Normal Mode Analysis for Nano-Scale Hydrodynamic Model Determination

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(Best viewed in Chrome Canary)

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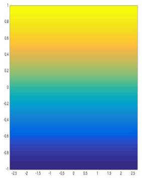
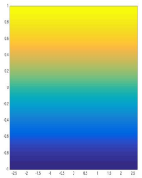
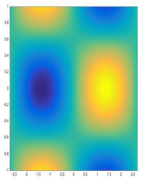


Motivation - *Determining "Hydrodynamical" Boundary (Inverse Problem)*



Model Problem - *Stokes Equation + Navier Slip Boundary Condition*



Analytical Results - *Eigenvalues & Eigenfunctions in Periodic Channels*

Microfluidic Dynamics

- At small scales (channel diameters from around $100nm$ to around $100\mu m$).
- If Navier-Stokes still holds,

$$\rho\left(\frac{\partial u}{\partial t} + u \cdot \nabla u\right) = -\nabla p + \eta \nabla^2 u + f,$$

  with

  - Low Reynolds number, $Re = \frac{\rho V L}{\mu} < 1000$.
  - Dissipation dominated by viscosity effects.
  - Fluid particles moving along smooth paths in laminar or layers.

Stokes Approximation, Boundary Slip

- Dropping inertial term (Stokes approximation), assuming zero body force and incompressibility,

$$\rho \partial_t v = -\nabla p + \nabla \cdot (\eta \nabla v),$$
$$\nabla \cdot v = 0.$$

- Instead of usual non-slip bounadry conditions, there is a slip at the solid surface due to intermediate Knudsen number,

$$u_{slip} = L_s \frac{\partial u_\tau}{\partial n}$$

Navier Slip Length

$L_s \approx L_{MFP}$

When $Kn = \frac{L_{MFP}}{H}$ small enough, non-slip boundary condition is accurate.

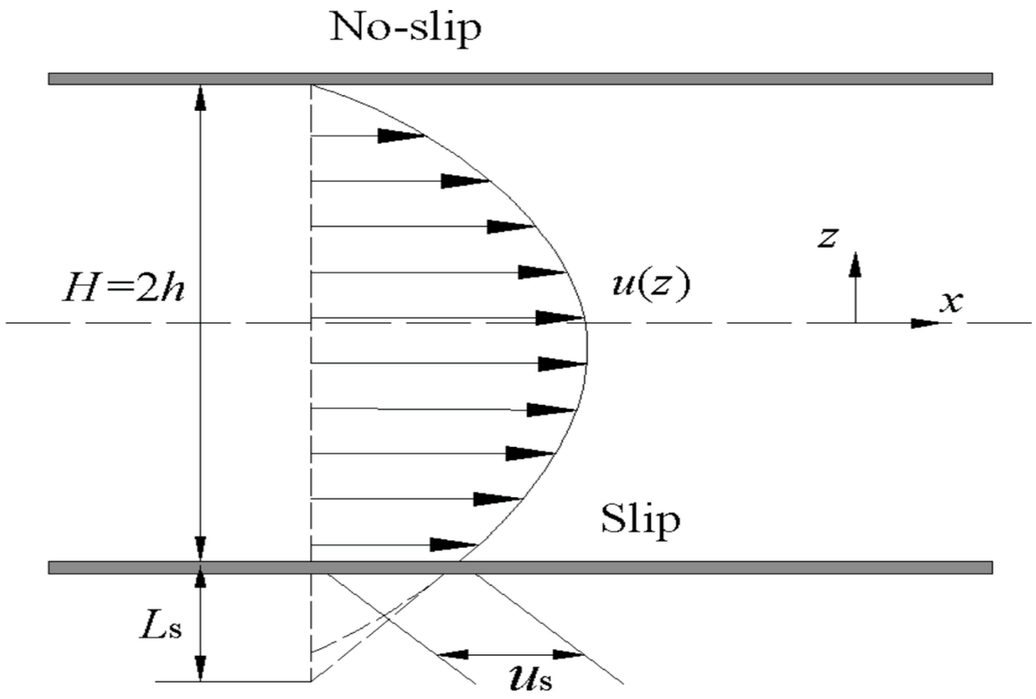


Image from http://www.mdpi.com/1422-0067/10/11/4638/htm.

