cdot \bar{\boldsymbol{\sigma}} = -\nabla p + \eta_s \nabla^2 \boldsymbol{u} + \boldsymbol{f} + \boldsymbol{F}_p$$

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

- How can we model polymer forces?

$$\boldsymbol{F}_p = \nabla \cdot \bar{\boldsymbol{\tau}} \qquad \frac{\partial \bar{\boldsymbol{\tau}}}{\partial t} = ???$$

Linear Maxwell Model



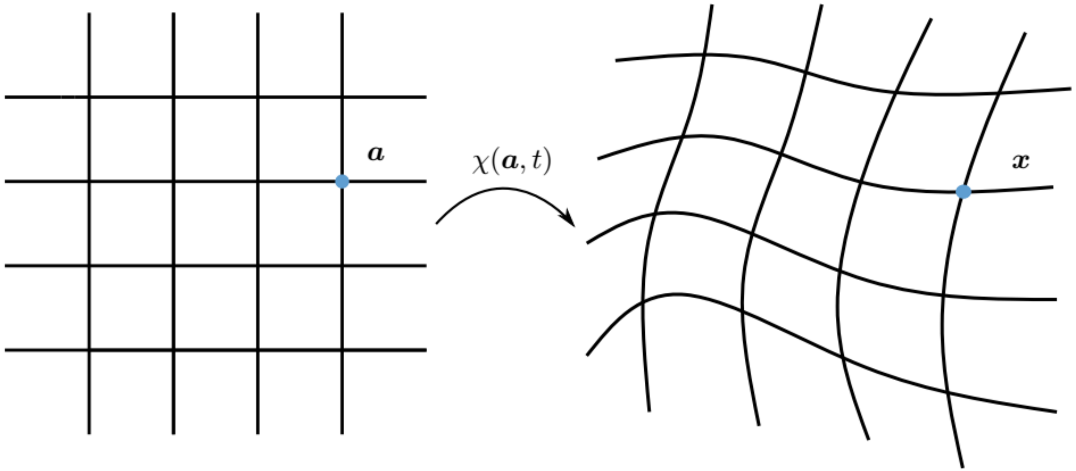
$$\sigma = \eta\dot{\gamma} \qquad\qquad \sigma = k\gamma$$

Maxwell Model: $\quad \sigma + \lambda\dot{\sigma} = \eta\dot{\gamma}, \quad \lambda := \dfrac{\eta}{k}$

$$\boxed{\sigma(t) = \frac{1}{\lambda}\int_{-\infty}^{t} e^{-\frac{t-t'}{\lambda}}\eta\dot{\gamma}(t')dt'}$$

Generalization to Three Dimensions

$$\sigma + \lambda \dot{\sigma} = \eta \dot{\gamma} \quad \xrightarrow{?} \quad \bar{\boldsymbol{\sigma}} + \lambda \frac{\partial \bar{\boldsymbol{\sigma}}}{\partial t} = \eta \dot{\bar{\boldsymbol{\gamma}}} \qquad \dot{\bar{\boldsymbol{\gamma}}} := \nabla \boldsymbol{u} + \nabla \boldsymbol{u}^\intercal$$



$$\overset{\nabla}{\bar{\boldsymbol{\sigma}}} := \frac{\partial \bar{\boldsymbol{\sigma}}}{\partial t} + (\boldsymbol{u} \cdot \nabla) \bar{\boldsymbol{\sigma}} - \bar{\boldsymbol{\sigma}} \cdot \nabla \boldsymbol{u} - (\nabla \boldsymbol{u})^\intercal \cdot \bar{\boldsymbol{\sigma}}$$

$$\sigma + \lambda \dot{\sigma} = \eta \dot{\gamma} \quad \xrightarrow{!} \quad \boxed{\bar{\boldsymbol{\tau}} + \lambda_p \overset{\nabla}{\bar{\boldsymbol{\tau}}} = \eta_p \dot{\bar{\boldsymbol{\gamma}}}}$$

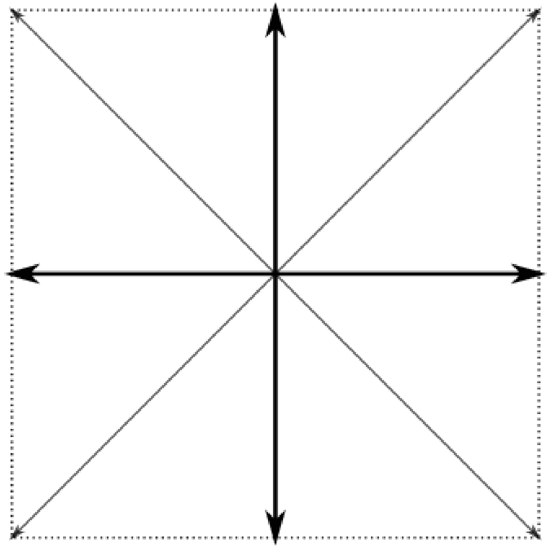
Differential Equations

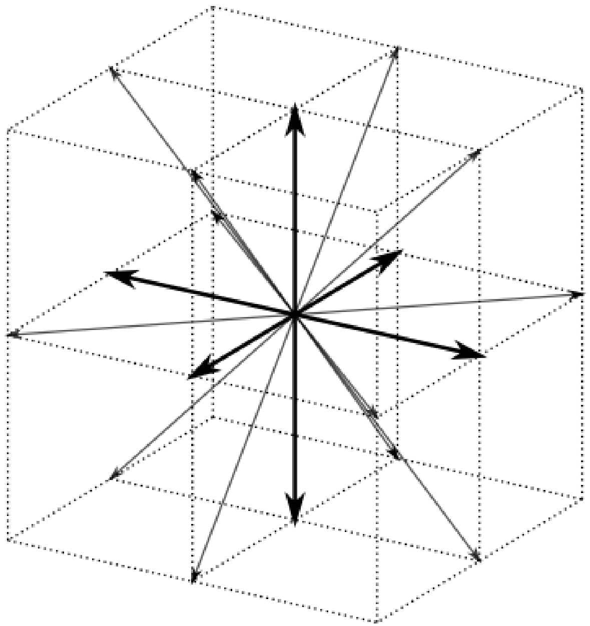
$$\rho \frac{\mathrm{D}\boldsymbol{u}}{\mathrm{D}t} = -\nabla p + \eta_s \nabla^2 \boldsymbol{u} + \boldsymbol{f} + \boldsymbol{F}_p$$

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

$$\frac{\partial \bar{\bar{\boldsymbol{\tau}}}}{\partial t} + (\boldsymbol{u} \cdot \nabla)\bar{\bar{\boldsymbol{\tau}}} = (\bar{\bar{\boldsymbol{\tau}}} \cdot \nabla \boldsymbol{u} + (\nabla \boldsymbol{u})^\intercal \cdot \bar{\bar{\boldsymbol{\tau}}}) + \frac{1}{\lambda_p}(\eta_p \dot{\bar{\bar{\gamma}}} - \bar{\bar{\boldsymbol{\tau}}})$$

