# 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?

## Equations of Motion

$$\dot{\mathbf{r}_\mathbf{i}} = \frac{\mathbf{p_i}}{m} + \dot{\gamma} y_i \mathbf{e_x} + \boxed{\frac{s}{T}\frac{\partial T_{conf}}{\partial \mathbf{r_i}}}$$

$$\dot{\mathbf{p}_\mathbf{i}} = \mathbf{F_i} - \dot{\gamma} p_{yi} \mathbf{e_x} - \boxed{\alpha \mathbf{p_i}}$$

$$\dot{s} = -Q\frac{(T_{conf} - T)}{T}$$

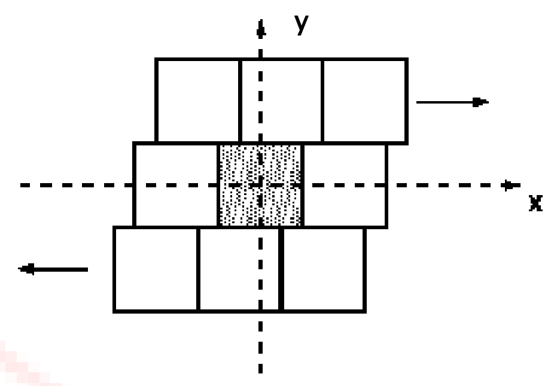
**Kinetic** **Configurational**

$$\sum_i \left\langle \frac{m v_i^2}{2} \right\rangle = \frac{3}{2} k T_{kin}$$

$$\frac{1}{k_B T_{conf}} = \left\langle \frac{\sum_i \frac{\partial^2 \Phi_0}{\partial \mathbf{r_i}^2}}{\sum_i \left(\frac{\partial \Phi_0}{\partial \mathbf{r_i}}\right)^2} \right\rangle$$

- Kinetic temperature defined by velocities, configurational defined by positions.

## Simulation Methods

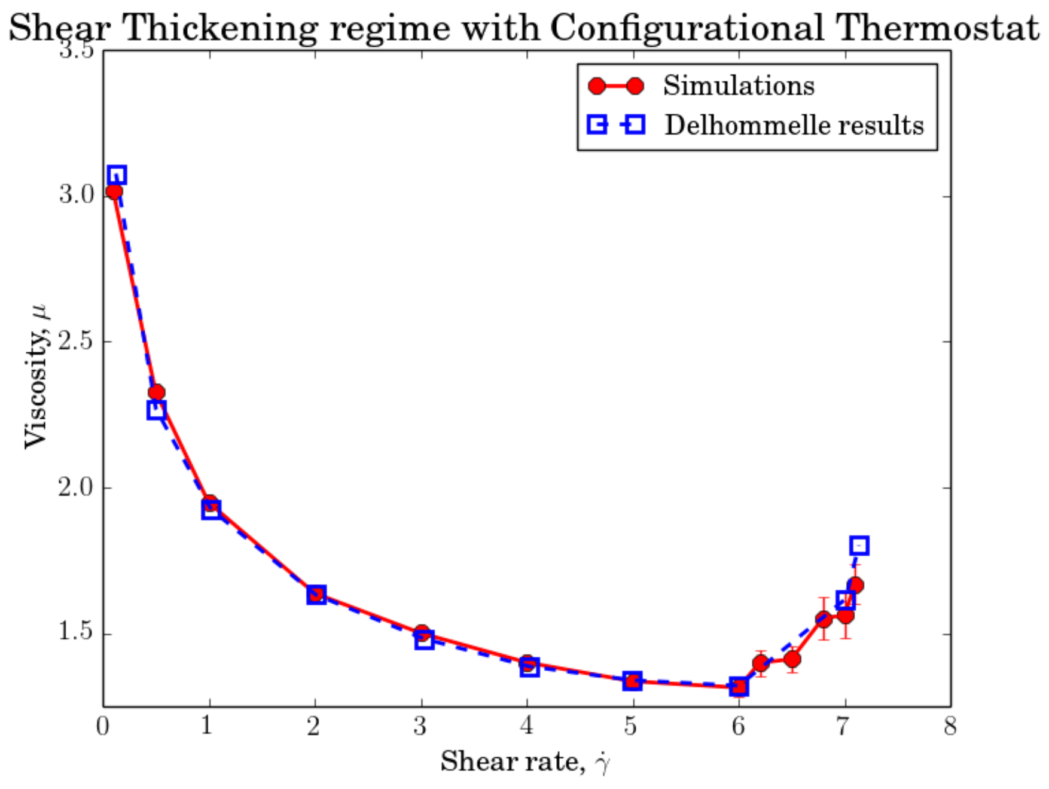


- Numerical Integration with 4th order Gear predictor-corrector algorithm.
- Lees Edwards boundary conditions (sliding brick)

