11th i-CoMSE Workshop: Mesoscale Particle-Based Modeling

Mississippi State University
July 21–25, 2025

Multiparticle collision dynamics II

Session 13: Coupling to boundaries I (wall-driven flow)

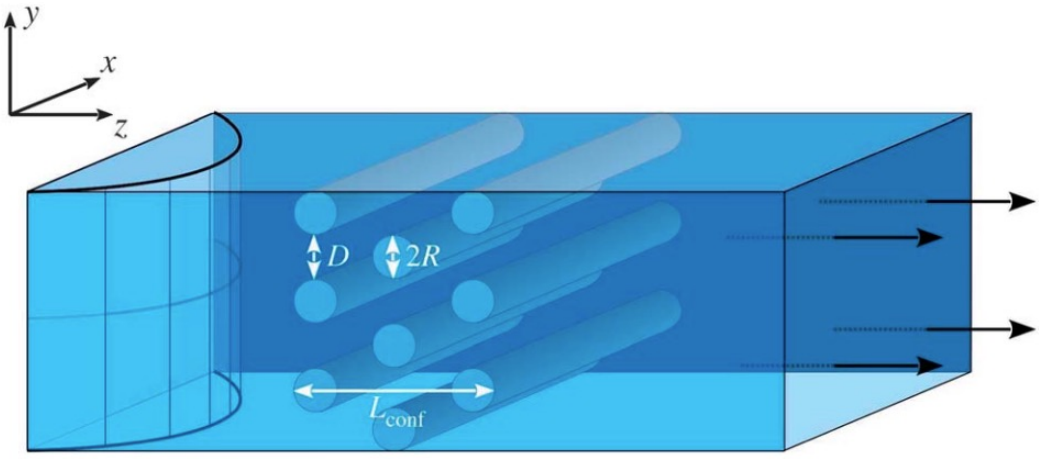
Fluid flow

https://corporate.exxonmobil.com/news/news-releases/2023/0919_exxonmobil-expands-chemical-production-at-baytown

