EFFECTS OF MOLECULAR DETAILS ON TWO-PHASE FLOWS THROUGH NANOPORES

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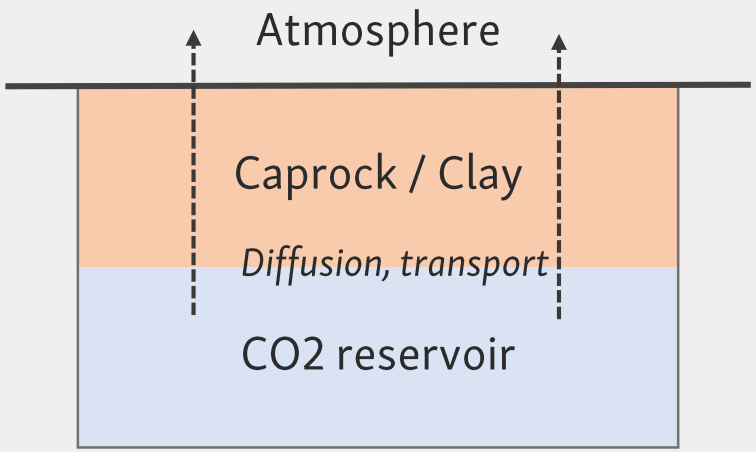
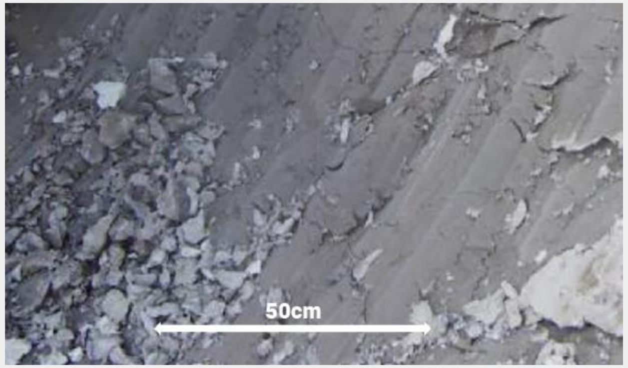
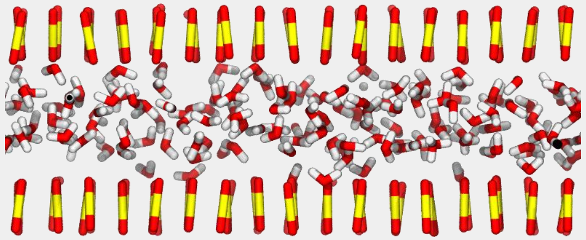
OVERVIEW

- Fluid–fluid flows through pore networks
- Multiscale problem
- Upscale multiphase transport properties from nanoscale
- Measuring nanoscale properties using molecular simulations







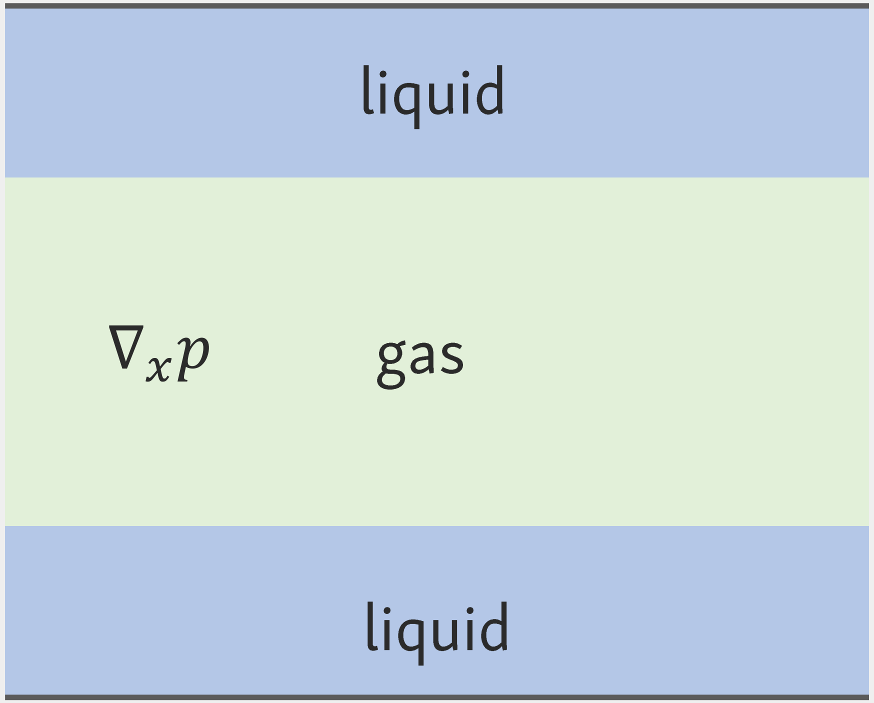
QUESTIONS

Can we measure nanoscopic transport properties?

