JUNE 5, 2019

TEXAS
The University of Texas at Austin

MANIPULATING SMALL DROPLETS IN MICROCHANNELS WITH COMPLEX FLUIDS

Blue Waters Symposium 2019

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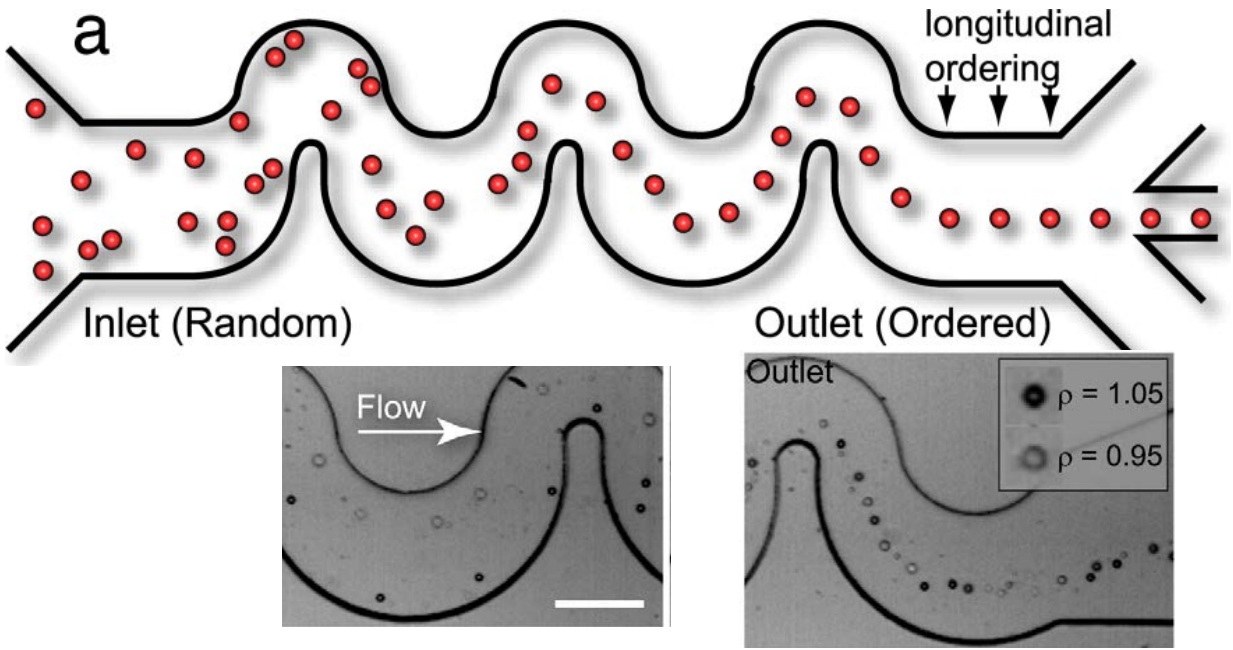
I use Blue Waters to engineer complex fluids and soft materials at the nanoscale.

Manipulating particles in microchannels

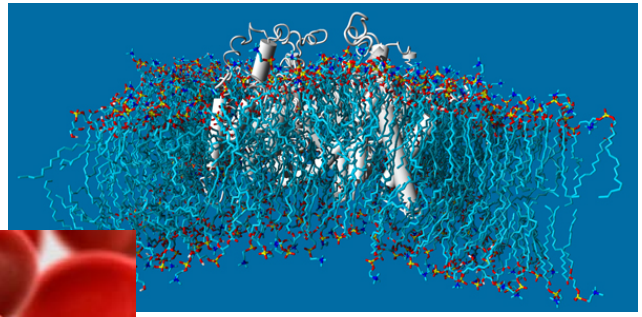


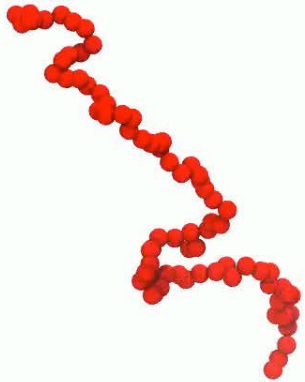
- filtration
- fractionation
- cell sorting
- oil recovery
- water treatment

How can we systematically engineer these processes?