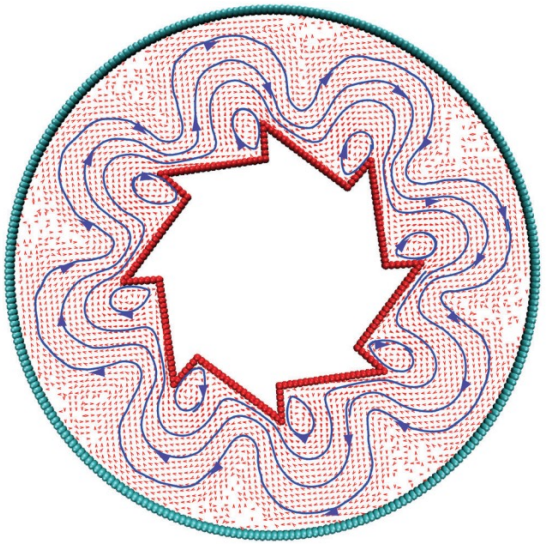
Fluid flow

https://www.tainstruments.com/discovery-core-rheometer/

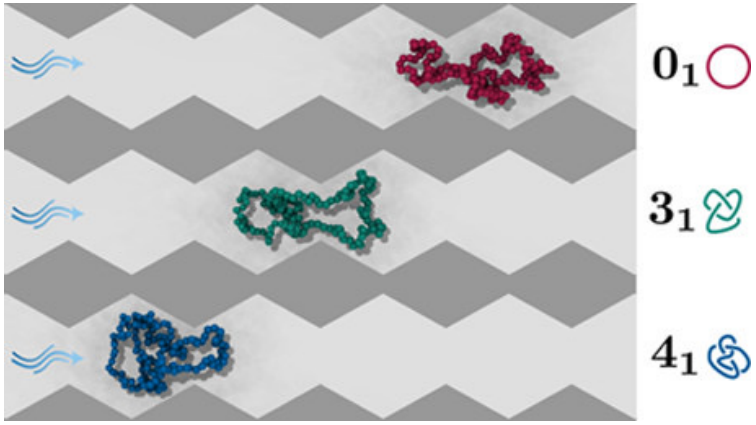
Fluid flow



A. Nikoubashman et al. *Soft Matter* **9**, 2603 (2013)



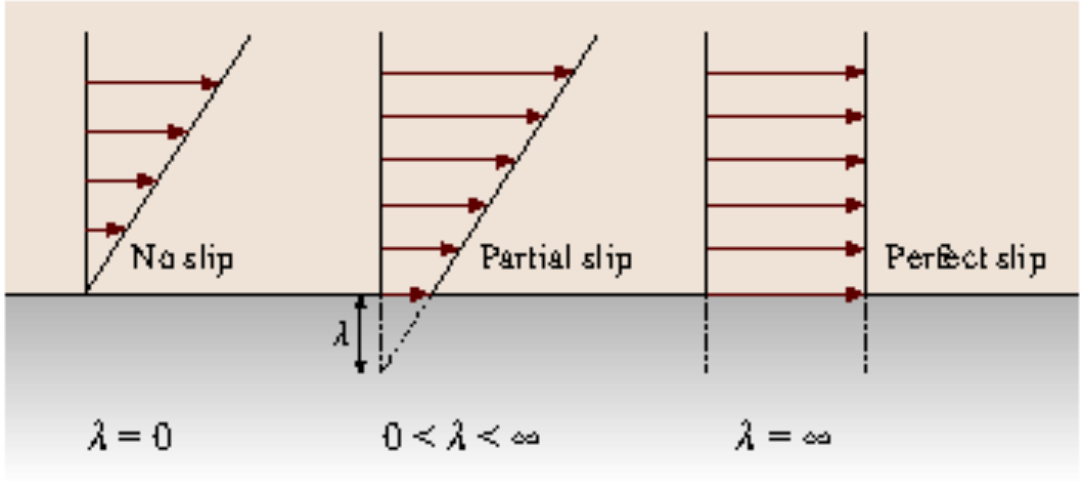
M. Yang and M. Ripoll. *Soft Matter* **12**, 8564 (2016)



L.B. Weiss et al.
Macromolecules **52**, 4111 (2019)

Solid boundaries and fluids

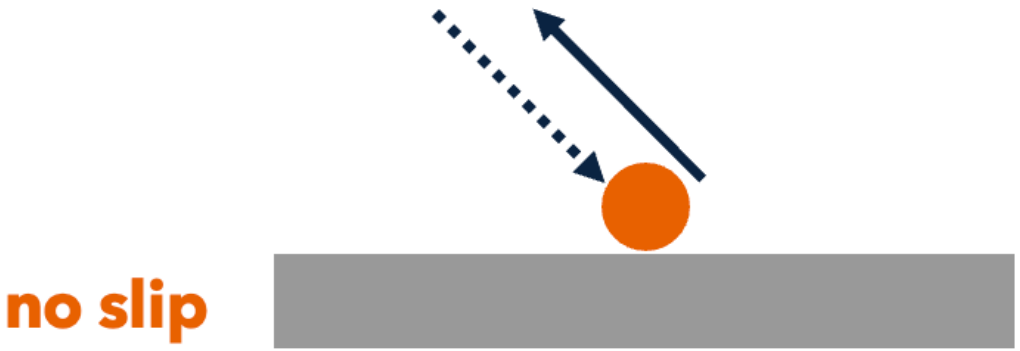
- Solid boundaries:
  - Prevent fluid from entering (no penetration)
  - *May* exert friction on the fluid (no slip, partial slip, perfect sliip)