Lattice Boltzmann





$$f_i(\boldsymbol{x} + \boldsymbol{c}_i \delta t, t + \delta t) = f_i(\boldsymbol{x}, t) + \frac{\delta t}{\lambda} \left(f_i^{\mathrm{eq}}(\boldsymbol{x}) - f_i(\boldsymbol{x}, t) \right)$$

Oldroyd-B Scheme

$$\rho \frac{\mathrm{D}\boldsymbol{u}}{\mathrm{D}t} = -\nabla p + \eta_s \nabla^2 \boldsymbol{u} + \boldsymbol{F}_p + \boldsymbol{f}$$

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

$$\frac{\partial \bar{\boldsymbol{\tau}}}{\partial t} + \underbrace{(\boldsymbol{u} \cdot \nabla)\bar{\boldsymbol{\tau}}}_{\bar{\boldsymbol{A}}_{\mathrm{adv}}(\bar{\boldsymbol{\tau}}, t)} = \underbrace{\left(\bar{\boldsymbol{\tau}} \cdot \nabla \boldsymbol{u} + (\nabla \boldsymbol{u})^{\intercal} \cdot \bar{\boldsymbol{\tau}}\right) + \frac{1}{\lambda_p}\left(\eta_p \dot{\bar{\boldsymbol{\gamma}}} - \bar{\boldsymbol{\tau}}\right)}_{\bar{\boldsymbol{A}}_{\mathrm{rel}}(\bar{\boldsymbol{\tau}}, t)}$$

Oldroyd-B Scheme

$$\rho \frac{\mathrm{D}\boldsymbol{u}}{\mathrm{D}t} = -\nabla p + \eta_s \nabla^2 \boldsymbol{u} + \boldsymbol{F}_p + \boldsymbol{f}$$

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

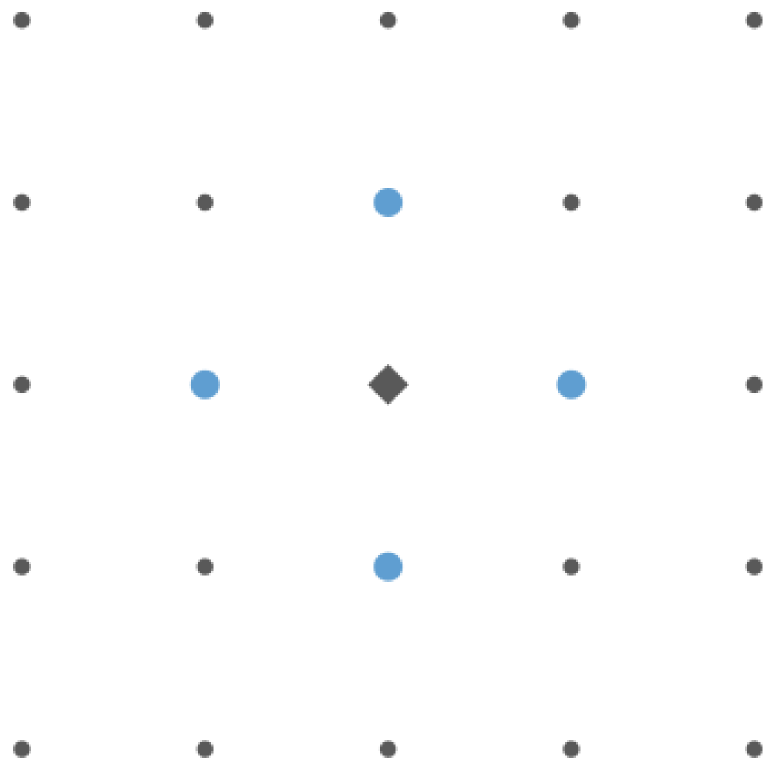
$$\bar{\boldsymbol{\tau}}(\boldsymbol{x}, t + \Delta t) = \bar{\boldsymbol{\tau}}(\boldsymbol{x}, t) - \Delta t \bar{\boldsymbol{A}}_{\mathrm{adv}}(\bar{\boldsymbol{\tau}}, t) + \Delta t \bar{\boldsymbol{A}}_{\mathrm{rel}}(\bar{\boldsymbol{\tau}}, t)$$

Velocity and Stress Derivatives

$$\bar{\boldsymbol{A}}_{\mathrm{rel}}(\bar{\boldsymbol{\tau}}, t) = \left(\bar{\boldsymbol{\tau}} \cdot \nabla \boldsymbol{u} + (\nabla \boldsymbol{u})^{\intercal} \cdot \bar{\boldsymbol{\tau}}\right)$$

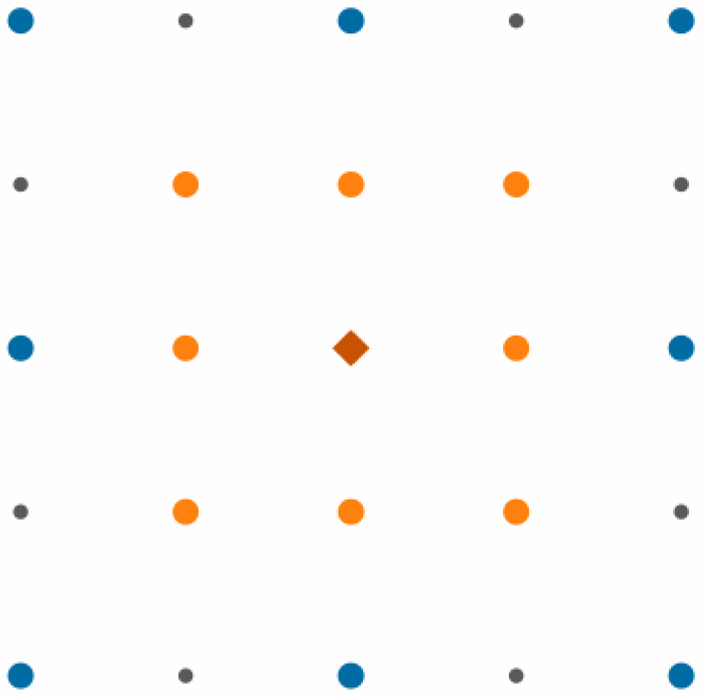
$$+ \frac{1}{\lambda_p} \left(\eta_p \dot{\bar{\boldsymbol{\gamma}}} - \bar{\boldsymbol{\tau}}\right)$$

