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

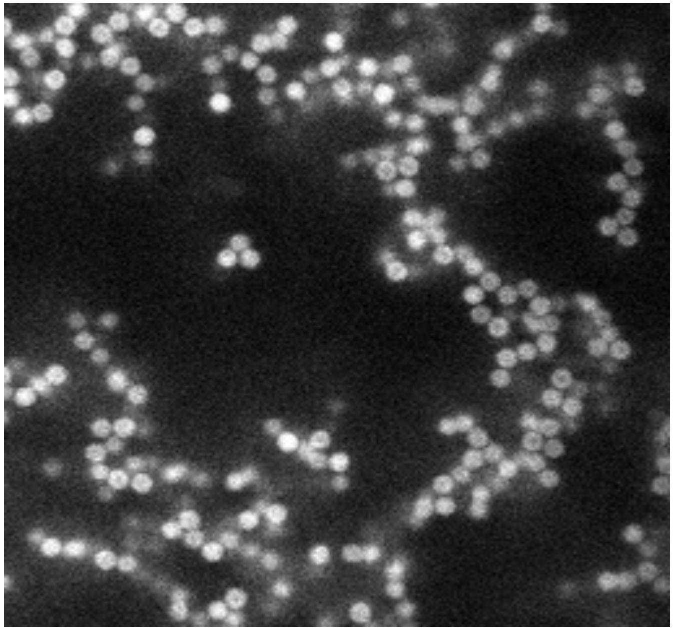
Mississippi State University
July 21–25, 2025

Multiparticle collision dynamics I

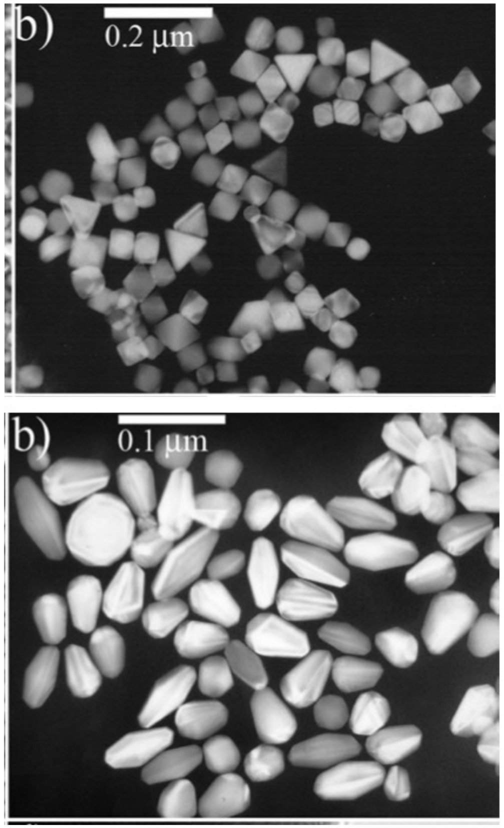
Session 12: Coupling to colloids

Nanoparticles / colloids

- Particles that are suspended in a solvent
  - Nanoparticle vs. colloid is usually around ~1 μm