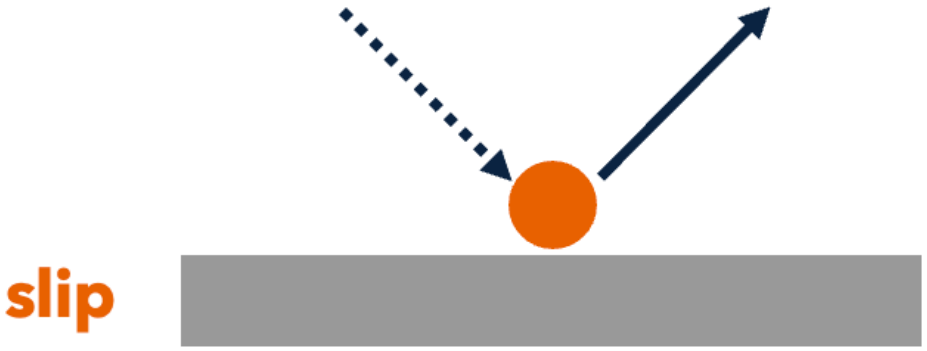


E. Lauga, M. Brenner, and H. Stone. Microfluidics: The No-Slip Boundary Condition (2007). https://doi.org/10.1007/978-3-540-30299-5_19

Solid boundaries in MPCD

- Bounce-back (specular reflection) of velocity relative to surface
  - Normal component is always reversed
  - Tangential component is reversed for no-slip

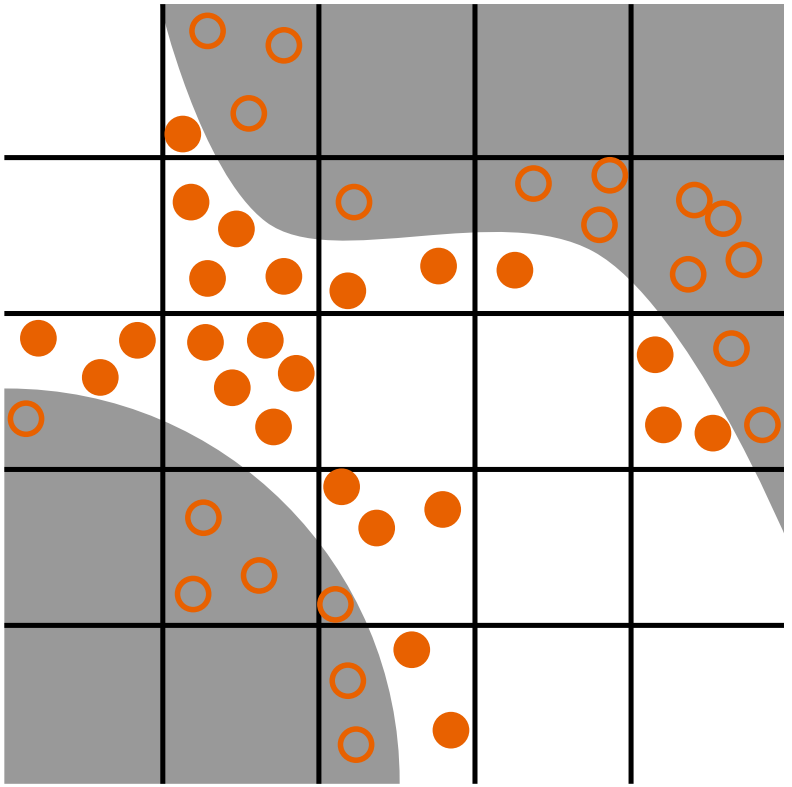




A. Lamura et al. *Europhys. Lett.* **56**, 319 (2001).

Solid boundaries in MPCD

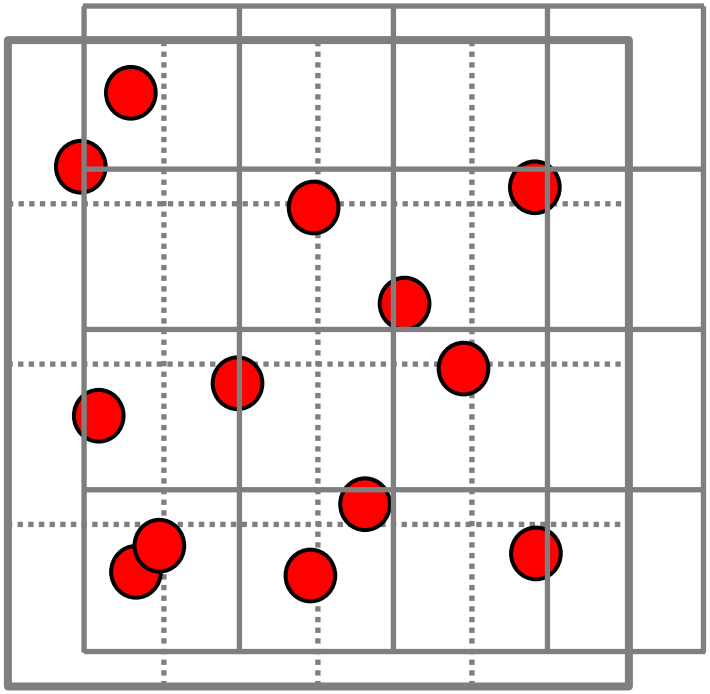
- Virtual particle filling
  - Cells near solid boundaries are “underfilled” in the collision, giving them different properties
  - Add particles inside these solid boundaries. Note: some caution needs to be taken to give the virtual particles the right statistics!