$$\boldsymbol{F}_p = \nabla \cdot \bar{\boldsymbol{\tau}}$$



Stress Advection

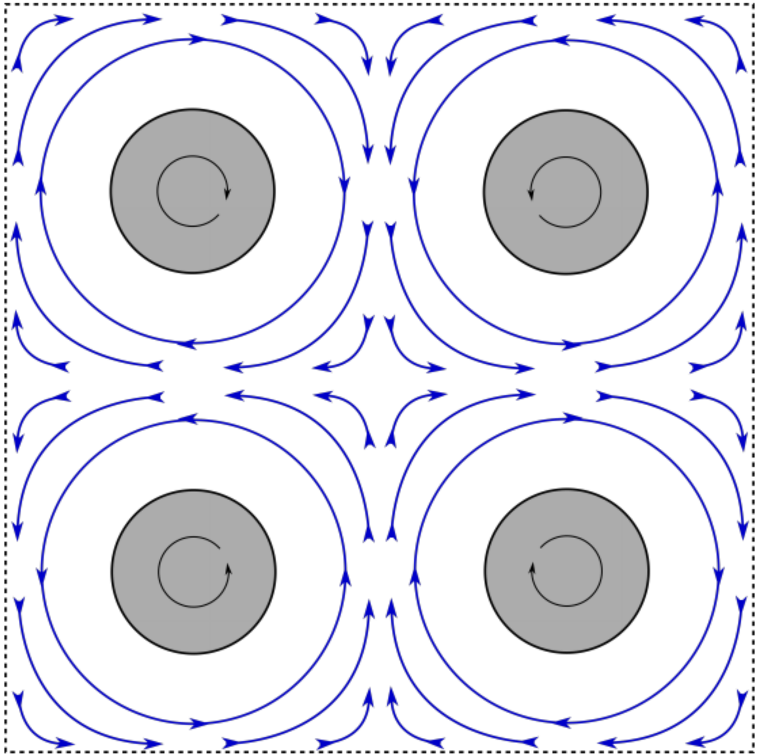
$$\bar{\boldsymbol{A}}_{\mathrm{adv}}(\bar{\boldsymbol{\tau}}, t) := (\boldsymbol{u} \cdot \nabla)\bar{\boldsymbol{\tau}}$$



$$\begin{aligned}\rho\delta t \bar{\boldsymbol{A}}_{\mathrm{adv}}(\bar{\boldsymbol{\tau}}, t) = {} & \frac{3}{2}\sum_{i=1}^{q} \bar{\boldsymbol{\tau}}(\boldsymbol{x}, t) f_i(\boldsymbol{x}, t) \\ & - 2\sum_{i=1}^{q} \bar{\boldsymbol{\tau}}(\boldsymbol{x} - \boldsymbol{c}_i\delta t, t) f_i(\boldsymbol{x} - \boldsymbol{c}_i\delta t, t) \\ & + \frac{1}{2}\sum_{i=1}^{q} \bar{\boldsymbol{\tau}}(\boldsymbol{x} - 2\boldsymbol{c}_i\delta t, t) f_i(\boldsymbol{x} - 2\boldsymbol{c}_i\delta t, t)\end{aligned}$$

Four-Roll Mill

$$\boldsymbol{f} = f \sin\left(\frac{2\pi}{L}x\right)\cos\left(\frac{2\pi}{L}y\right)\boldsymbol{e}_x - f\cos\left(\frac{2\pi}{L}x\right)\sin\left(\frac{2\pi}{L}y\right)\boldsymbol{e}_y \longrightarrow \boldsymbol{u} = \alpha(x, -y)$$



$$\epsilon := \alpha\lambda_p \propto \mathrm{Wi}$$

Sol'n near Central Point:

$$\tau_{xx}(0,y) = \frac{2\eta_p\alpha}{1-2\epsilon} + C|y|^{\frac{1-2\epsilon}{\epsilon}}$$

$$\tau_{yy}(0,y) = -\frac{2\eta_p\alpha}{1+2\epsilon} + C|y|^{\frac{1+2\epsilon}{\epsilon}}$$

$$\tau_{xy}(0,y) = 0$$

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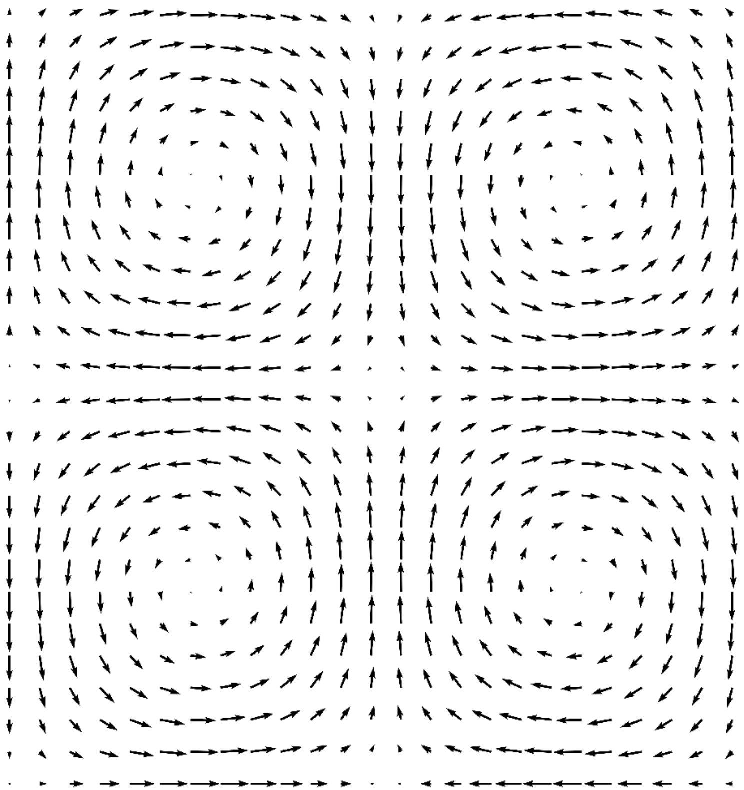