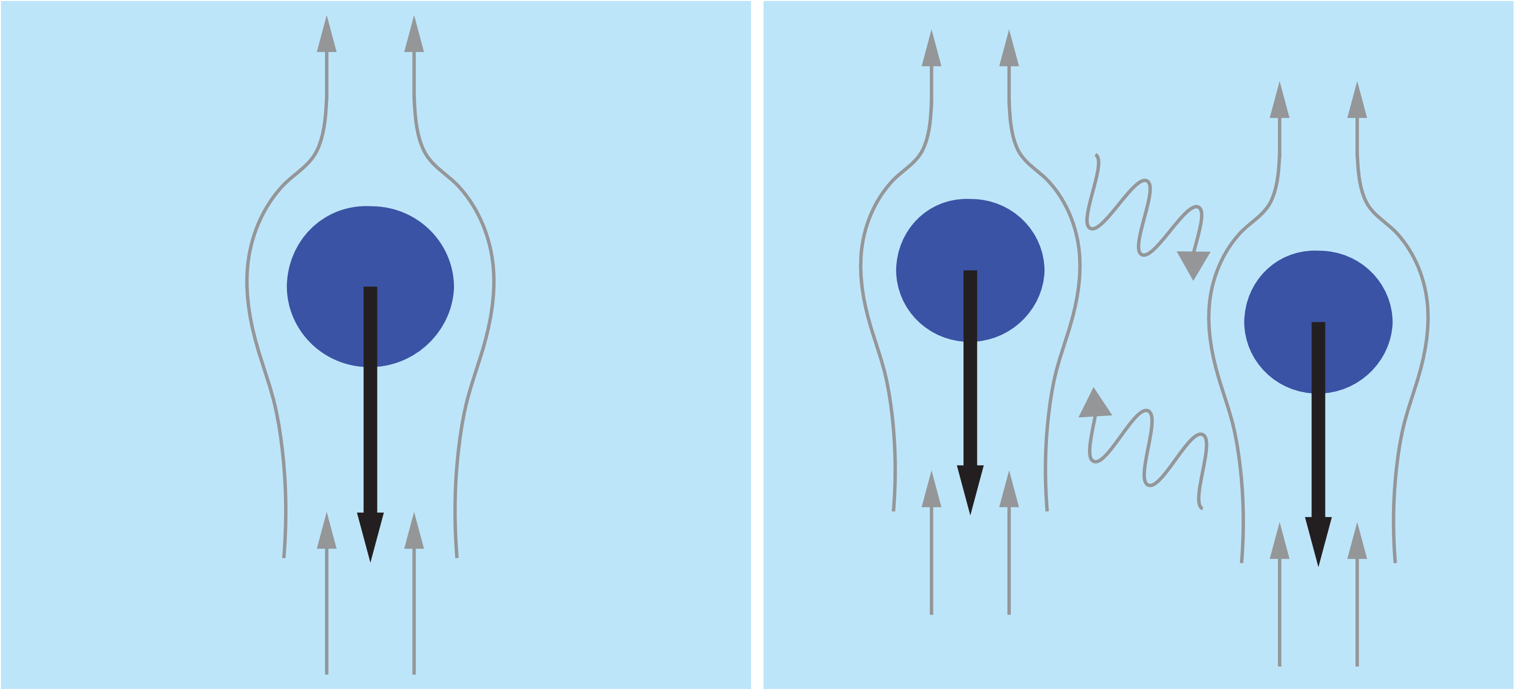
https://faculty.college.emory.edu/sites/weeks/lab/gelpage



J. Zhang et al. *Adv. Funct. Mater.* **17**, 3295 (2007)

Nanoparticles / colloids

- **Objective:** model hydrodynamic interactions on particles and between particles
  - Can play an important role on both individual and collective dynamics

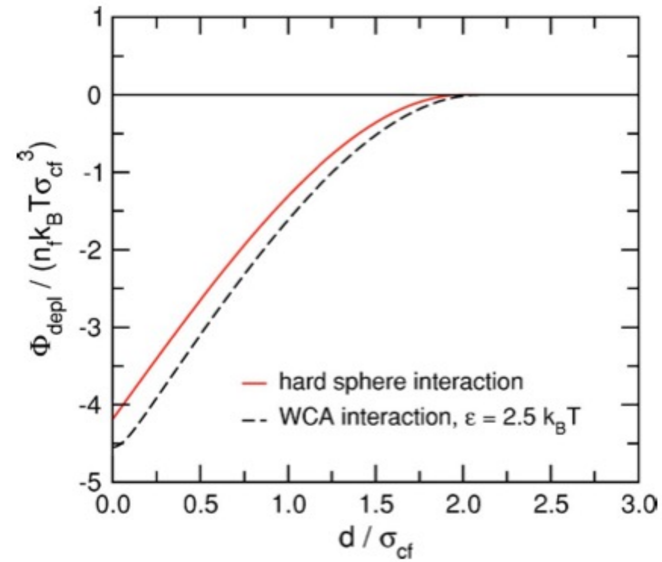


Nanoparticles / colloids in MPCD

- Central pairwise potentials (like WCA)

Similarly, the colloid-fluid interaction takes the WCA form

$$\varphi_{cf}(r) = \begin{cases} 4\epsilon_{cf}\left[\left(\frac{\sigma_{cf}}{r}\right)^{12} - \left(\frac{\sigma_{cf}}{r}\right)^{6} + \frac{1}{4}\right] & (r \leqslant 2^{1/6}\sigma_{cf}), \\ 0 & (r > 2^{1/6}\sigma_{cf}). \end{cases} \tag{17}$$



J.T. Padding and A.A. Louis. *Phys. Rev. E* **74**, 031402 (2006).