Can we model the flow with continuum fluid dynamics?

NANOPORE SYSTEM

- Gas + partially saturated pores
- Pore diameters 5 nm to 30 nm
- Pressure gradient through pore
- Gravity is negligible

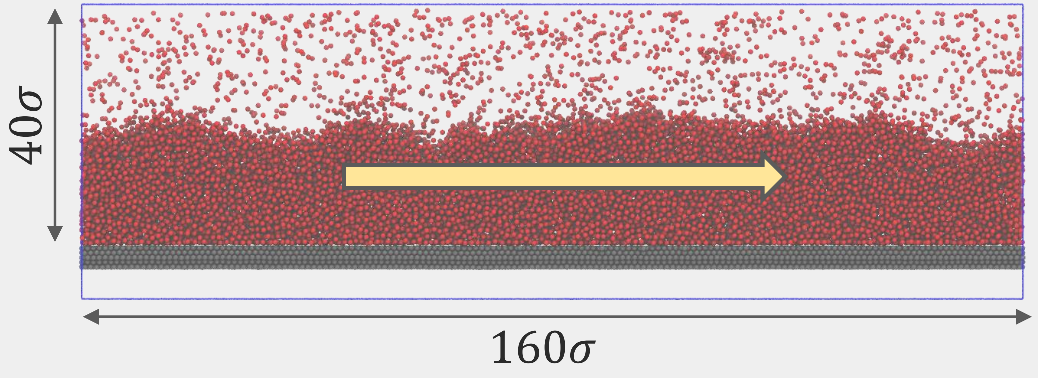


MOLECULAR DYNAMICS (MD) SIMULATIONS

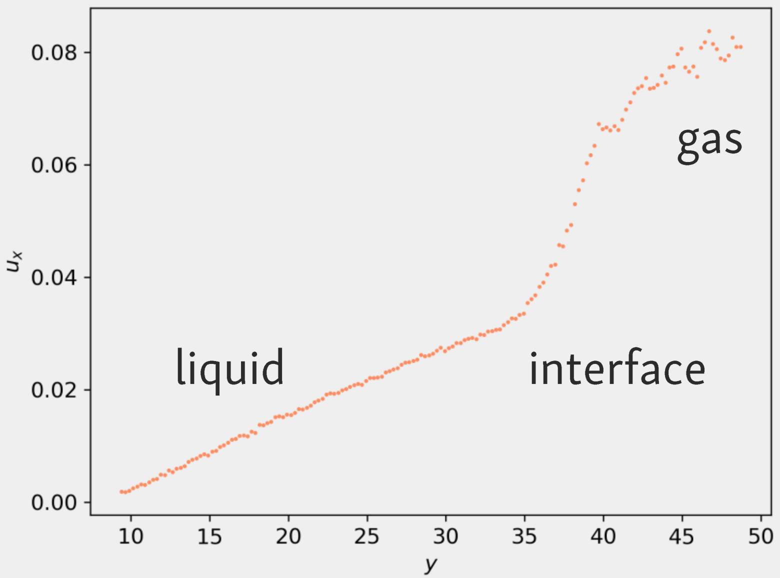
- Atomic detail
- Molecular interactions tuned to obtain physical properties (e.g. surface tensions γ, density ρ, viscosity μ, slip lengths δ)
- Classical physics (Newtonian)

- Computer experiment!