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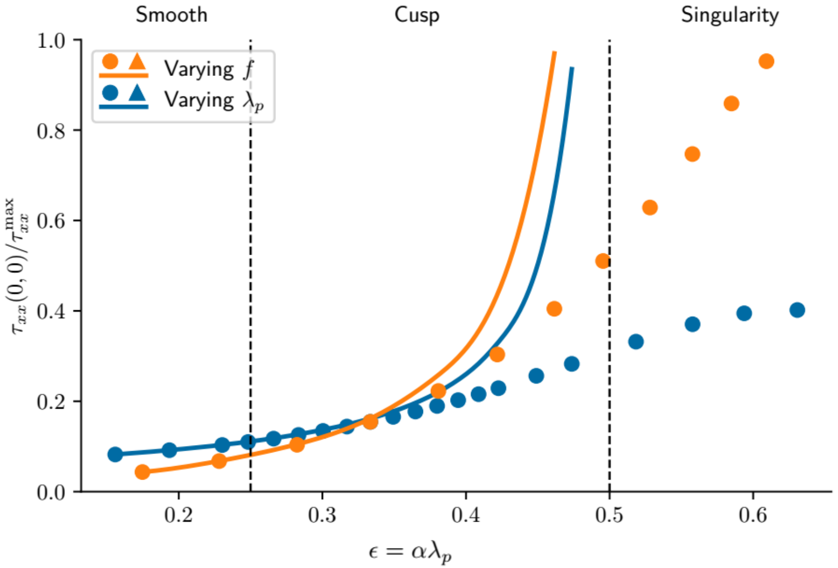
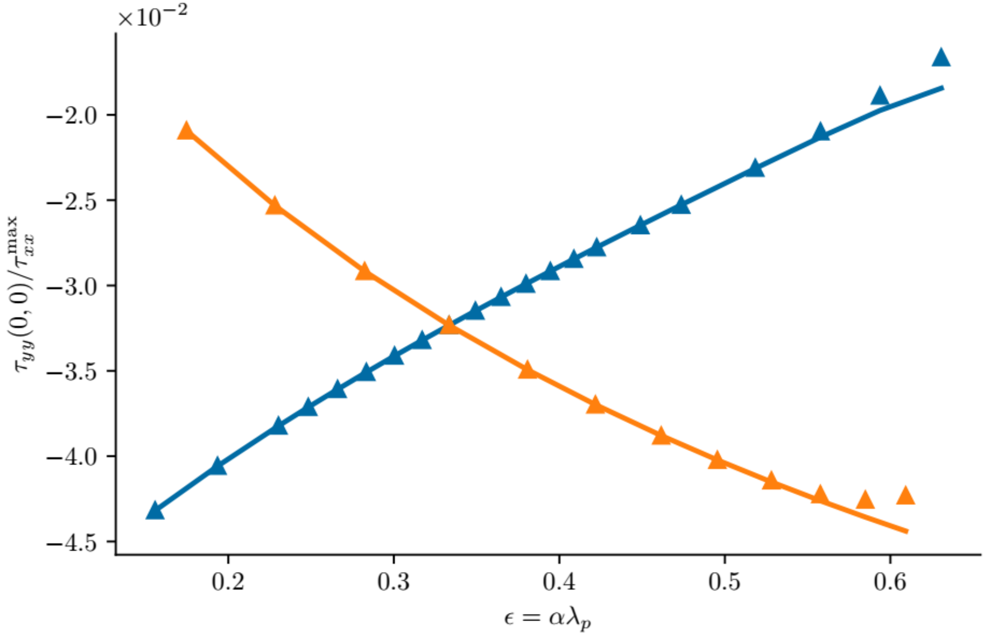
Center Point Stress

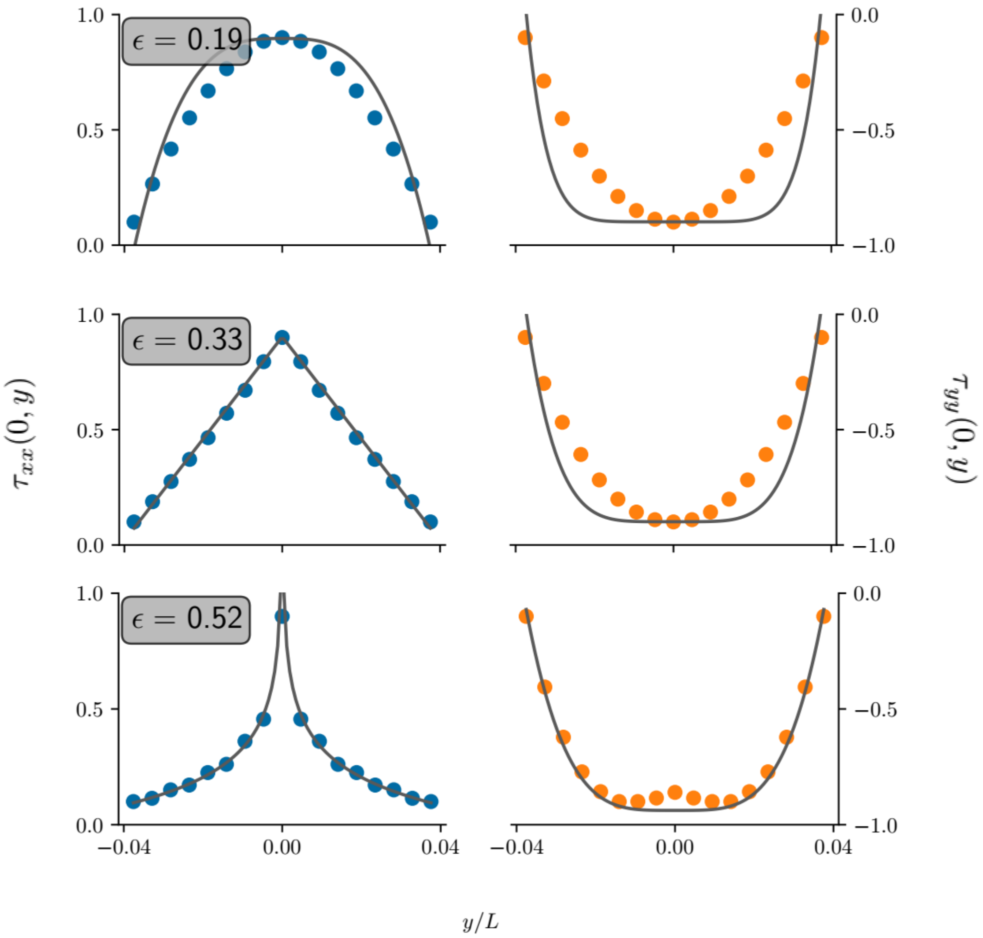


$$\tau_{xx}(0,0) = \frac{2\eta_p\alpha}{1-2\epsilon}$$

$$\tau_{yy}(0,0) = -\frac{2\eta_p\alpha}{1+2\epsilon}$$



Center Line Stress

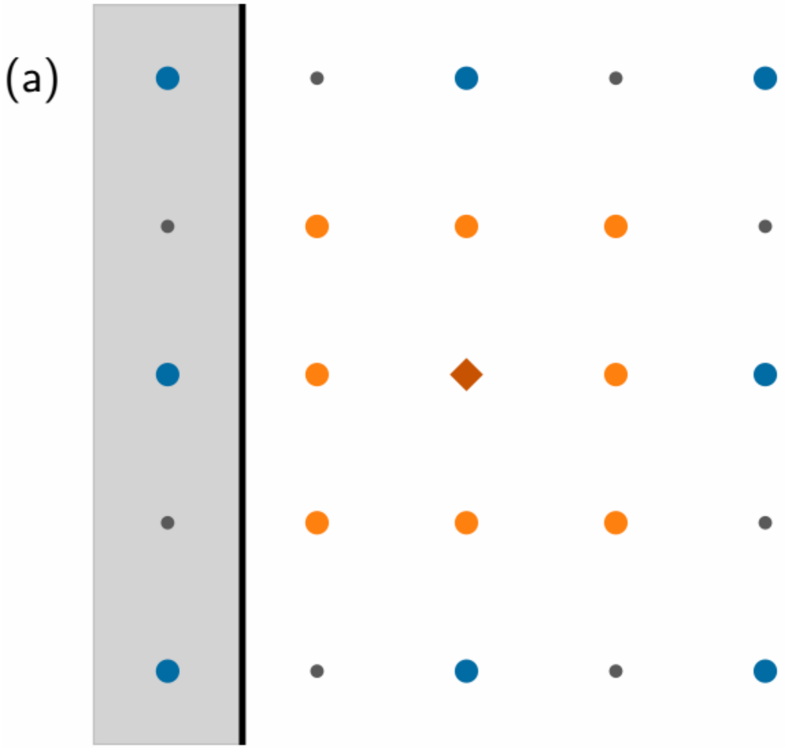


$$\tau_{xx}(0, y) = \frac{2\eta_p \alpha}{1 - 2\epsilon} + C|y|^{\frac{1-2\epsilon}{\epsilon}}$$