A. Lamura et al. *Europhys. Lett.* **56**, 319 (2001).
D.S. Bolintineanu et al. *Phys. Rev. E* **86**, 066703 (2012).

Solid boundaries in MPCD

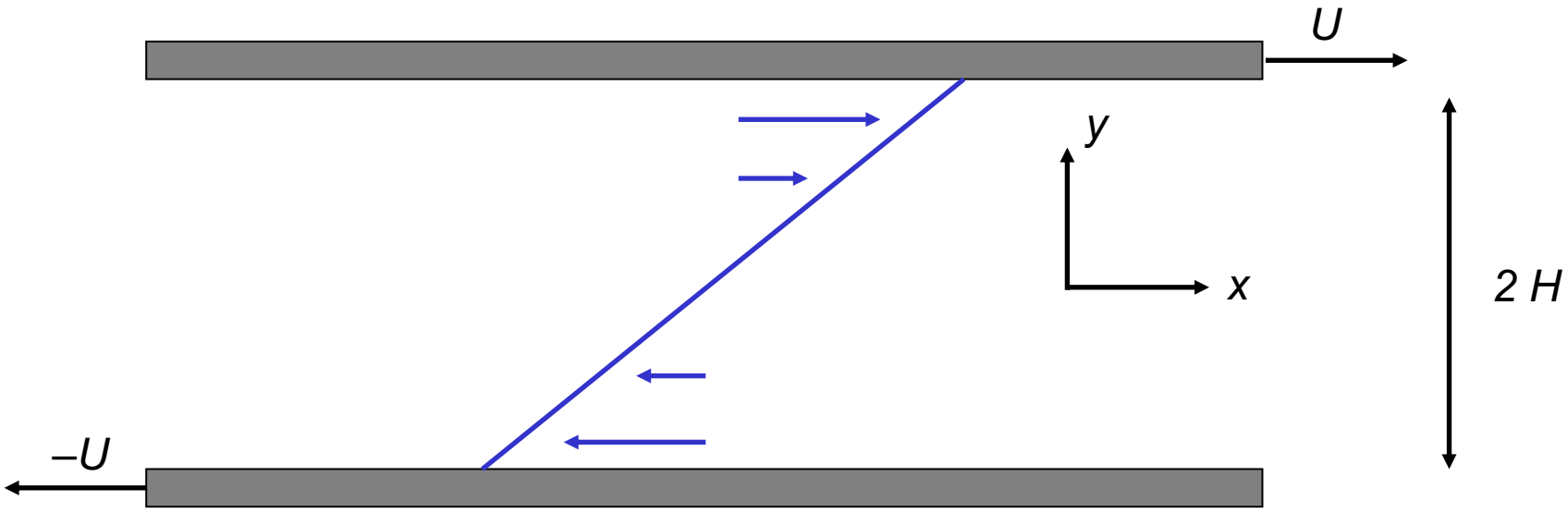
- Grid shifting
  - If many particles stay in the same cell, they become correlated, and the correlations are influenced by flow.
  - This breaks what is called *Galilean invariance*.
  - One way to mitigate this effect is to randomly shift the grid before each collision.



T. Ihle and D.M. Kroll. *Phys. Rev. E* **63**, 020201(R) (2001).

Exercise: Couette flow

- Wall-driven flow is created when a fluid is in contact with a moving surface.



$$u_x(y) = U\frac{y}{H}$$