## Benchmarking code

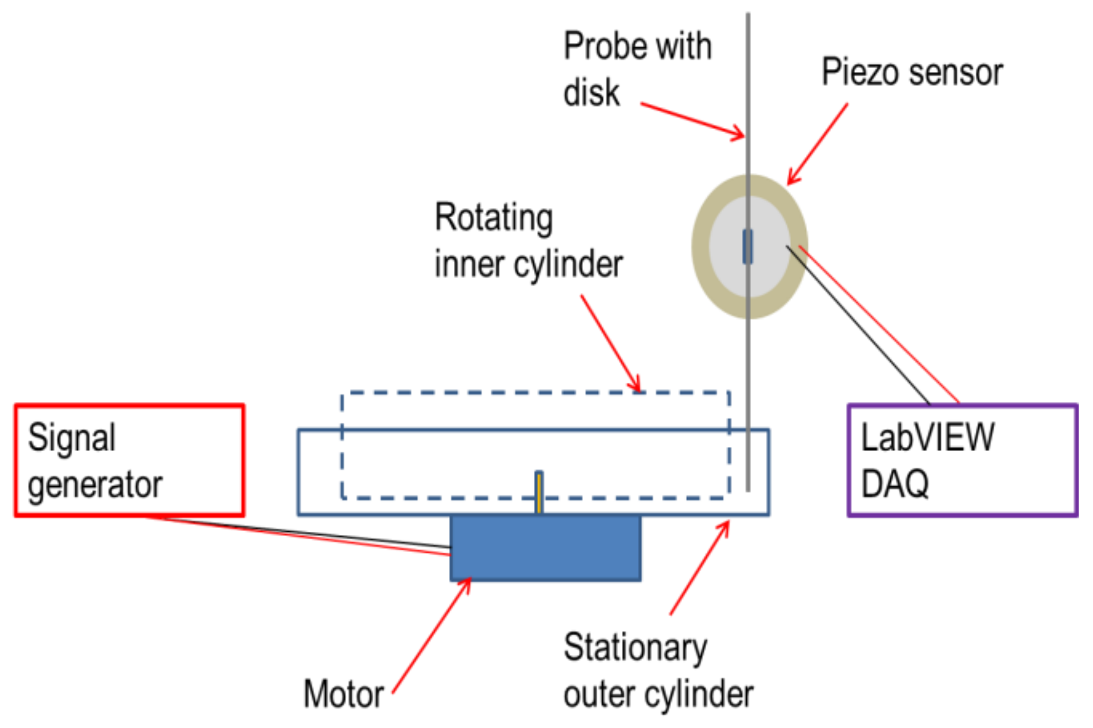
Comparison of shear thickening regime with configurational thermostat [1].