$$\tau_{yy}(0, y) = -\frac{2\eta_p \alpha}{1 + 2\epsilon} + C|y|^{\frac{1+2\epsilon}{\epsilon}}$$

$$\epsilon = \alpha \lambda_p \propto \mathrm{Wi}$$

Boundaries

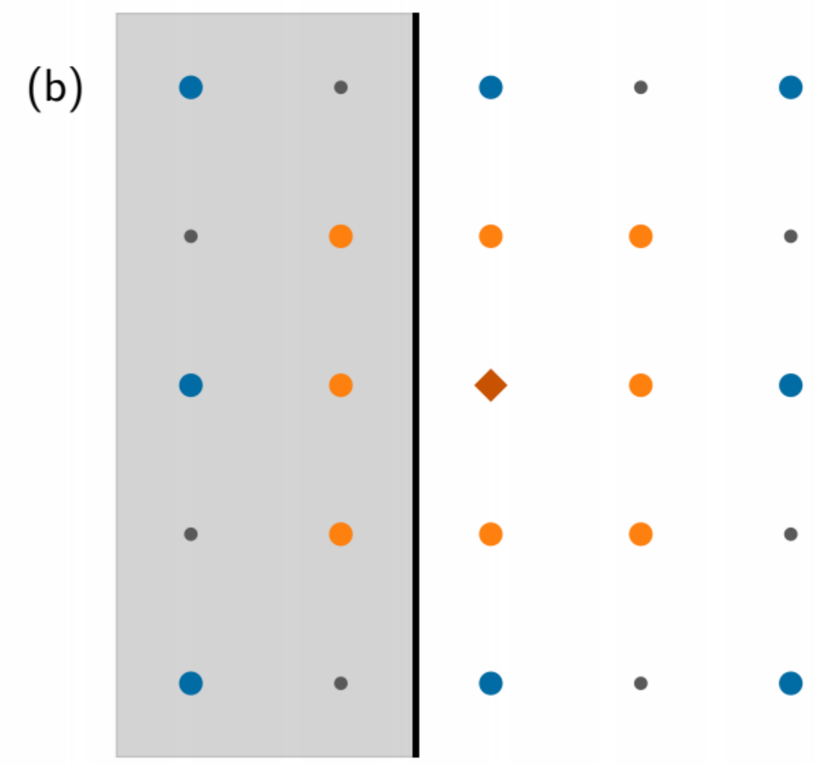


✓ $\boldsymbol{F}_p = \nabla \cdot \bar{\boldsymbol{\tau}}$

✓ $\dot{\bar{\gamma}} := \nabla \boldsymbol{u} + \nabla \boldsymbol{u}^{\intercal}$

✗ $\bar{\boldsymbol{A}}_{\mathrm{adv}}(\bar{\boldsymbol{\tau}}, t) := (\boldsymbol{u} \cdot \nabla)\bar{\boldsymbol{\tau}}$

Boundaries



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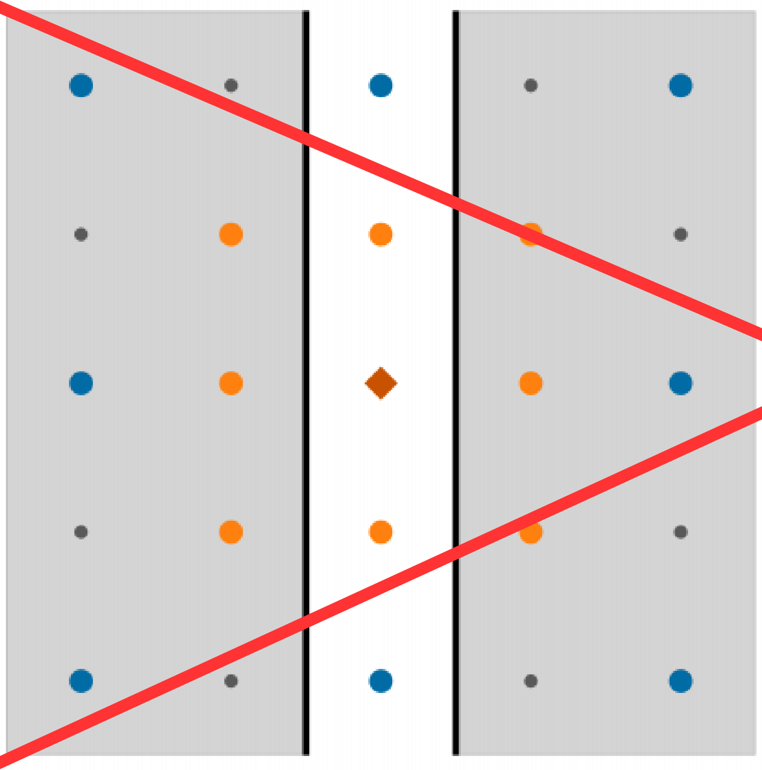
Boundaries

(c)



$$\boldsymbol{F}_p = \nabla \cdot \bar{\boldsymbol{\tau}}$$

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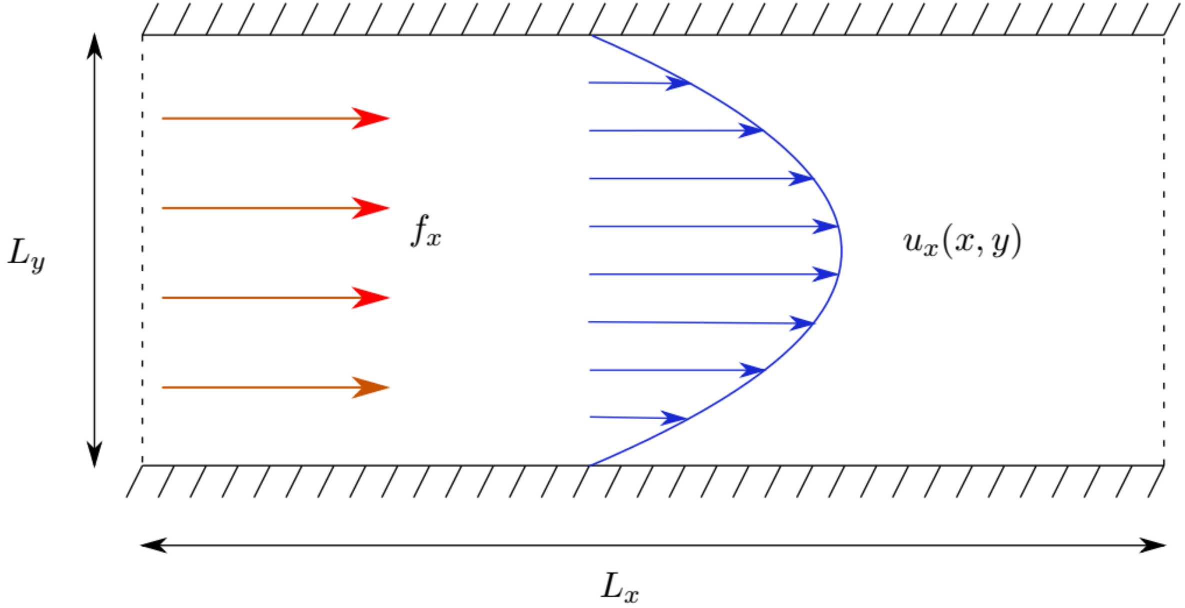
$$\bar{\boldsymbol{A}}_{\mathrm{adv}}(\bar{\boldsymbol{\tau}}, t) := (\boldsymbol{u} \cdot \nabla)\bar{\boldsymbol{\tau}}$$

