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

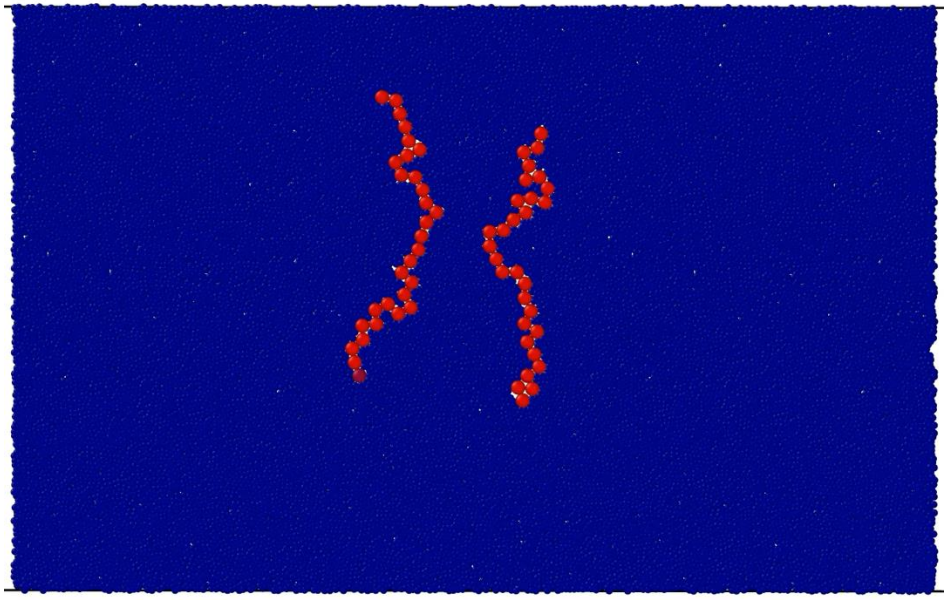
Mississippi State University
July 21-25, 2025

Topic: Polymer Solutions with MPCD

Polymer solutions with MPCD

Why?

- Hydrodynamics are important and interesting!

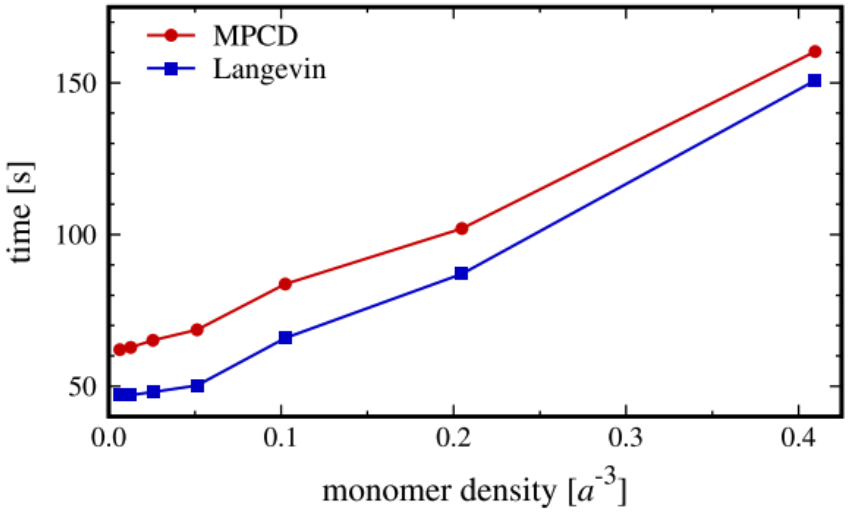


- Impact equilibrium transport properties, diffusion coefficients, etc.
- very important for nonequilibrium processes, flow, shear, etc.

Polymer solutions with MPCD

Dilute Polymer solutions:

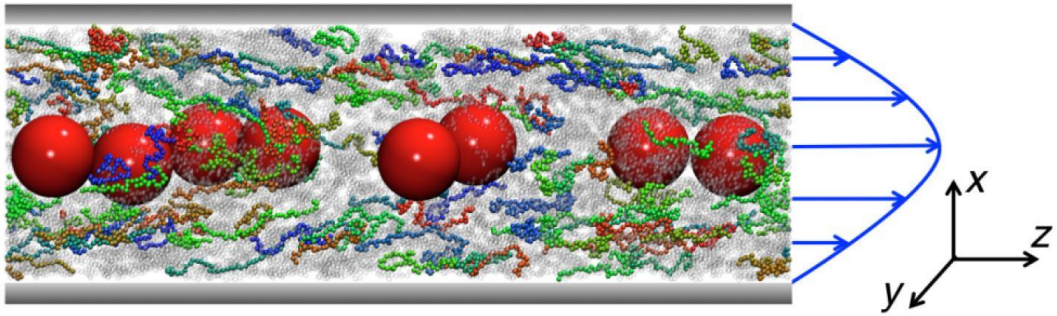
- **Explicit** solvent – full hydrodynamic interactions, etc. but very expensive
- **Implicit** solvent (Langevin, Brownian) – only indirect solvent effects, no hydrodynamic interactions, very cheap
- **MPCD** – some hydrodynamic interactions, only ~20% more expensive than Langevin!