Nanopore system, accelerate along x axis

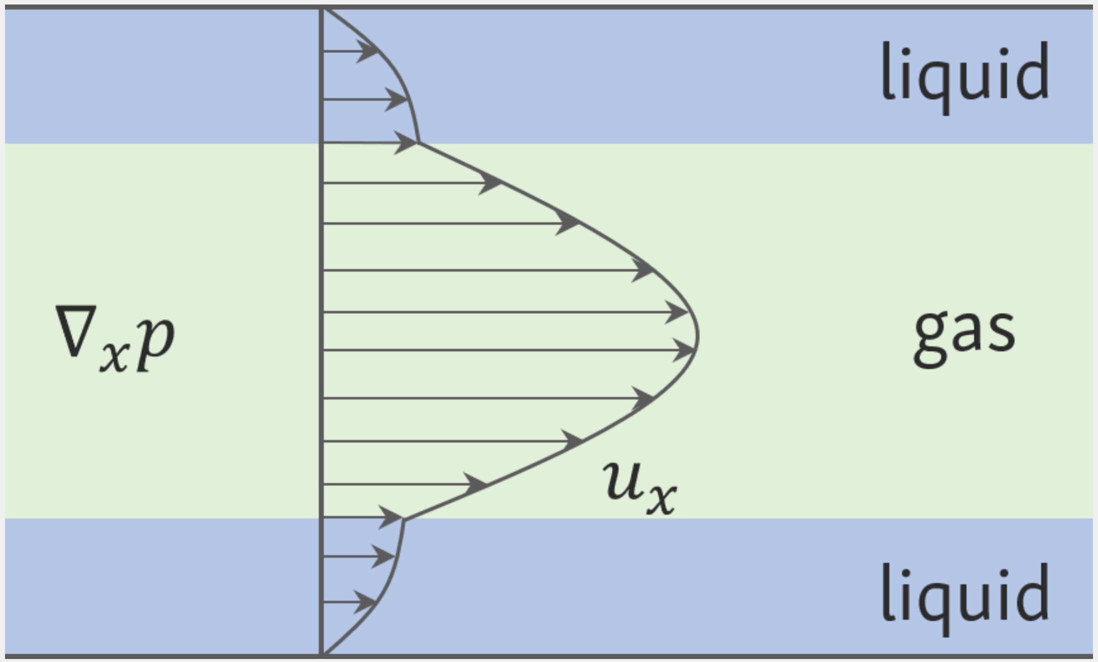


Steady state velocity profile



MACROSCOPIC MODELING OF PORE FLOW

- Poiseuille flow
  (pressure grad. or external force)
- Navier-Stokes equations
  + boundary conditions
  → analytical solution for u_x
- Separate fluid phases,
  constant density, viscosity, etc.