Poiseuille Flow

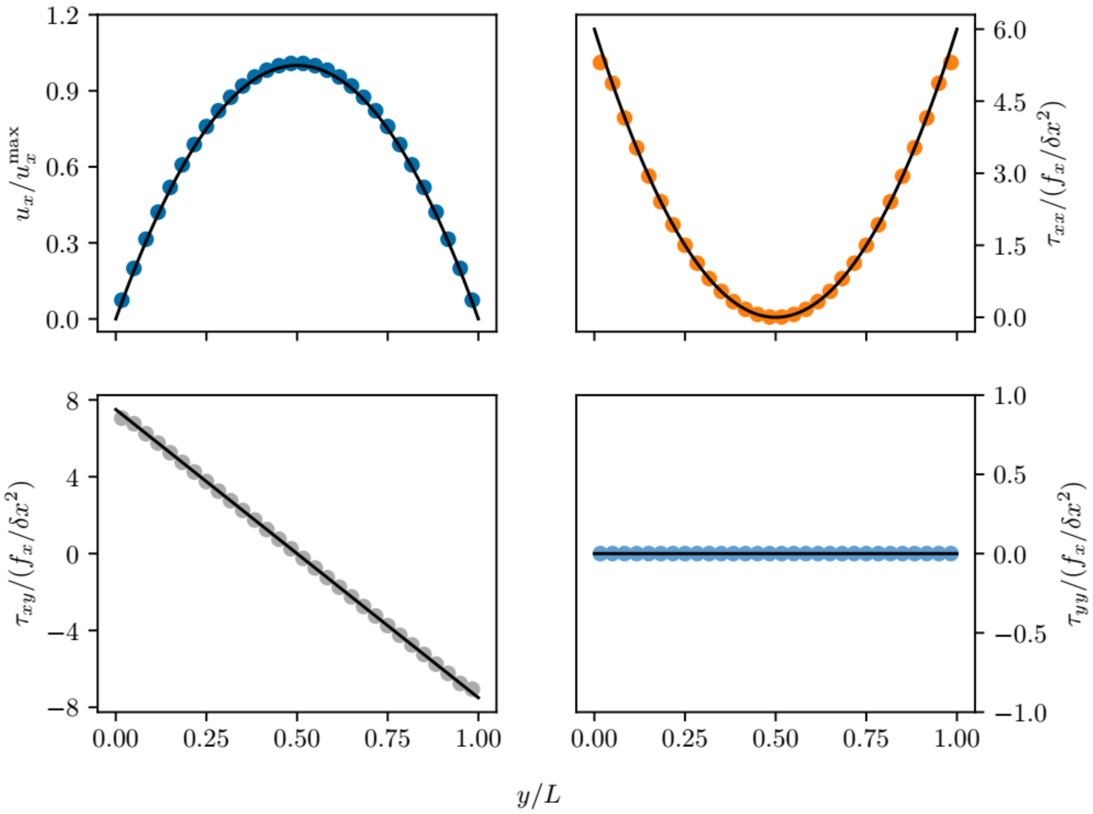


$$u_x = -\frac{f_x}{2}\left(\frac{y^2 - L_y y}{\eta_s + \eta_p}\right)$$

$$u_y = 0$$

$$\boxed{\tau_{xx} = 2\lambda_p \eta_p \left(\frac{\partial u_x}{\partial y}\right)^2 \qquad \tau_{xy} = \eta_p \frac{\partial u_x}{\partial y} \qquad \tau_{yy} = 0}$$