- $T_{conf}$=0.722
- n= N/V=0.844
- N= 1372 particles
- L-J potential



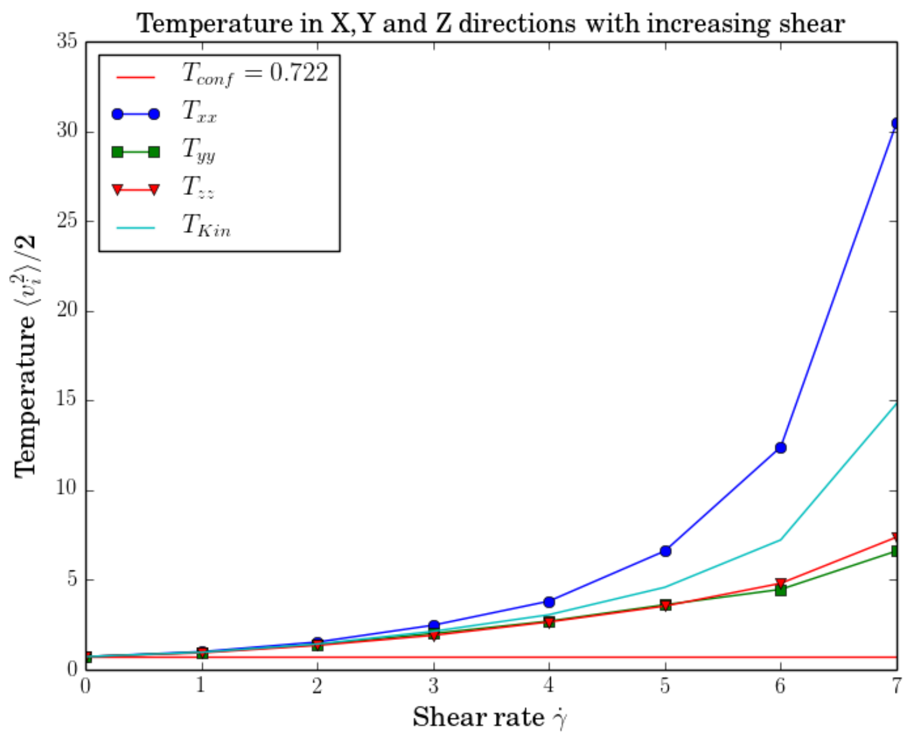
## Experimental Method

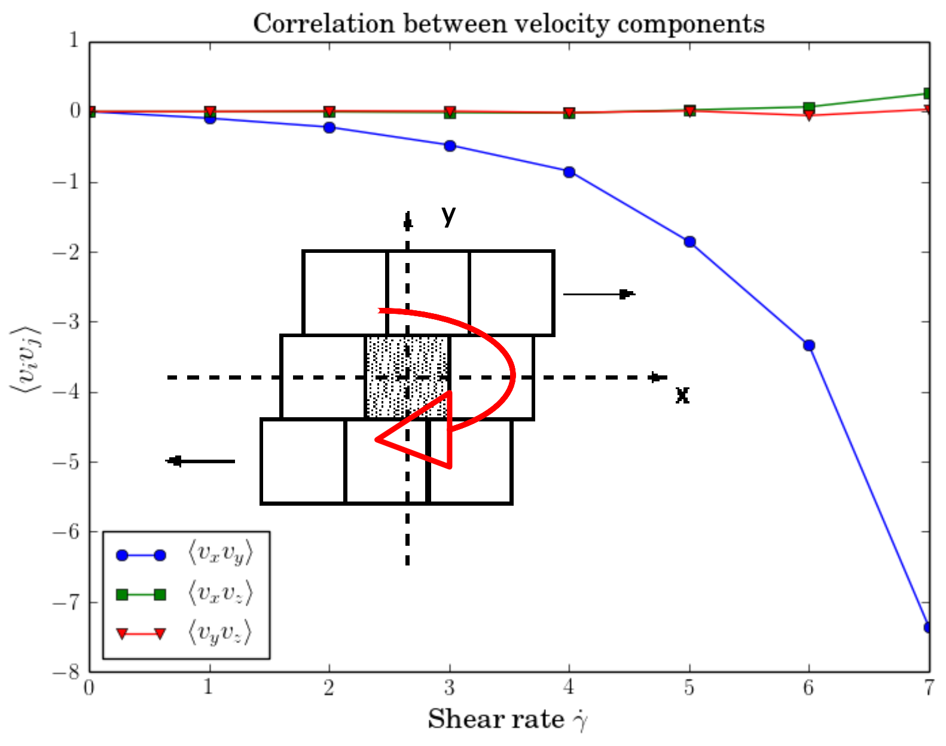
- Couette system with densely packed colloidal particles.
- Intermittent jamming detected by needle and piezo sensor inserted in system.
- Magnitude of jamming event related to voltage