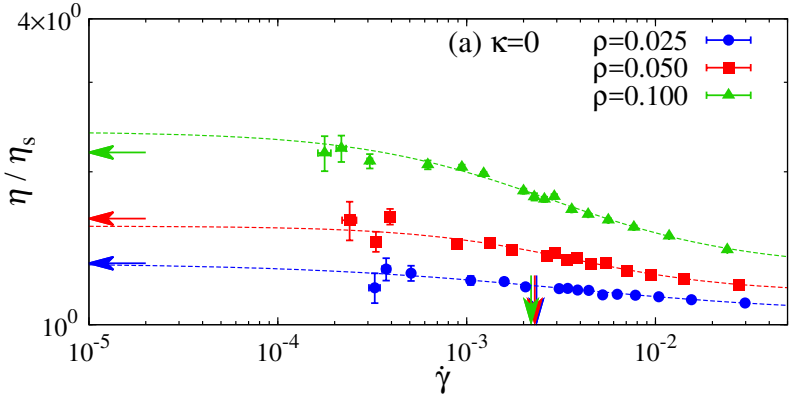
Di Carlo et al., *PNAS* **104**, 18892 (2007).

Complex fluids





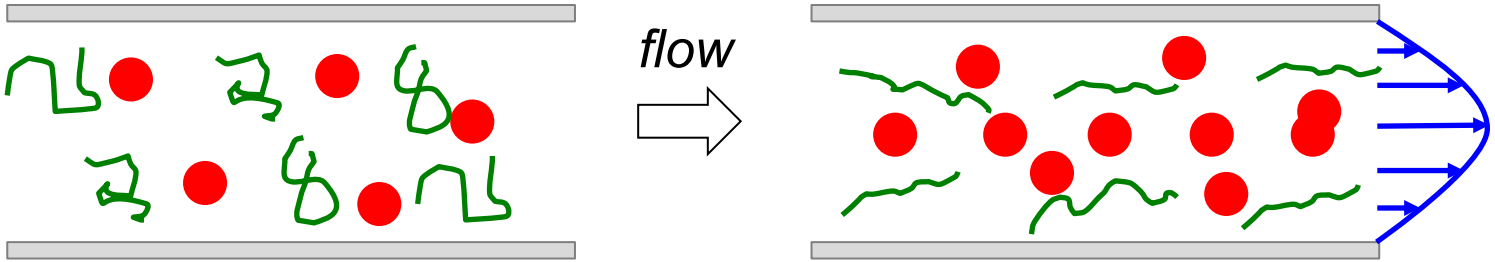
microscopic → macroscopic



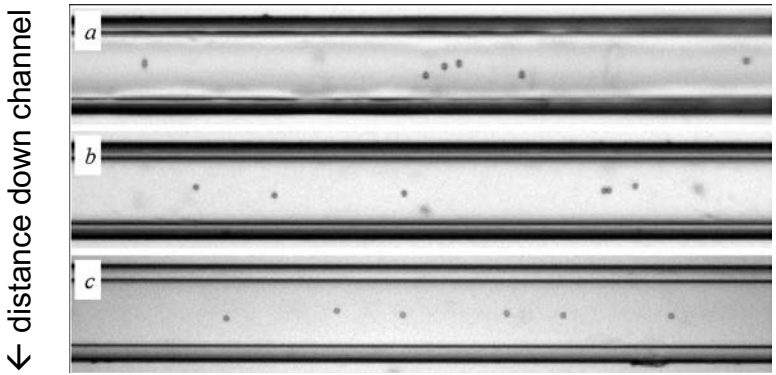
A. Nikoubashman and M.P. Howard. *Macromolecules* **50**, 8279 (2017).

Cross-stream migration

Addition of a viscoelastic component induces migration in Poiseuille flow



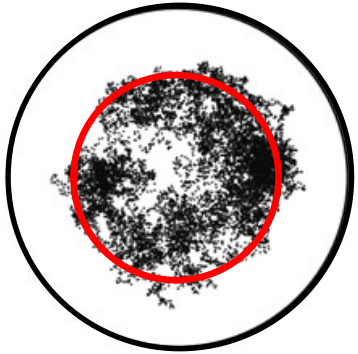
What happens when the particles become “small”?



D'Avino et al., *Lab Chip* **12**, 1638 (2012).

Cross-stream migration at the nanoscale

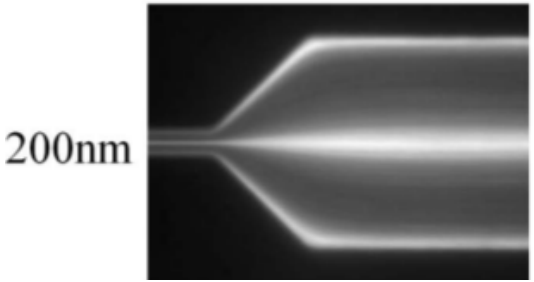
Brownian motion



Prohm et al., *Eur. Phys. J. E* **35**, 80 (2012).