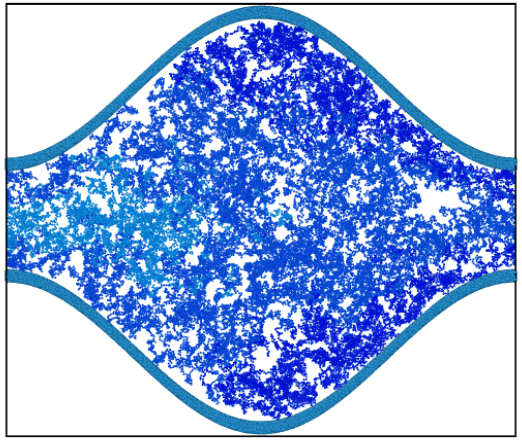
Howard, Michael P., Athanassios Z. Panagiotopoulos, and Arash Nikoubashman. "Efficient mesoscale hydrodynamics: Multiparticle collision dynamics with massively parallel GPU acceleration." Computer Physics Communications 230 (2018): 10-20.

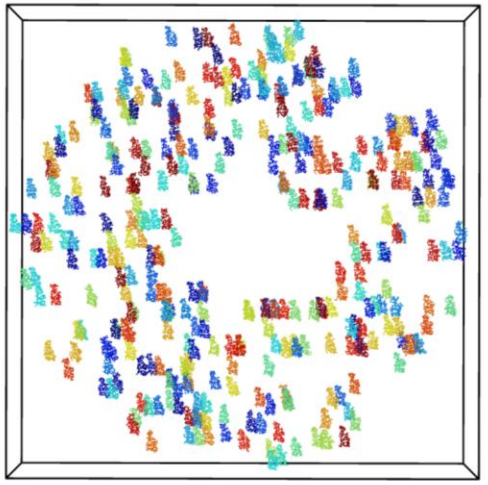
Polymer solutions with MPCD

Flow through various geometries



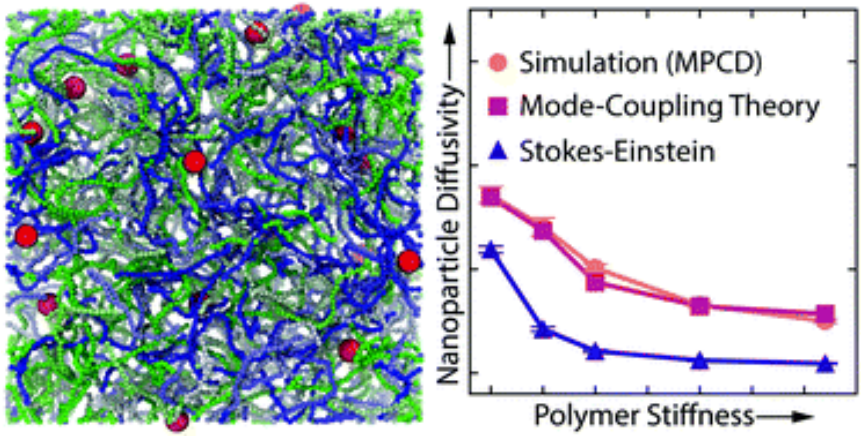
Howard, Nikoubashman, Palmer "Modeling hydrodynamic interactions in soft materials with multiparticle collision dynamics." Current Opinion in Chemical Engineering 23 (2019): 34-43. DOI:10.1016/j.coche.2019.02.007