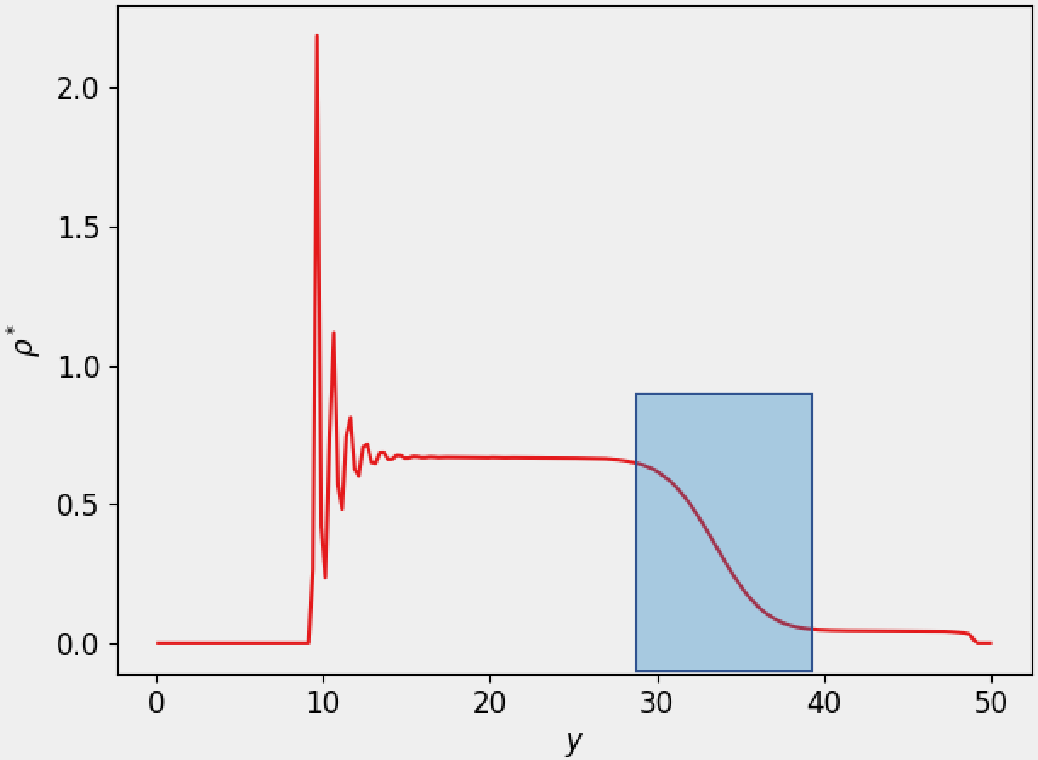


NOVEL FEATURES ON NANOSCALE

- Molecular layering at walls
- Fluid–fluid interfaces not thin: must be modeled

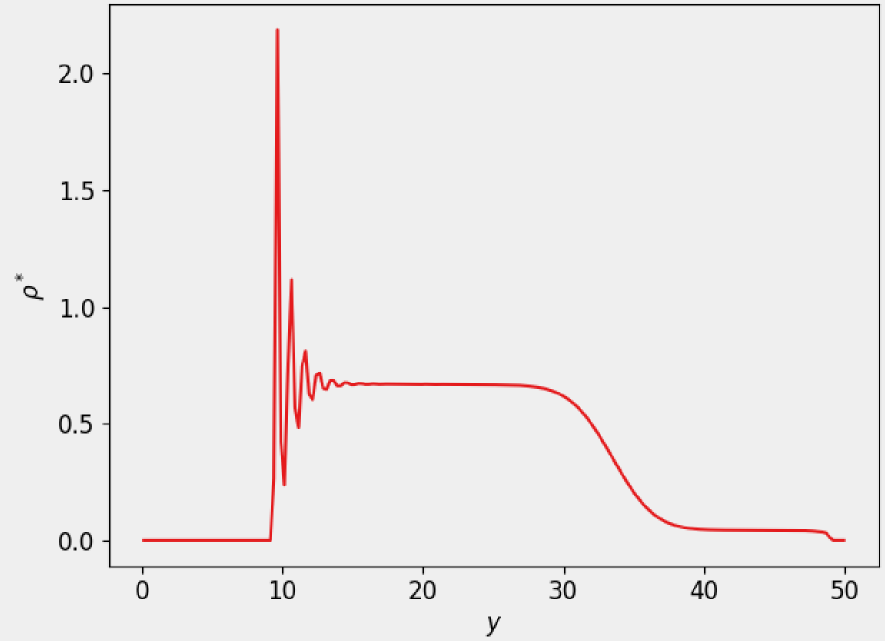
- How do these affect the modeling?