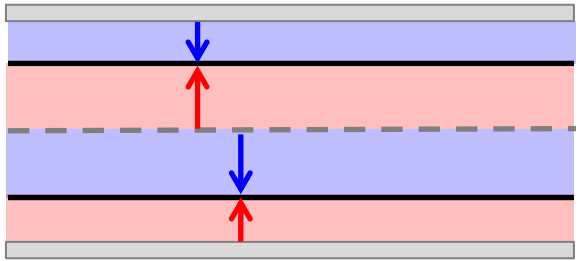
Comparable length scales

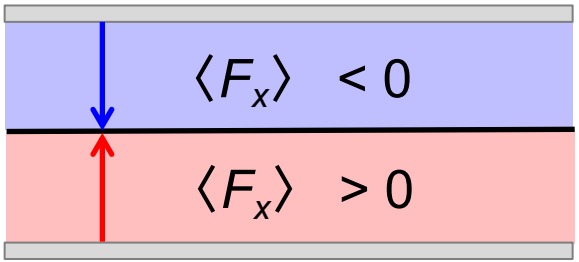
PEO R_e ~ 300 nm



Kim et al., *Lab Chip* **12**, 2807 (2012).

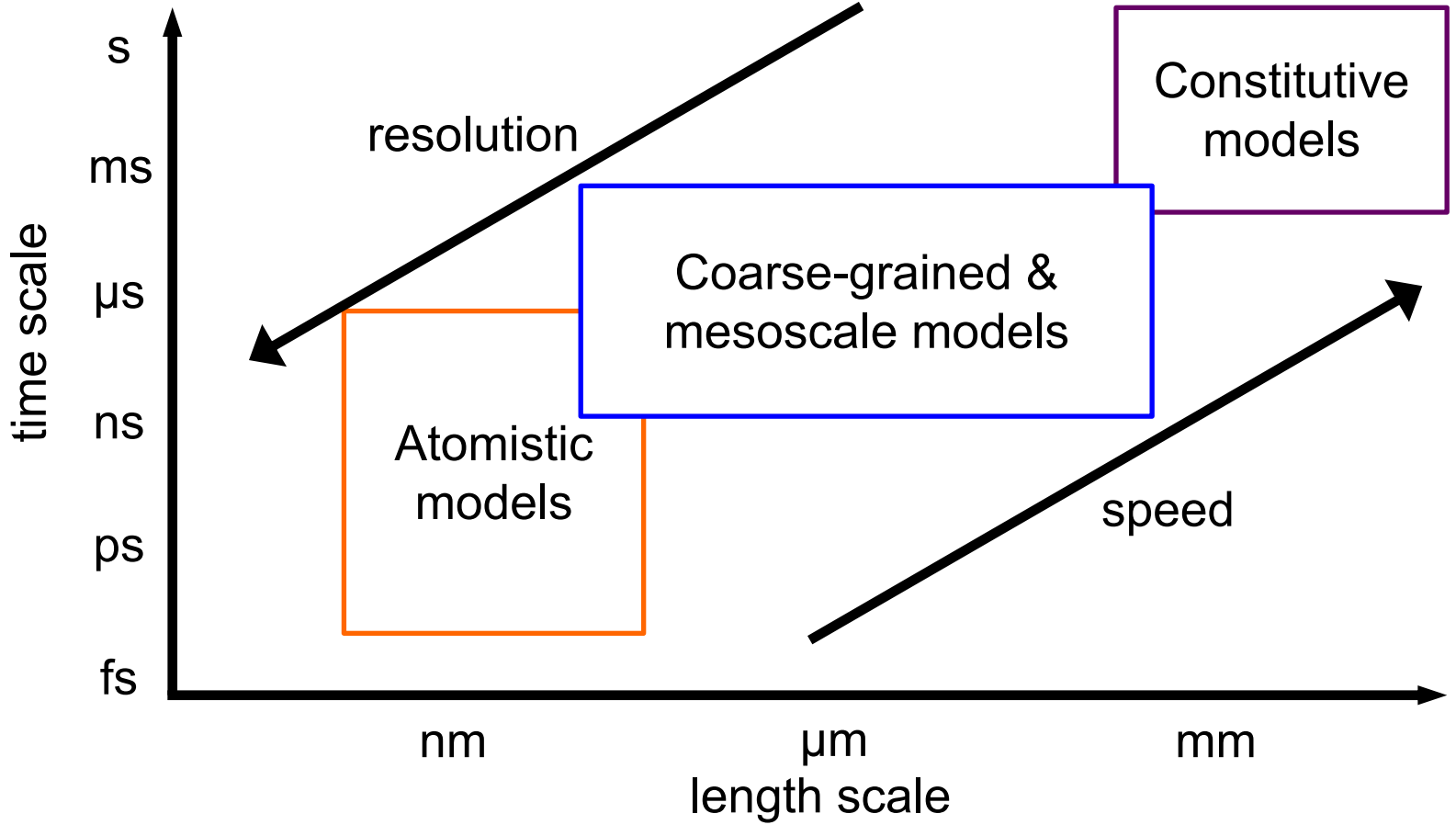
Average force on particles $\langle F_x \rangle$ gives average direction of movement