Even Narrower Channels

- If channel width is only around 100σ, the model above fails again due to the presence of density boundary layer.

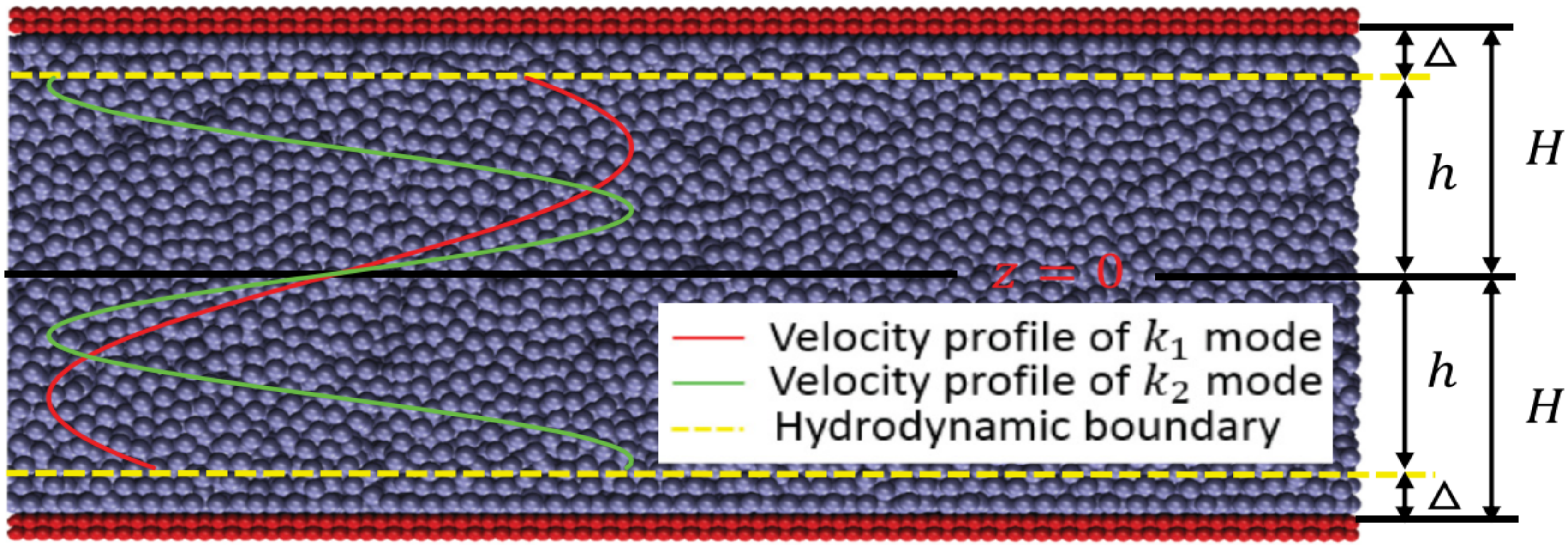


Image from [Ping Sheng et al., Physical Review E, 2015]

Molecular Dynamics

- Model validation and determining model parameters directly from MD simulation.
- At equilibrium, the system experiences thermal fluctuations (FDT).
- In linear response regime, longevity of a specific mode U can be determined by:
  - Calculating its autocorrelation function
    $$C_U(\Delta t) = \frac{\left\langle \left(\sum_{i=1}^{N} v_i(t{=}t_0) U(x_i,y_i) \right) \left(\sum_{i=1}^{N} v_i(t{=}t_0{+}\Delta t) U(x_i,y_i) \right) \right\rangle}{\left\langle \left(\sum_{i=1}^{N} v_i(t{=}t_0) U(x_i,y_i) \right) \left(\sum_{i=1}^{N} v_i(t{=}t_0) U(x_i,y_i) \right) \right\rangle}.$$
  - $\tau_{decay} \approx -\frac{1}{[\ln(C_U)]'}.$

Matching Spectral Fingerprints

Take U from a one-parameter group by fixing k.