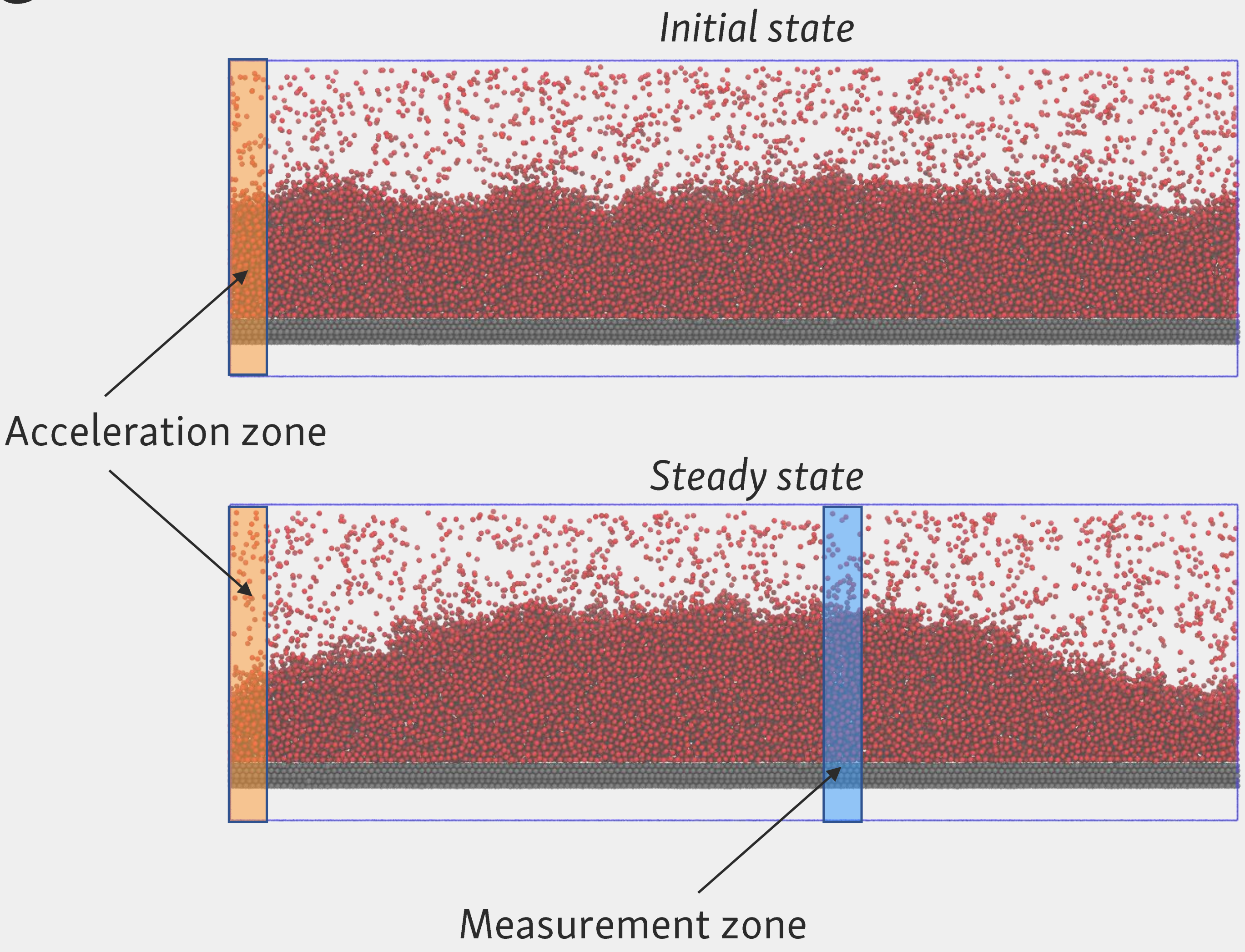
Density profile across channel



MOLECULAR LAYERING

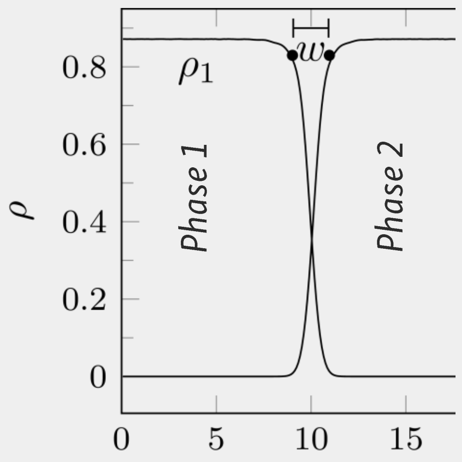
- Density and viscosity variation
- Accelerate in part of system, measure far away