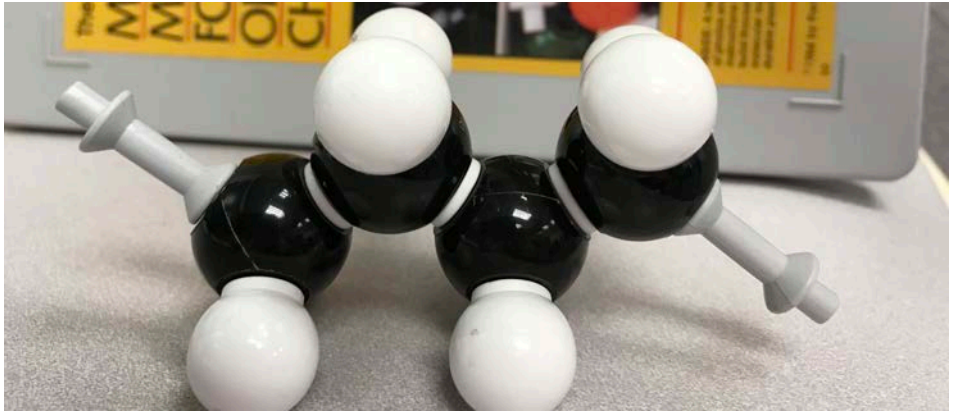


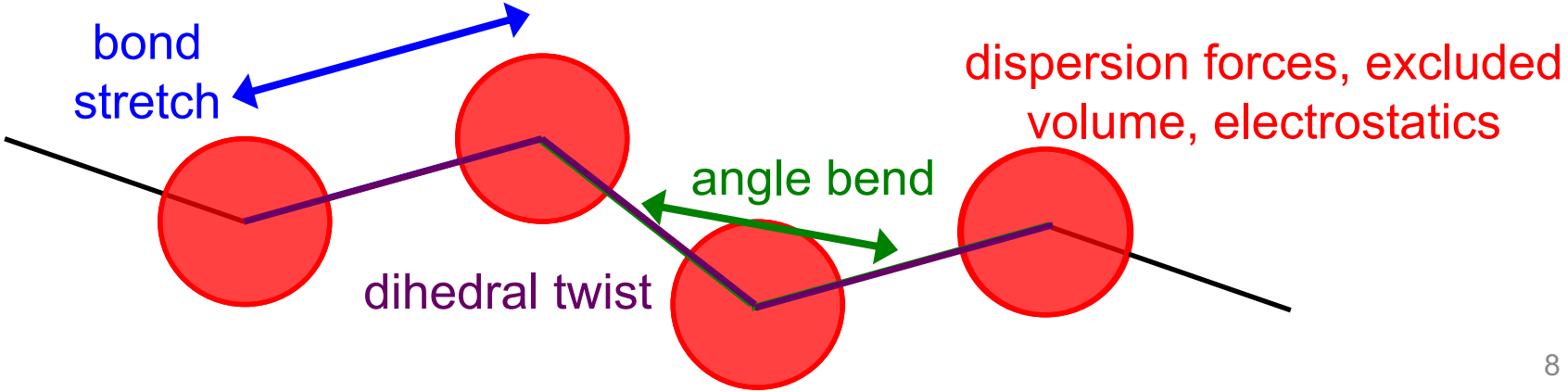
$\langle F_x \rangle = 0$

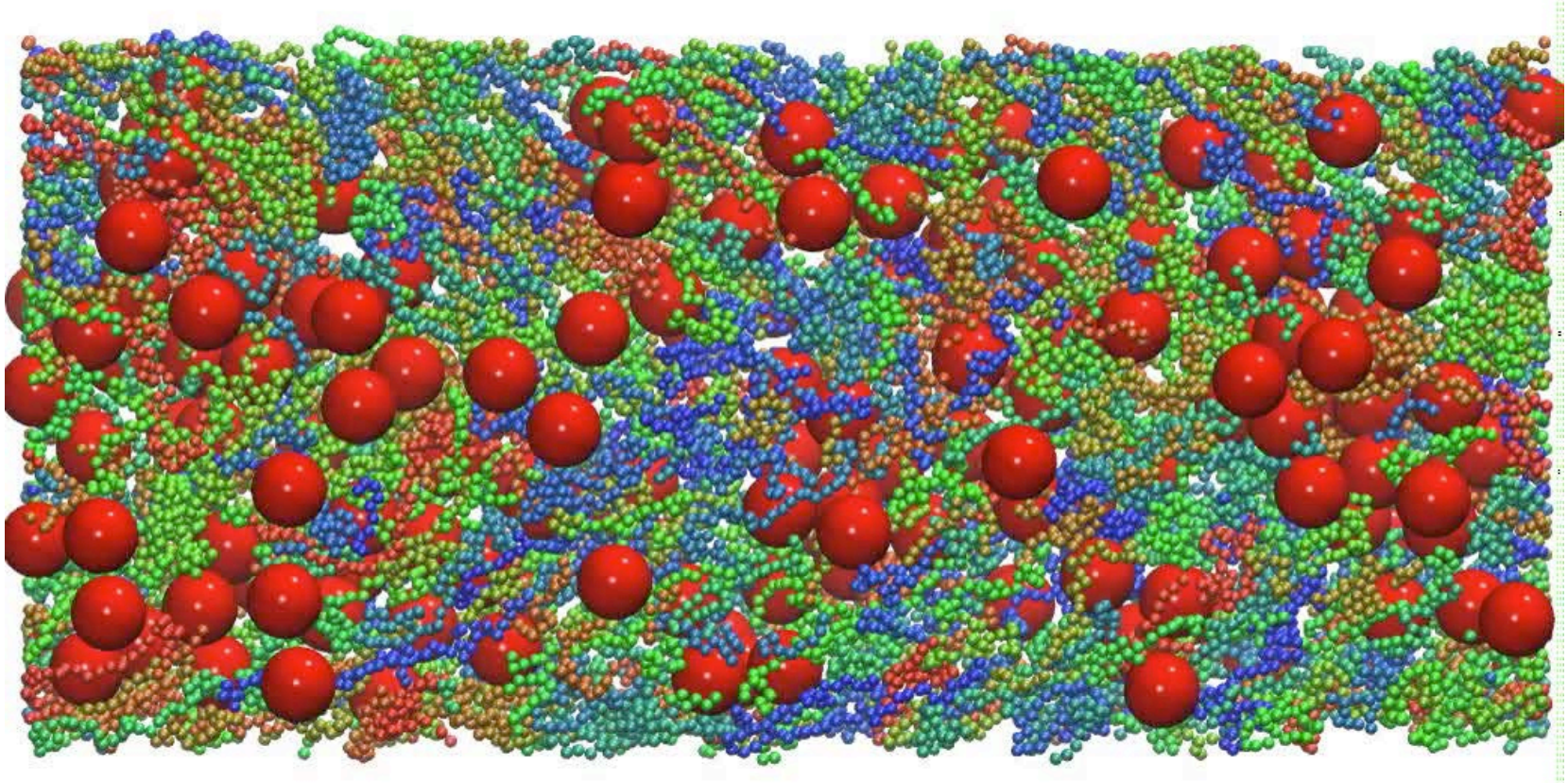
Mesoscale modeling



Coarse-grained models