Pouiseuille Steady State

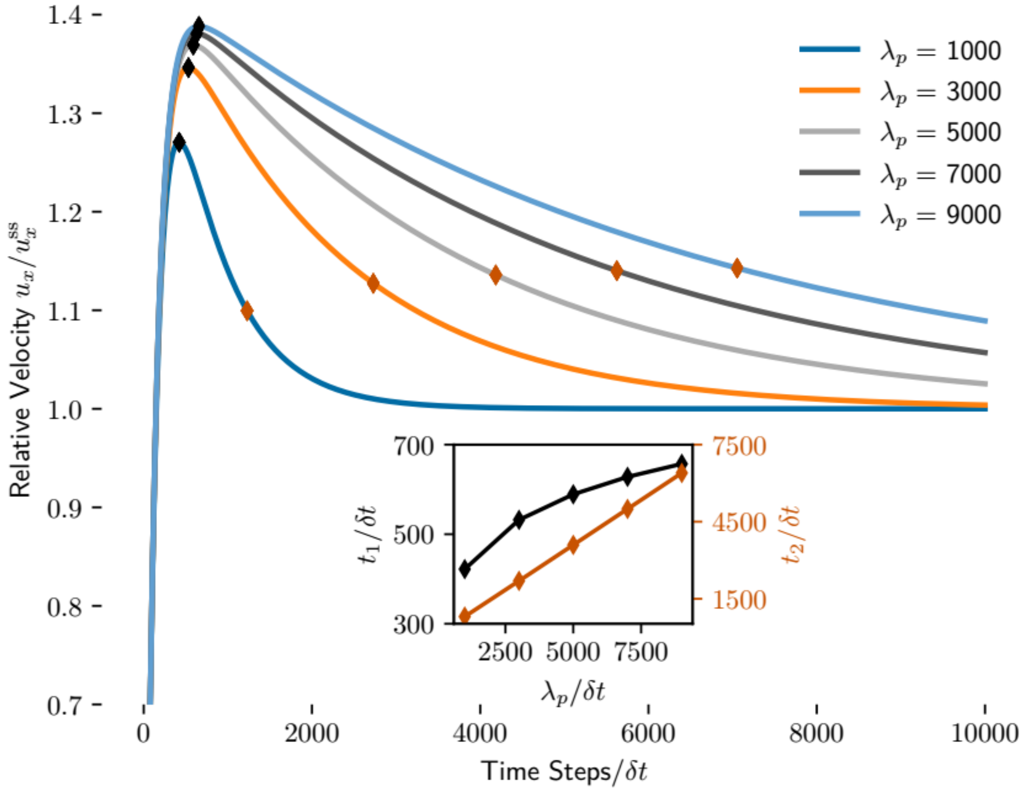


$$u_x = -\frac{f_x}{2}\left(\frac{y^2 - L_y y}{\eta_s + \eta_p}\right)$$

$$\tau_{xx} = 2\lambda_p \eta_p \left(\frac{\partial u_x}{\partial y}\right)^2$$

$$\tau_{xy} = \eta_p \frac{\partial u_x}{\partial y}$$

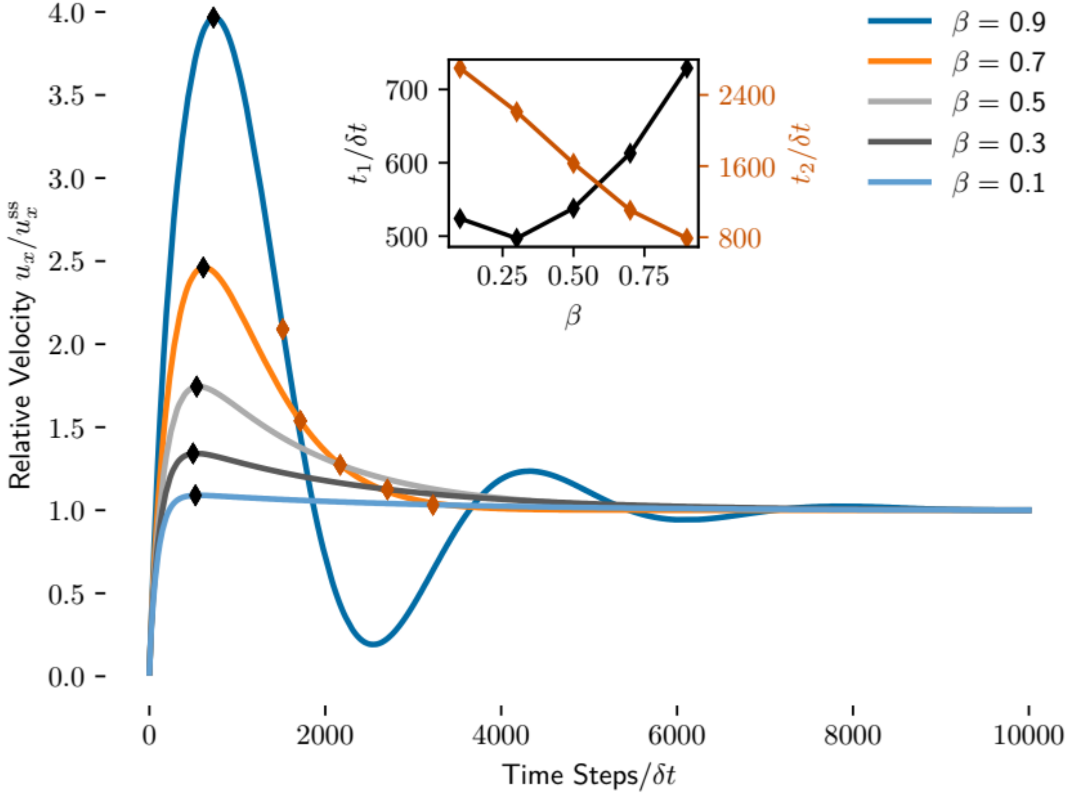
Velocity Overshoot



t_1 : Time of maximum

t_2 : Decay time

Velocity Overshoot

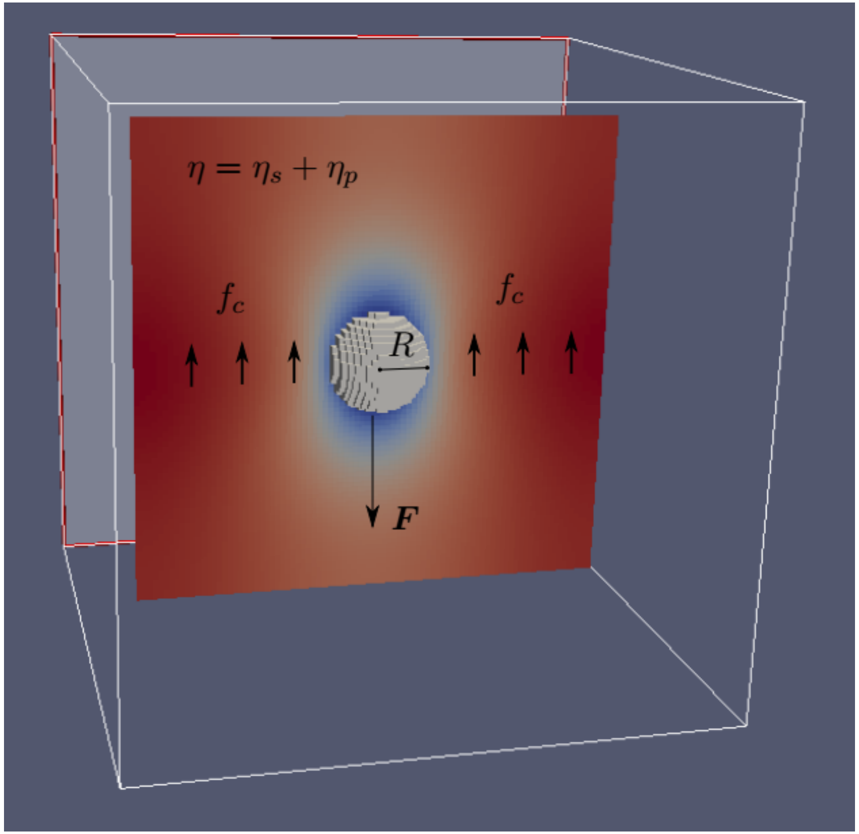


$$\beta = \frac{\eta_p}{\eta_s + \eta_p}$$

t_1 : Time of maximum