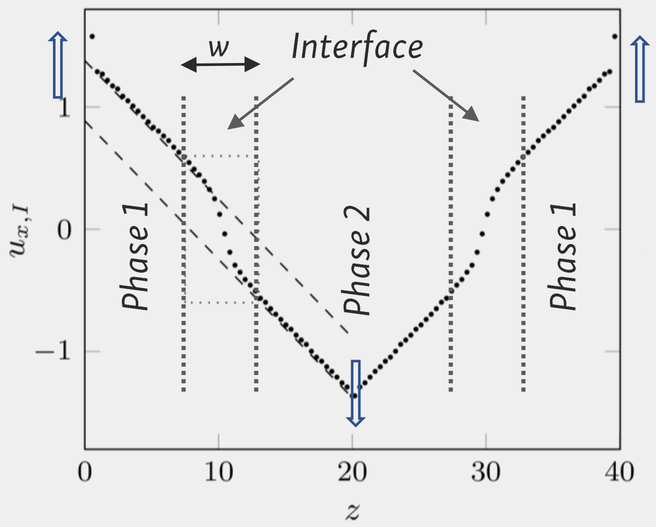




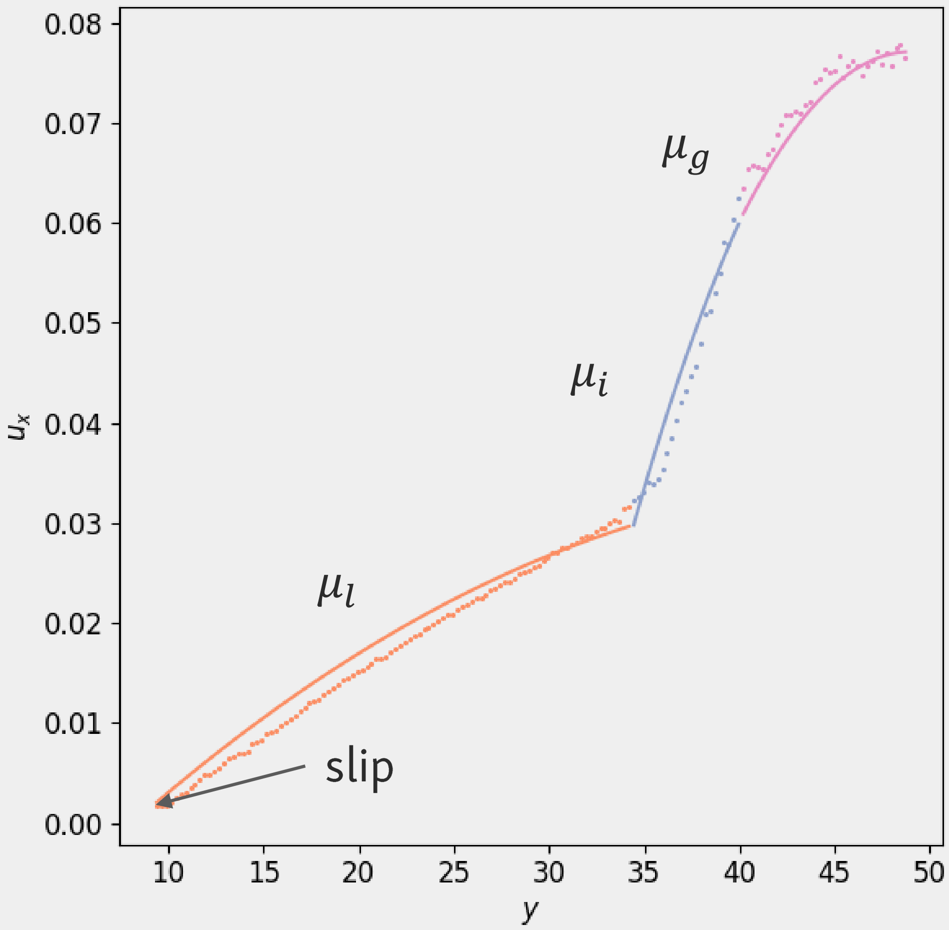
INTERFACIAL VISCOSITY

- Can measure effective viscosity of fluid–fluid interfaces
- Good agreement with Navier-Stokes solution*