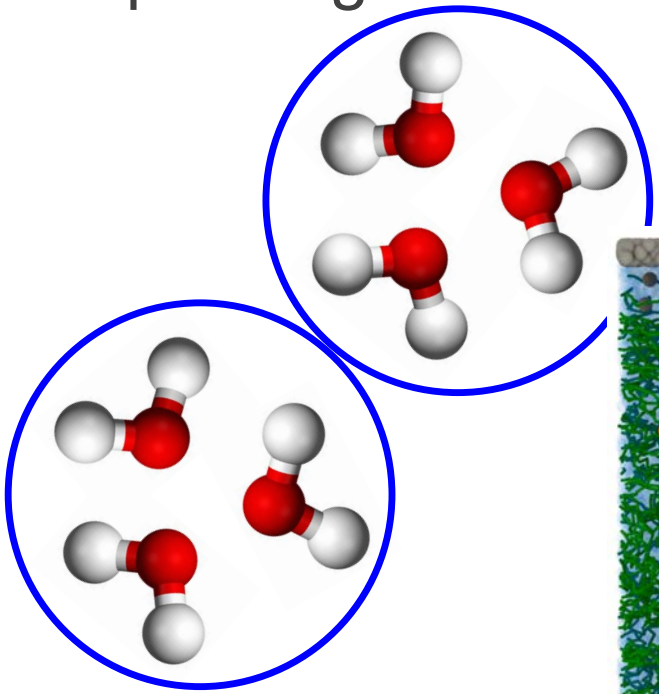




A. Nikoubashman et al., *J. Chem. Phys.* **140** 094903 (2014).
M.P. Howard et al., *J. Chem. Phys.* **142**, 224908 (2015).

What happens if the particles are droplets or cells that deform?