t_2 : Decay time

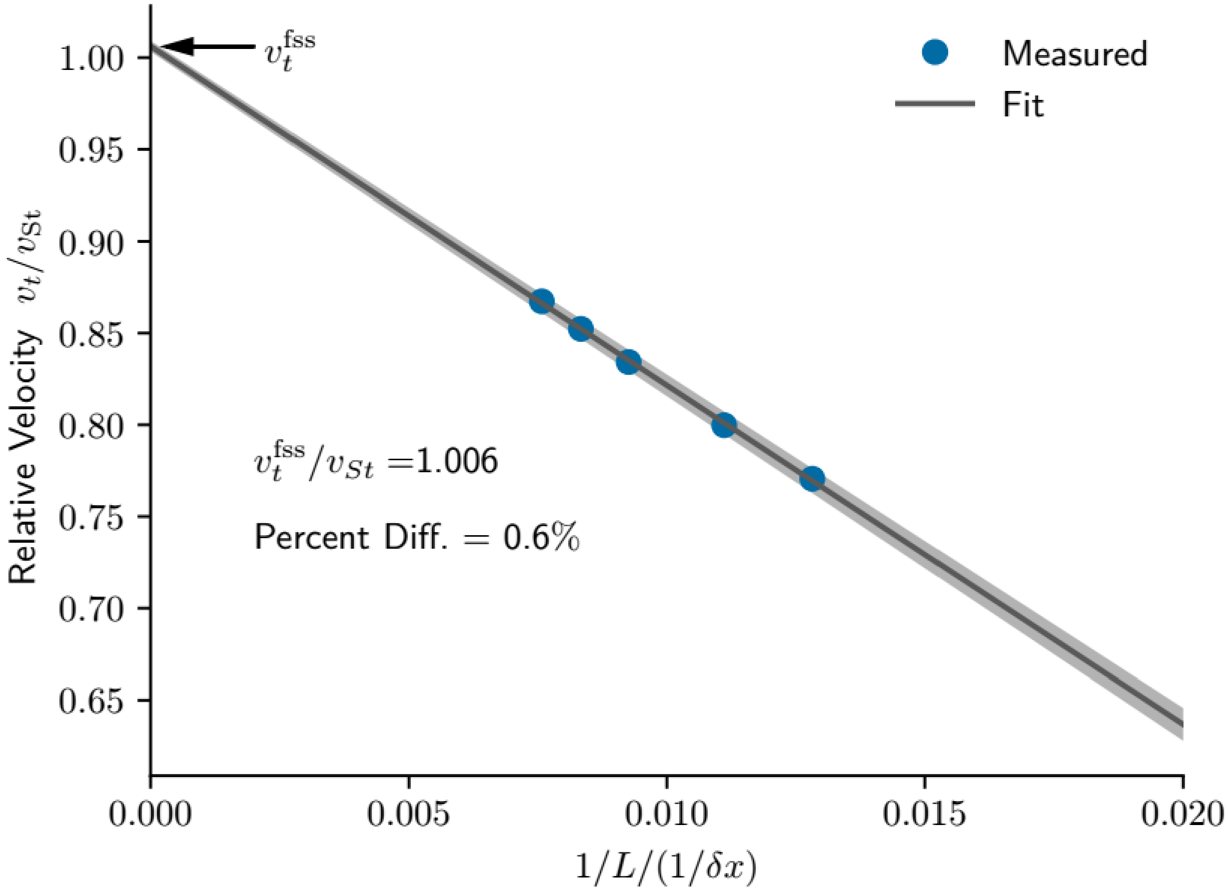
MD with Moving Boundary Conditions



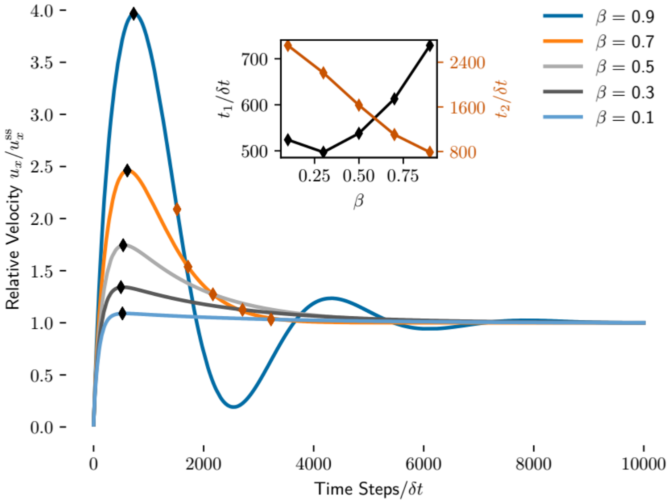
$$\boldsymbol{v}_{\mathrm{St}} \approx \frac{\boldsymbol{F}}{6\pi(\eta_s + \eta_p)R}$$

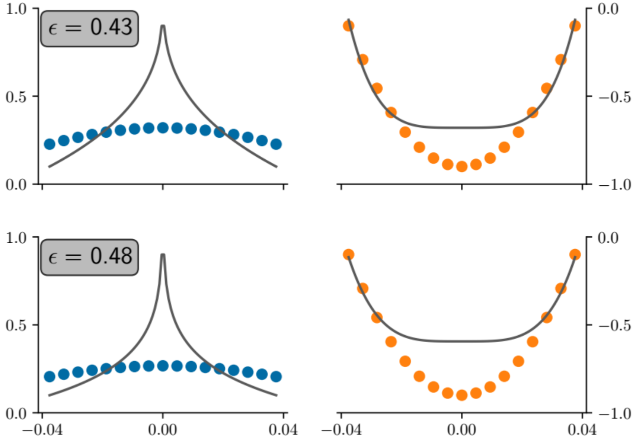
$$\boldsymbol{f}_c = \frac{\boldsymbol{F}}{n_c} \qquad n_c \approx L^3 - \frac{\frac{4}{3}\pi R^3}{\delta x^3}$$

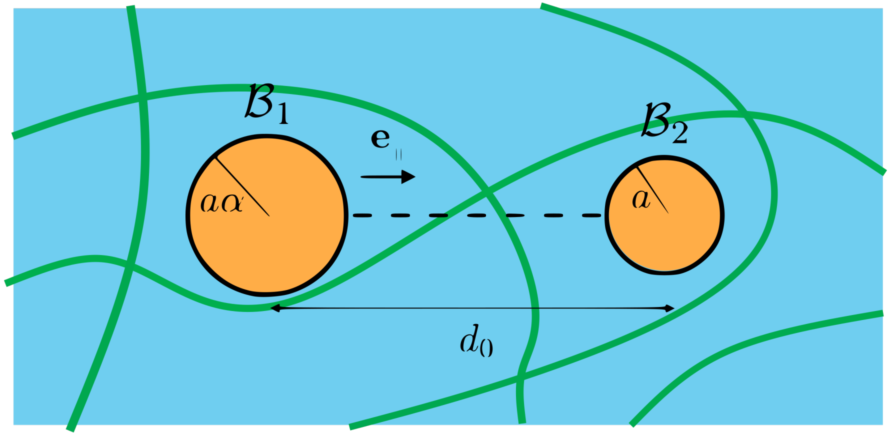
Stokes Law FSS

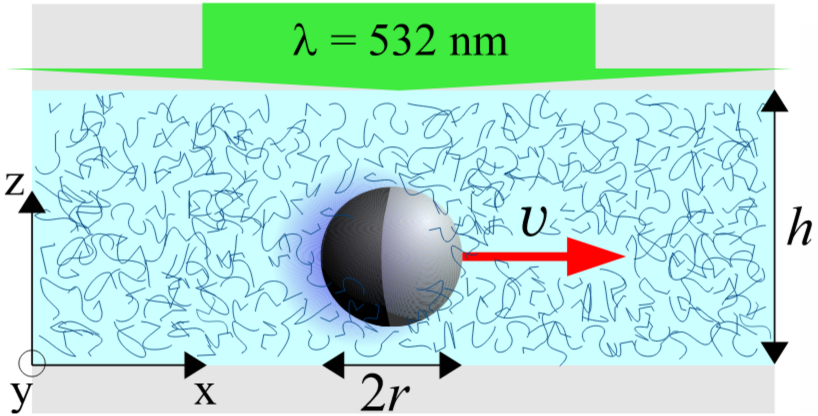


Conclusion and Outlook









Thank You!