Plot τ_{decay} against λ, and obtain eigenvalues as local peaks.

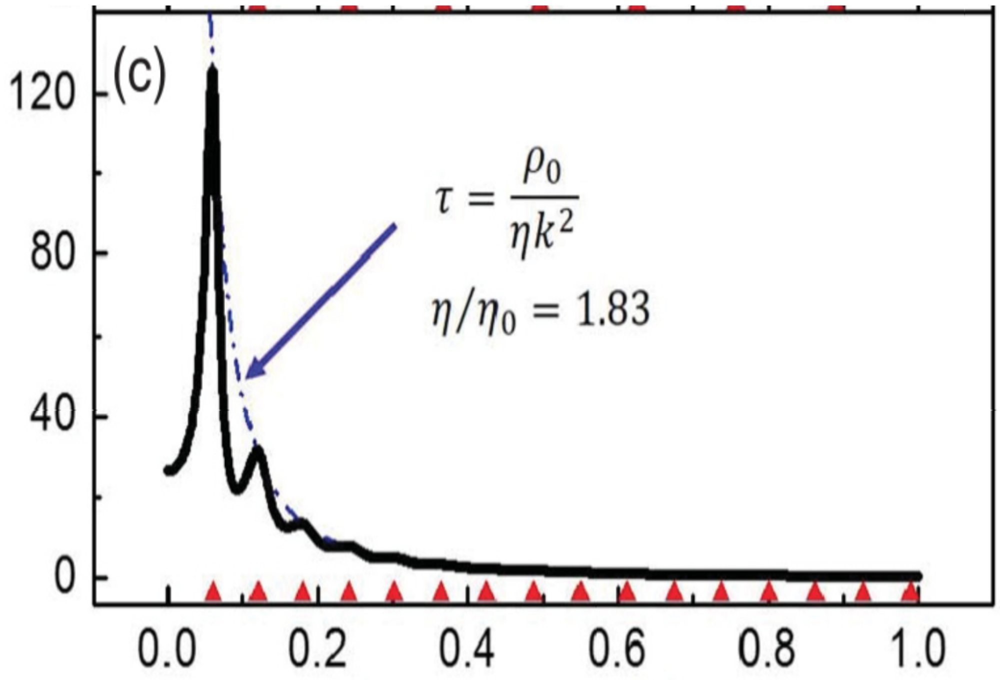


Image from [Ping Sheng et al., Physical Review E, 2015]

Even Narrower Channels Cont.