Droplet migration

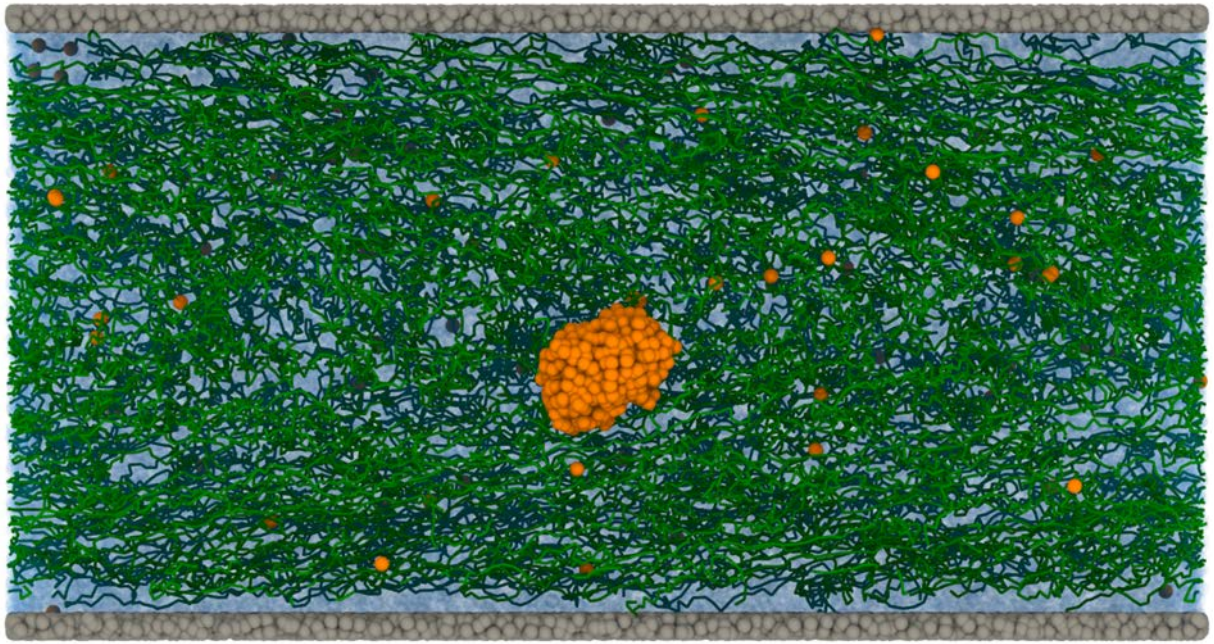


$$\mathbf{F} = \mathbf{F}_{\mathrm{C}} + \mathbf{F}_{\mathrm{R}} + \mathbf{F}_{\mathrm{D}}$$

repulsive force

random force

drag force



Why Blue Waters

Large parametric design space

4 polymers
x 3 polymer concentrations
x 5 flow rates
x 5 replicas

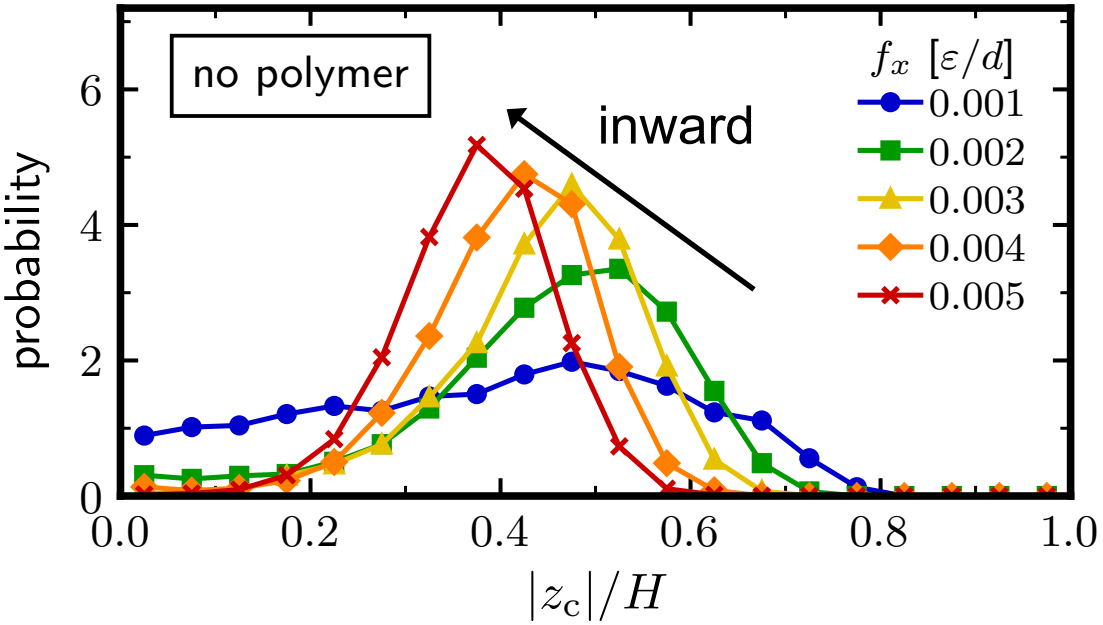
Large coarse-grained model

384,000 particles
= 4 GPUs for 48 hours

(HOOMD-blue)