## Shear Thickening with CT Thermostat

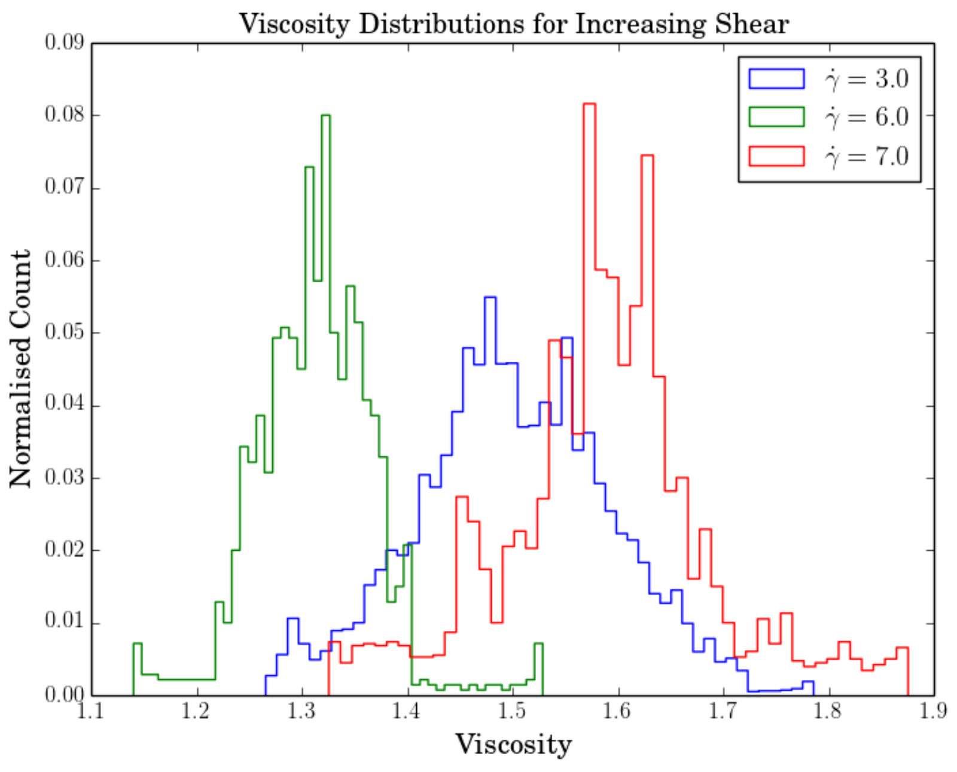
- Use of configurational thermostat leads to shear thickening regimes for this system.
- Kinetic degrees of freedom allowed to fluctuate – no lane formation observed.
- Kinetic temperature differs in X, Y and Z directions.
- Strong correlation between X and Y velocity components (Reynolds stress).

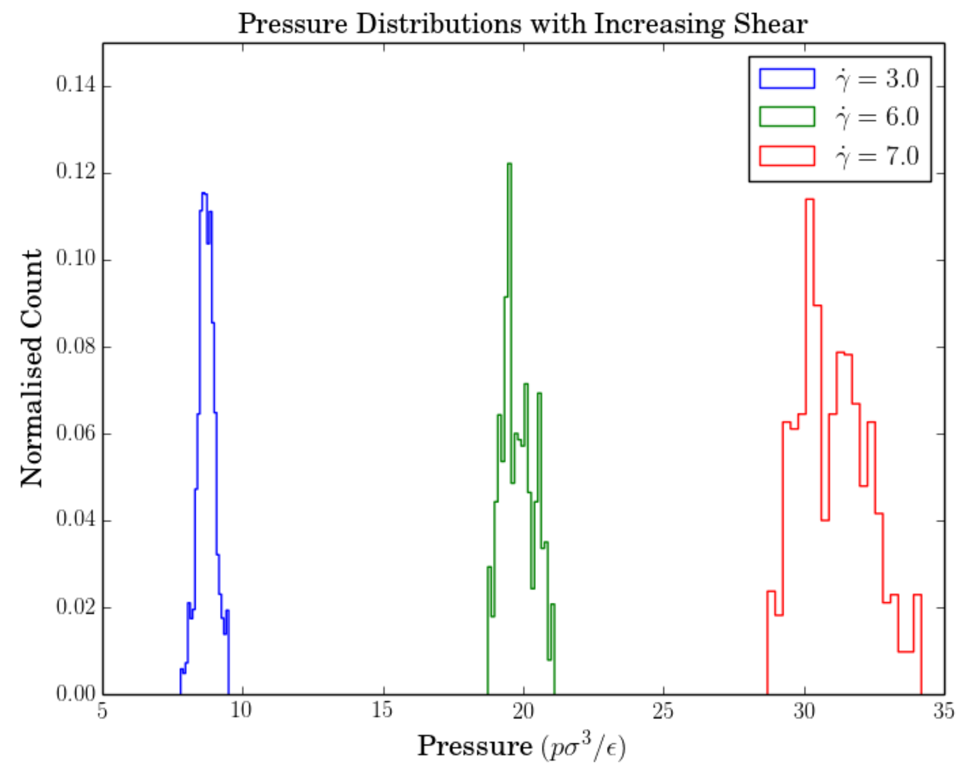




## System Properties

- 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.

1. *"Non-Newtonian Behaviour in Simple Fluids", J. Delhommelle* et al, J. Chem Phys. 120 (13), 2004.