- A modified model can be derived in this way

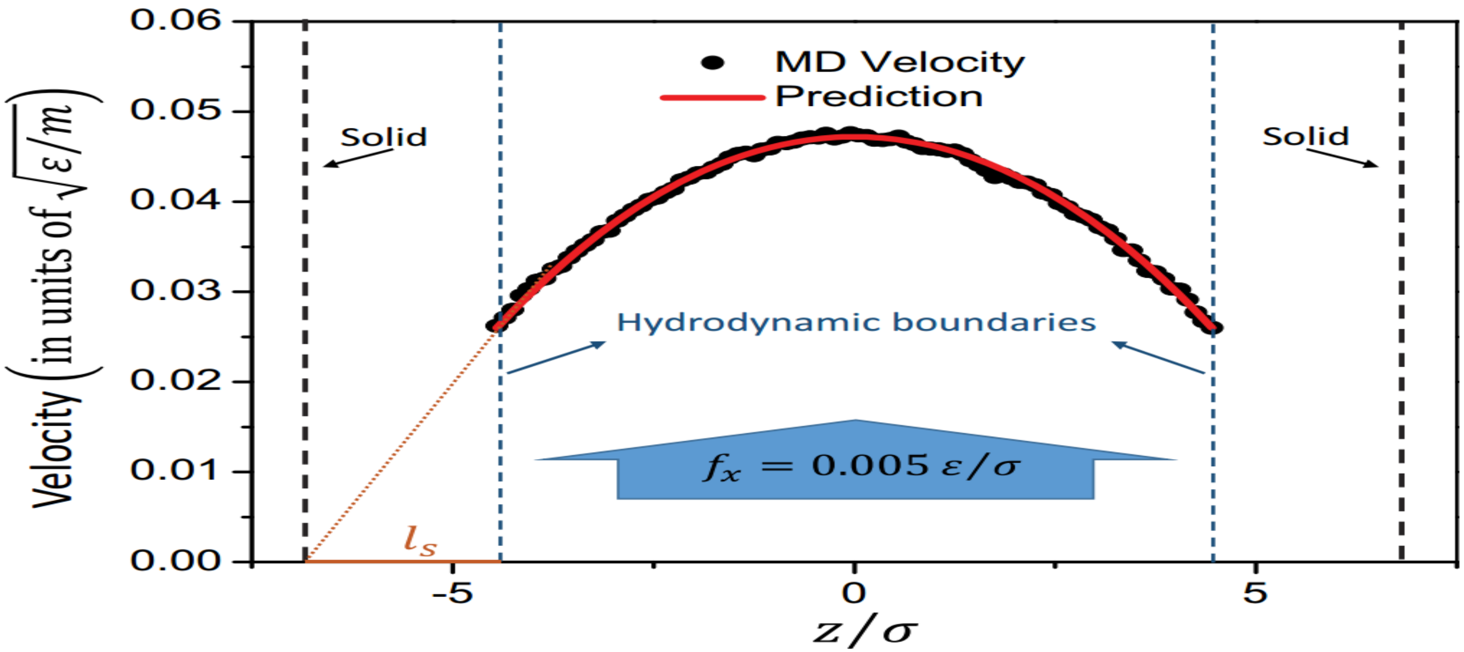


Image from [Ping Sheng et al., Physical Review E, 2015]

However..

- One obvious caveat is that not all families of eigenfunctions are investigated.
- To validate the conjectured model above, we have to obtain the full set of eigenfunctions of the model.

Existing Results

- Taking $l_s = 0$, the problem reduces to the one considered by Steven A. Orszag in 1986.
- Later, Orszag's results are applied to analyse accuracy and stability of Chorin's projection method and its variants. See, for example [Weinan E and Jianguo Liu, 1995, 1996].

A 1D System

- We consider the domain to be a 2D periodic channel
$$\Omega = [-l, l] \times [-h, h].$$
- The generalized eigenvalue problem can be written as
$$\nabla^2 u + \lambda u = \nabla p,$$
$$\nabla \cdot u = 0.$$
- Subject to periodic boundary conditions at $x = \pm l$:
$$u(x + 2l, y) = u(x, y), \qquad p(x + 2l, y) = p(x, y),$$
and slip boundary conditions at $y = \pm h$:
$$l_s \partial_y u_x = \mp u_x .$$
- Key observation: pressure Poisson equation is a Laplace equation!

Solution Procedure

- Solutions to the eigenvalue problem is of the form
$$u_k(x, y) = \hat{u}_k(y)e^{ikx},$$
$$p_k(x, u) = \hat{p}_k(y)e^{ikx},$$
where $k \in \frac{\pi}{l}\mathcal{Z}$.
- General solution to the pressure Poisson equation:
$$\hat{p}_k(x, y) = c_1 e^{ky} + c_2 e^{-ky}.$$
- Then from Stokes equation,
$$\hat{u}_{k,x}(x, y) = a_x e^{ik_\lambda y} + b_x e^{-ik_\lambda y} + \frac{ik}{\lambda}(c_1 e^{ky} + c_2 e^{-ky}),$$
$$\hat{u}_{k,y}(x, y) = a_y e^{ik_\lambda y} + b_y e^{k_\lambda y} + \frac{ik}{\lambda}(c_1 e^{ky} - c_2 e^{-ky}),$$

Solution Procedure (2)

- Now, the solution is fully determined by six constants
$$Par = [a_x, a_y, b_x, b_y, c_1, c_2]^T.$$
- Using boundary conditions and incompressibility constraints, the eigenvalue problem is reduced to a linear system
$$A(h, l, l_s, \lambda)Par = 0,$$
where A is a 6×6 matrix.
- For the problem to have nontrivial solutions, the characteristic equation has to be satisfied
$$det(A) = 0.$$