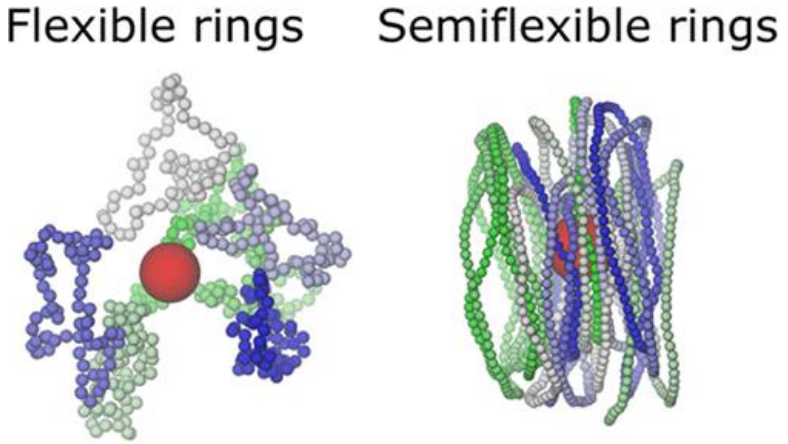


Polymer solutions with MPCD

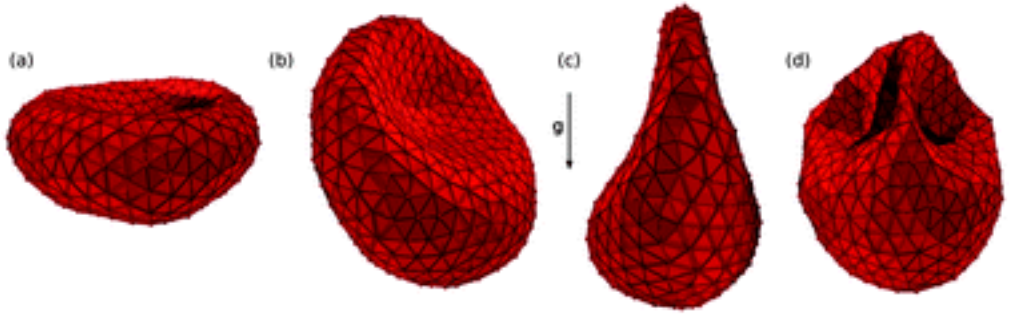
Complex systems



Chen, Renjie, et al. "Influence of polymer flexibility on nanoparticle dynamics in semidilute solutions." Soft Matter 15.6 (2019): 1260-1268.

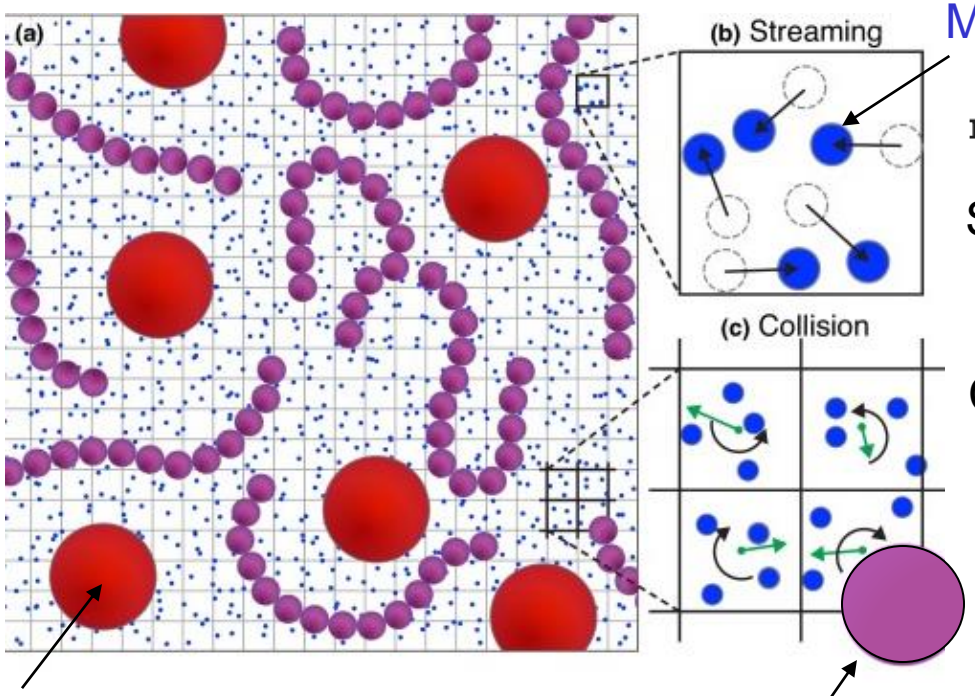


Kotkar, Shivraj B., et al. "Dynamics of Nanoparticles in Solutions of Semiflexible Ring Polymers." The Journal of Physical Chemistry B 128.50 (2024): 12586-12596.



Peltomäki, Matti, and Gerhard Gompper. "Sedimentation of single red blood cells." Soft Matter 9.34 (2013): 8346-8358.

Coupling



MPCD particles

$$\mathbf{r}_i(t+\Delta t) = \mathbf{r}_i(t) + \mathbf{v}_i(t)\Delta t,$$

Streaming step:

No change

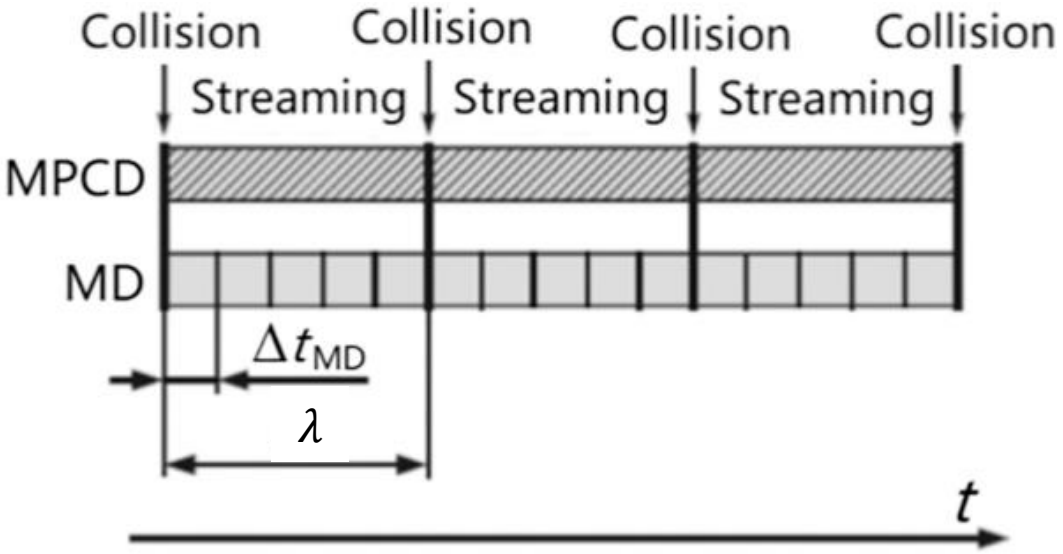
Collison step:

treat MD particles like MPCD particles (bin, rotate velocities)

NP/Colloids

polymer monomers

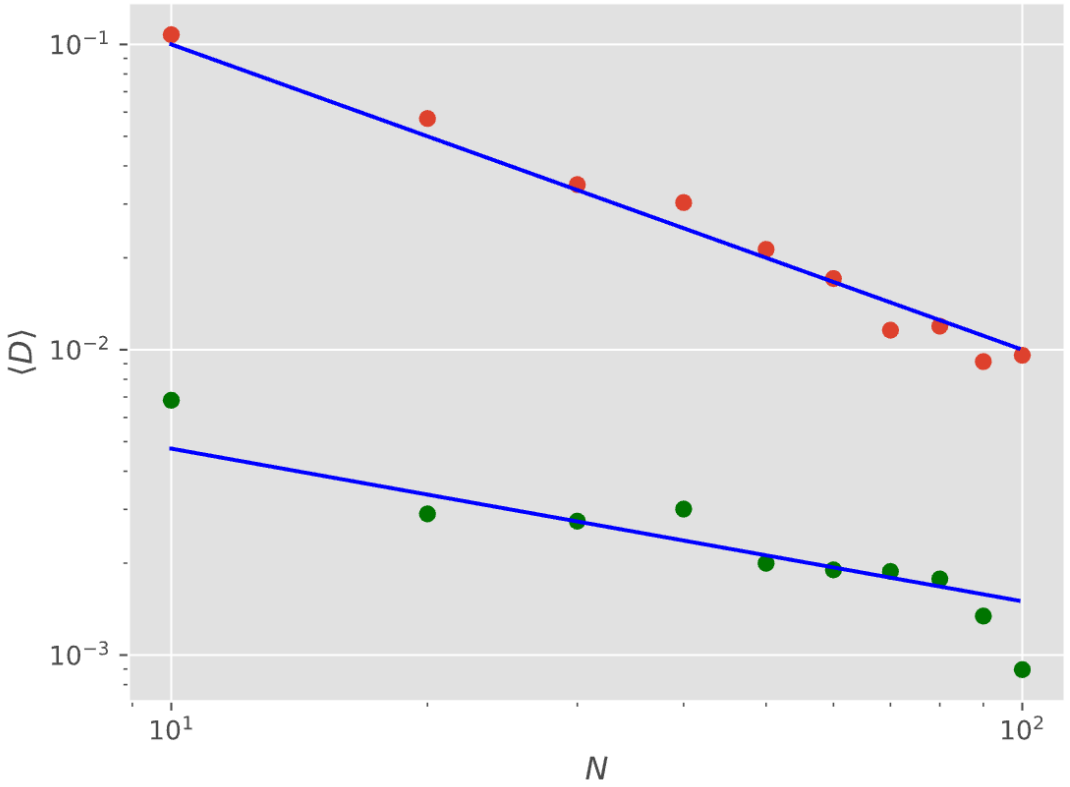
Coupling


Collision
Collision
Collision
Collision
Streaming
Streaming
Streaming
MPCD
MD
Δt_{MD}
λ
t

Exercise

Objective:

- Perform simple polymer solution simulation with MPCD
- Calculate the diffusion coefficient and compare to theory and Langevin simulation



Limitations of MPCD as polymer solvent

- No solvent phase coexistence:
  - No multiphase flow
  - No liquid interfaces
  - No explicit evaporation simulations

- Hydrodynamic interactions only on the scale of the grid