Non–Equilibrium Molecular Dynamics of Jamming in Thermostatted Shear Flows
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Summary
- Jamming occurs in a multitude of different systems on various length and time scales.
- Underlying mechanisms are not clearly understood.
- Can simulations verify behaviour and patterns found in experiments?
- Can manipulation of thermostats mimic the hydrodynamic interactions?

Experimental Method
- Couette system with densely packed colloidal particles.
- Intermittent jamming detected by needle and piezo sensor inserted in system.
- Magnitude of jamming event related to voltage

Shear Thickening with CT Thermostat
- Use of configurational thermostat leads to shear thickening regimes for this system.
- Kinetic degrees of freedom allowed to fluctuate – no lane formation observed.
- Kinetic temperature differs in X, Y and Z directions.
- Strong correlation between X and Y velocity components (Reynolds stress).

System Properties
- Histograms of fluctuations in viscosity at particular shear rates obtained.
- Similarly, pressure distributions were also obtained.
- Evident broadening of distribution occurring at highest shear rates, indicating larger fluctuations in stresses during shear thickening.

Conclusions
- Shear thickening regime obtained using configurational thermostat.
- By thermostatting configurationally; velocities are allowed to freely deviate from streamline, giving insight to Reynolds stress.
- Currently parallelising code to simulate larger systems and obtain longer trajectories for better statistics in shear thickening regime.

Equations of Motion
\[
\dot{r}_i = \frac{p_i}{m} + \gamma y_i e_x + \frac{s}{T} \frac{\partial T_{conf}}{\partial r_i}
\]
\[
\dot{p}_i = F_i - \gamma p_{yi} e_x - \alpha p_i
\]
\[
\dot{\theta} = -Q \left( \frac{T_{conf} - T}{T} \right)
\]

Simulation Methods
- Numerical Integration with 4th order Gear predictor–corrector algorithm.
- Lees Edwards boundary conditions (sliding brick)

Benchmarking code
Comparison of shear thickening regime with configurational thermostat [1].
- \( T_{conf} = 0.722 \)
- \( n = N/V = 0.844 \)
- \( N = 1372 \) particles
- L–J potential