- Potential drawbacks
  - Expensive (we wanted to get rid of pair potentials for the solvent!)
  - No tangential forces (slip)

Nanoparticles / colloids in MPCD

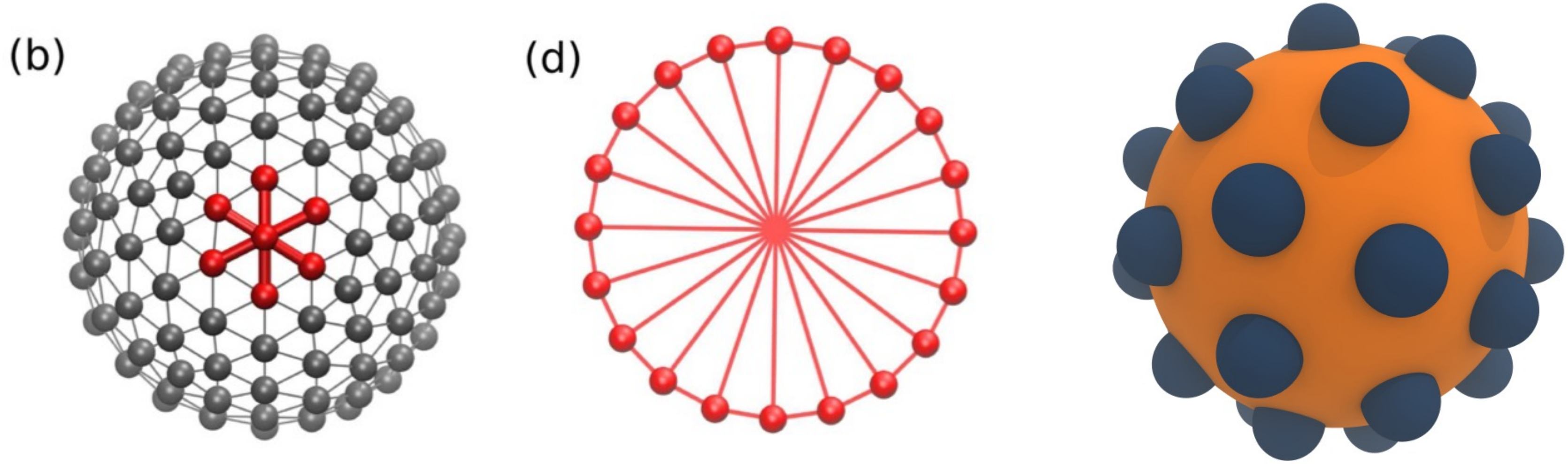
- Bounce-back coupling
  - Reflect the velocity when particle hits, or
  - Draw new particle velocities

Ex: J.K. Whitmer and E. Luijten. *J. Phys.: Condens. Matter* **22**, 104106 (2010).

- Potential drawbacks
  - Needs collision detection (as expensive as computing pairwise interactions)
  - May introduce artificial forces (like depletion)
  - How to handle collisions in cells near surfaces of particles (will discuss this problem more in upcoming sessions)

Nanoparticles / colloids in MPCD

- Collision coupling
  - Discretize surface of the particle
  - Surface particles participate in collision step (rather than streaming step)

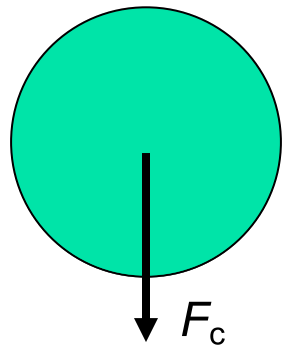


S. Poblete et al. *Phys. Rev. E* **90**, 033314 (2014).

- Potential drawbacks
  - Constructing the particle model is more challenging
  - Need to hold shape of the particle together (stiff springs)

Exercise: Sedimentation of a sphere

- Sedimentation is the process of a colloidal particle falling through a fluid, usually due to a density mismatch.



$$U_{\mathrm{c}} = F_{\mathrm{c}}/\gamma$$

$$\gamma = 3\pi\mu d$$

- Force balance: sum of forces on colloids and solvent must match

$$N_{\mathrm{c}}F_{\mathrm{c}} + N_{\mathrm{s}}F_{\mathrm{s}} = 0$$

- Finite-size effects: periodic boundary conditions slow the motion of the particle compared to being in an infinite volume.

Questions

- How to construct the model?
  - We have a tool for converting STL files to HOOMD inputs if you are interested!
- What should the density of surface particles be? Does it matter?
- What can go wrong?
  - Shape gets too floppy if springs are too soft
  - Simulation blows up if bad integration of springs
- Tradeoff in signal-to-noise ratio for applied force, may get physical instabilities if force is too large for suspensions
- Can I simulate active particles? Yes, with the right model!