Measured velocity + model

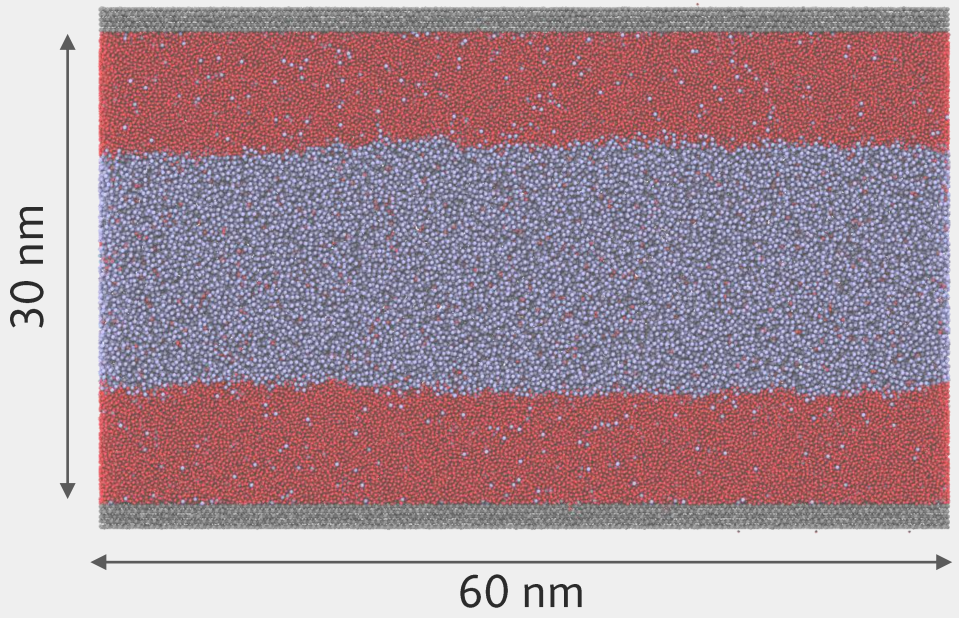


TOWARDS A UNIFIED VIEW

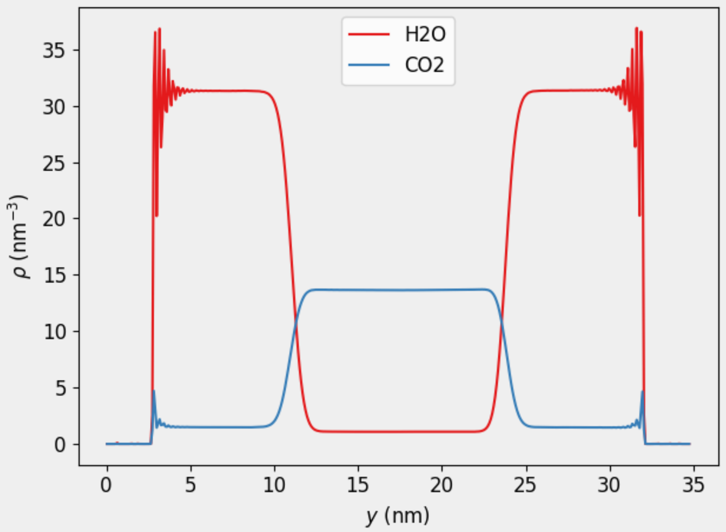
- Avoid layering problems for external forces
- Fluid–fluid interfaces important on nanoscale
- Can be treated as separate phase

- Local modeling of properties from local concentrations?

Supercritical CO_2 + H_2O



Density profiles, partial mixing



THANK YOU FOR LISTENING!

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REFERENCES

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MODEL SOLUTION

$$u_x(y) = \frac{\nabla_x p\, y^2}{2\mu_i} + A_i y + B_i \quad \text{for each phase } i$$

$$A_i = \frac{\mu_1 A_1}{\mu_i}$$

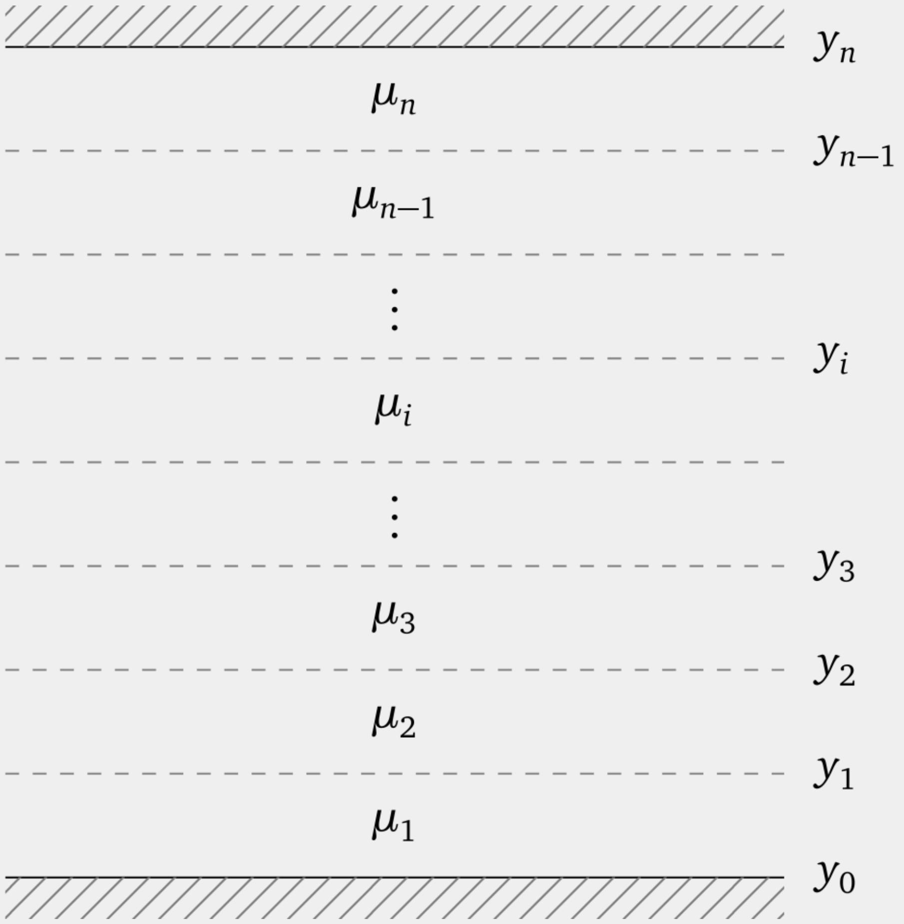
$$B_i = \frac{\nabla_x p\, y_{i-1}^2}{2} \frac{\mu_i - \mu_{i-1}}{\mu_i\, \mu_{i-1}} + (A_{i-1} - A_i)\, y_{i-1} + B_{i-1}$$