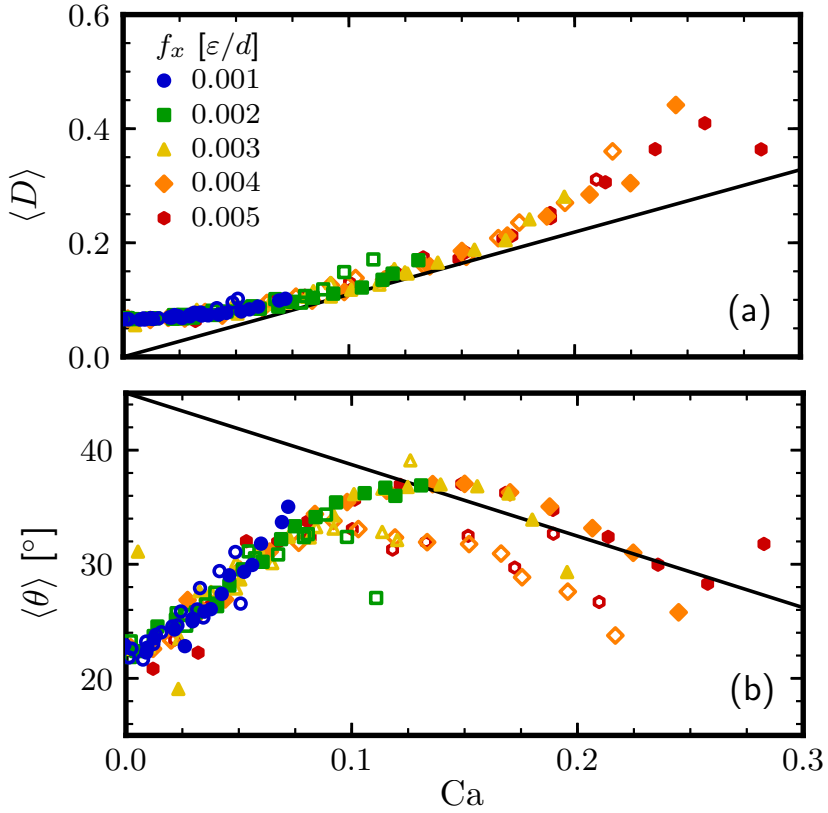
Blue Waters is the only system available to us with the GPU resources needed!

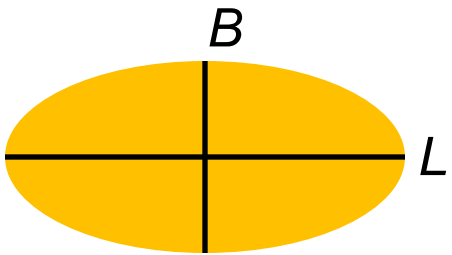
Droplet in a neat solvent is different from a rigid particle



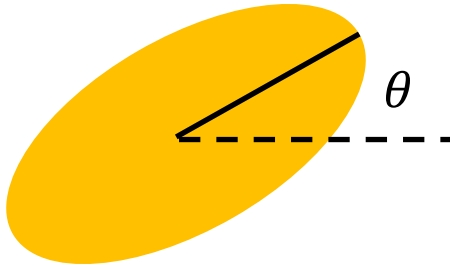
M.P. Howard et al., *Soft Matter* **15**, 3168 (2019).