Results

- When $k = 0$, there are two cases:
  - Asymmetric: $\tan(\sqrt{\lambda}h) = -l_s\sqrt{\lambda}, u_{0\lambda} = [\sin(\sqrt{\lambda}y), 0]^T$.
  - Symmetric: $\cot(\sqrt{\lambda}h) = l_s\sqrt{\lambda}, u_{0\lambda} = [\cos(\sqrt{\lambda}y), 0]^T$.
- When $k \neq 0$, also two cases ($k_\lambda = \sqrt{\lambda - k^2}$):
  - $k_\lambda \cot(k_\lambda h) - k \coth(kh) - l_s\lambda = 0$.

$$u_{k\lambda} = e^{ikx} \begin{bmatrix} ik\cosh(ky) - ik_\lambda \frac{\cosh(kh)}{\sin(k_\lambda h}\cos(k_\lambda y) \\ k\sinh(ky) - k\frac{\sinh(kh)}{\sin(k_\lambda h)}\sin(k_\lambda y) \end{bmatrix}$$

  - $k_\lambda \tan(k_\lambda h) + k \tanh(kh) + l_s\lambda = 0$.

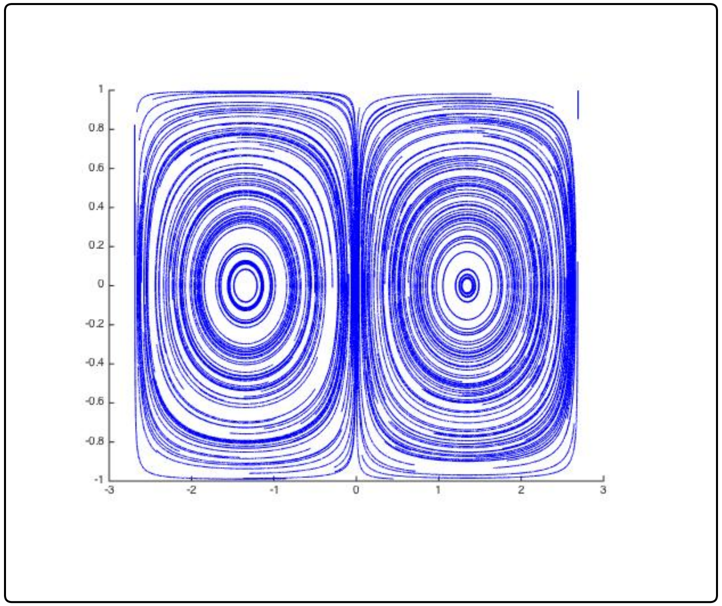
$$u_{k\lambda} = e^{ikx} \begin{bmatrix} ik\sinh(ky) - ik_\lambda \frac{\cosh(kh)}{\cos(k_\lambda h}\sin(k_\lambda y) \\ k\cosh(ky) - k\frac{\cosh(kh)}{\cos(k_\lambda h)}\cos(k_\lambda y) \end{bmatrix}$$

Discussion

- **Theorem**: Each eigenvalue λ obtained is monotonically decreasing in Navier length l_s.
  Proof: Directly calculate $\partial\lambda/\partial l_s$ via implicit function theorem.
- More slip = more dissipation on ALL modes.
- A counterintuitive fact: Numerical tests show that the first antisymmetric mode for $k = 0$ and the first mode for $k = 1$ has close eigenvalues even when $l/h \longrightarrow \infty$.

Summary

- A normal mode analysis is carried out for Stokes equation subject to Navier slip boundary conditions.
- Link to previous studies is drawn.
- Application to determining hydrodynamics boudary conditions is discussed.



Thanks for your attention!

Wish List

- A generic numerical method would be nice to have to deal with
  - Two phase flow
  - General geometry
- BIM might be preferable for this task, being more friendly to shifted inverse iteration / Arnoldi iteration.