$$A_1 = -\nabla_x p \frac{\frac{1}{\mu_1}\left(\lambda^- y_0 - \frac{y_0^2}{2}\right) + \frac{1}{\mu_n}\left(\lambda^+ y_n + \frac{y_n^2}{2}\right) + \frac{1}{2}\sum_{i=1}^{n-1}\left(y_i^2\, \frac{\mu_{i+1} - \mu_i}{\mu_{i+1}\mu_i}\right)}{\lambda^- - y_0 + \frac{\mu_1}{\mu_n}(\lambda^+ + y_n) + \mu_1 \sum_{i=1}^{n-1}\left(y_i\, \frac{\mu_{i+1} - \mu_i}{\mu_{i+1}\mu_i}\right)}$$

$$B_1 = \frac{\nabla_x p}{\mu_1}\left(\lambda^- y_0 - \frac{y_0^2}{2}\right) + A_1(\lambda^- - y_0)$$

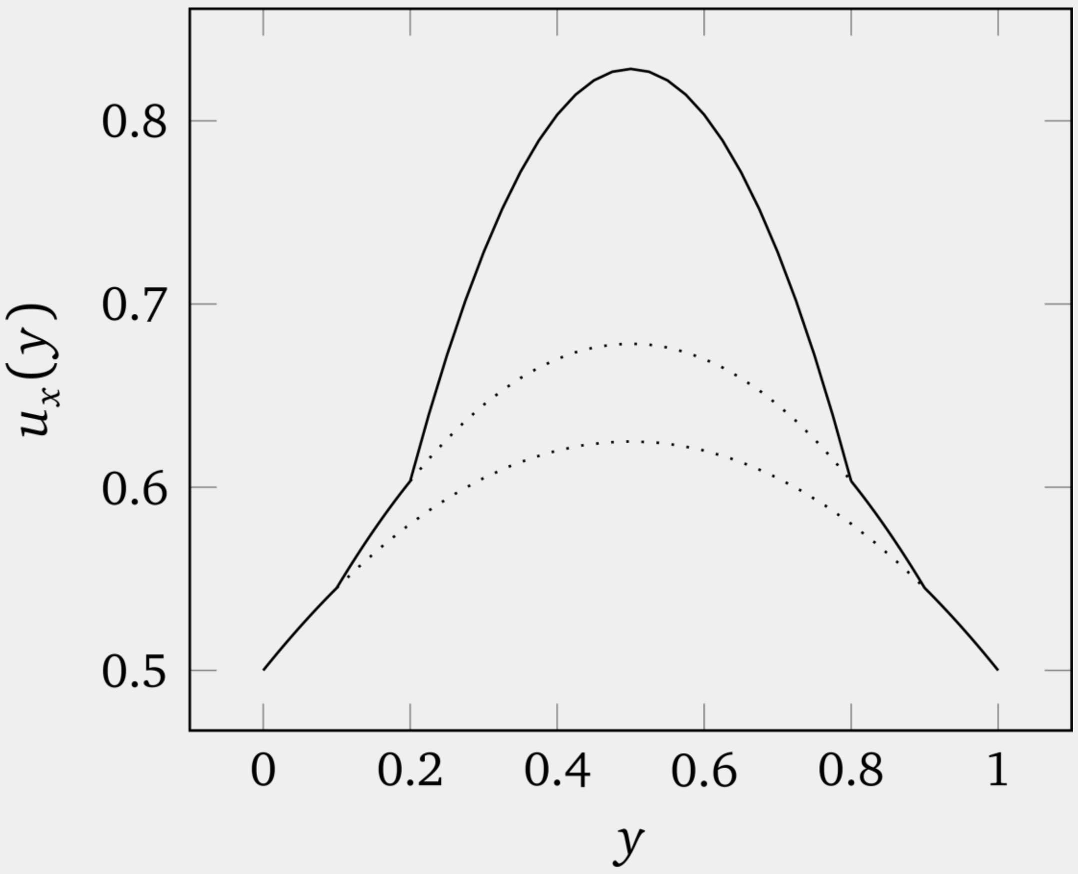
μ_i: viscosity, $\lambda^{-,+}$: lower and upper wall slip coeffs.

n fluid phases in channel



MODEL SOLUTION EXAMPLES

Two-phase flow + interface, symmetric



Five-phase flow, asymmetric