Droplet shape depends on the local flow





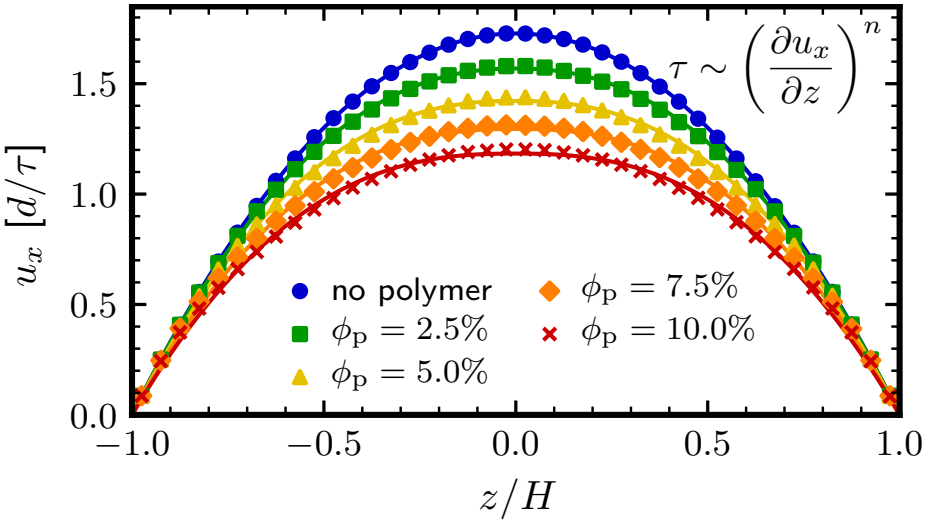
$$D = \frac{L - B}{L + B}$$



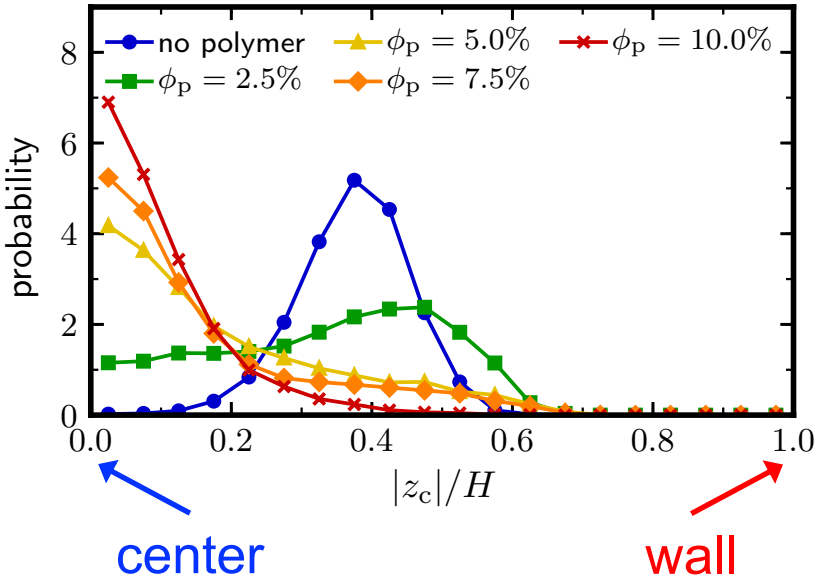
M.P. Howard et al., *Soft Matter* **15**, 3168 (2019).

Flow and droplet position depend on polymer concentration

Solution is non-Newtonian for higher polymer concentrations.



Droplet moves inward with increasing polymer concentration.



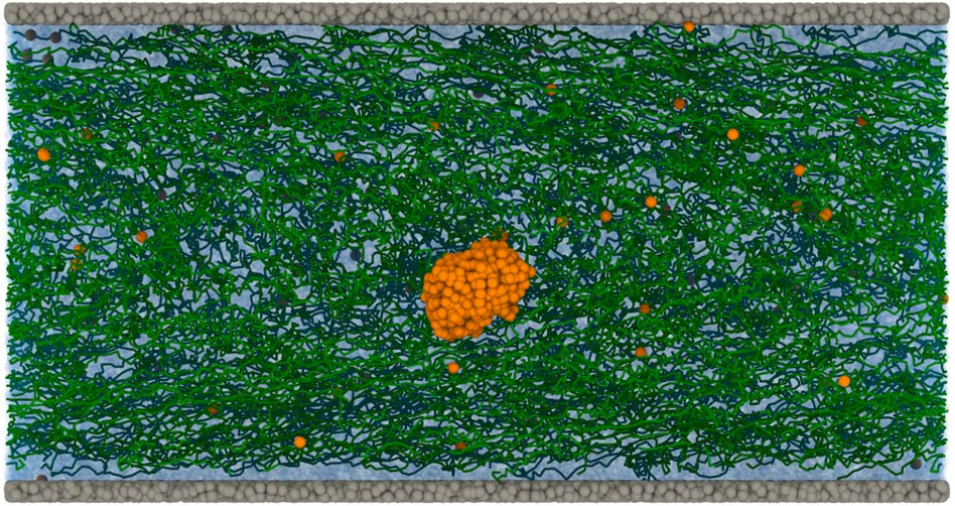
M.P. Howard et al., *Soft Matter* **15**, 3168 (2019).

Conclusions

Polymer solutions can be used to manipulate droplets in microchannels.

Droplet position and shape depend on the polymer solution and flow.

Important for applications like membrane filtration or cell sorting.



M.P. Howard et al., *Soft Matter* **15**, 3168 (2019).

All software has been released open source on GitHub: mphoward/azplugins

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BLUE WATERS SUSTAINED PETASCALE COMPUTING