The Role of Thermostats in Simulations of Jamming

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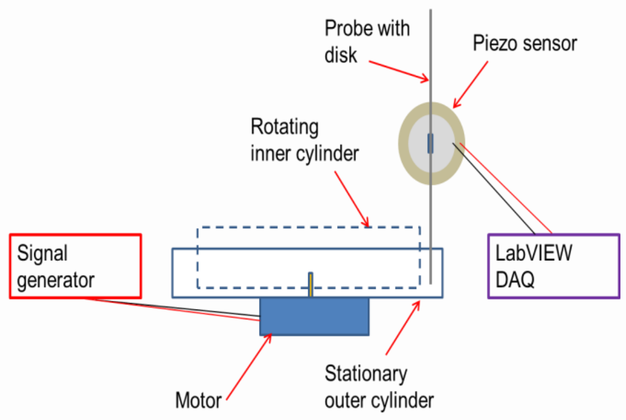
Summary

- 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



Equations of motion

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

$$\dot{\mathbf{p_i}} = \mathbf{F_i} - \dot{\gamma} p_{yi} \mathbf{e_x} - \alpha \mathbf{p_i}$$

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

Kinetic

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

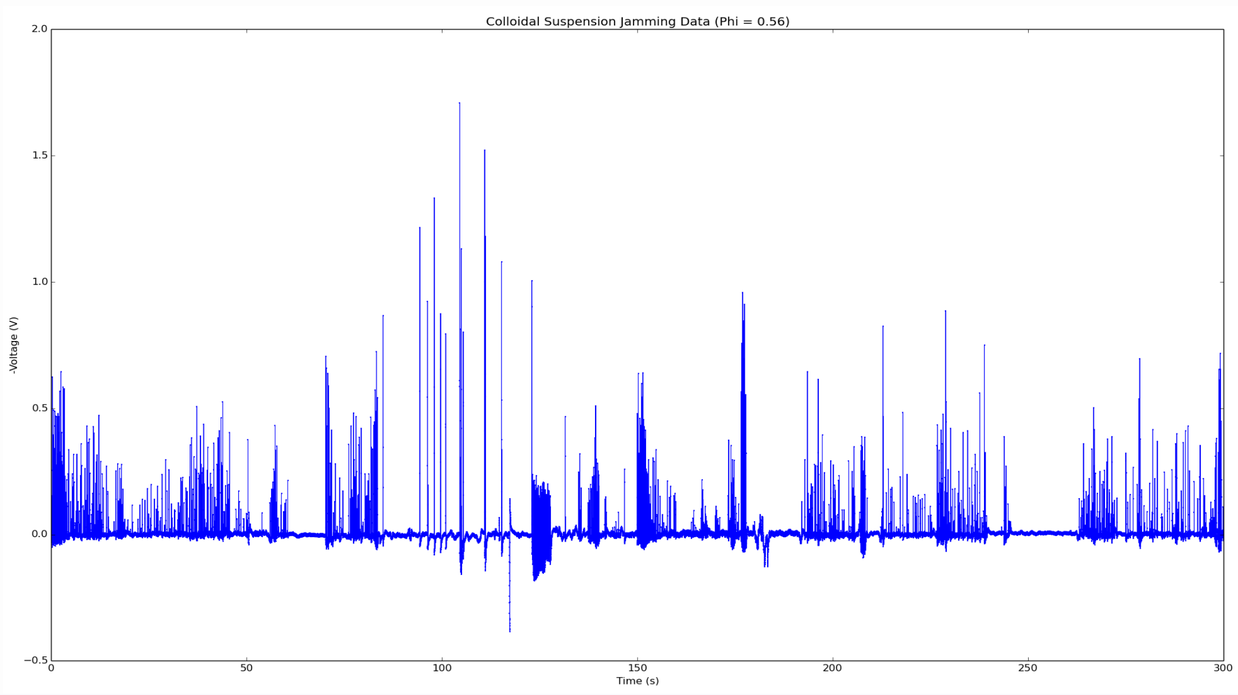
Configurational

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

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

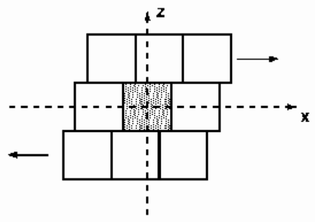
Experimental Data Analysis

By gathering voltage data over time it is possible to analyse how the internal forces fluctuate as the system moves between jammed and flowing states.



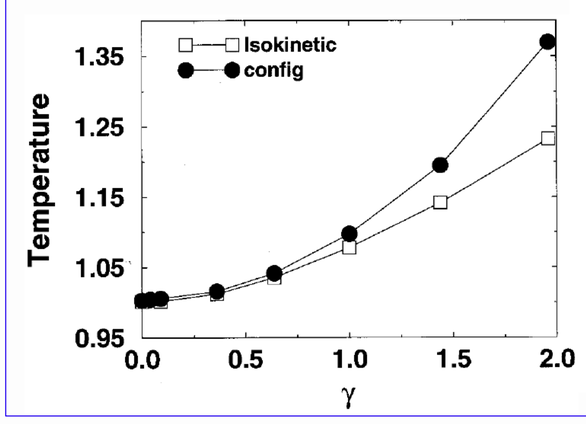
Simulation Methods

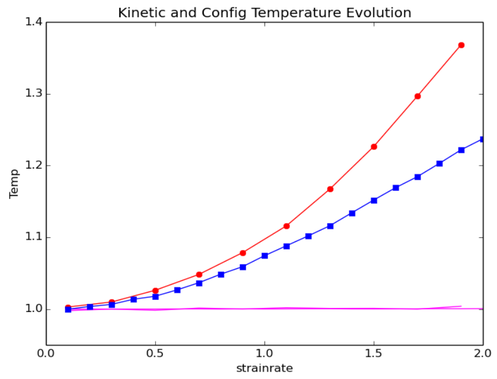
- Numerical Integration with 4th order Gear predictor-corrector algorithm
- Lees Edwards & periodic boundary conditions (sliding brick)



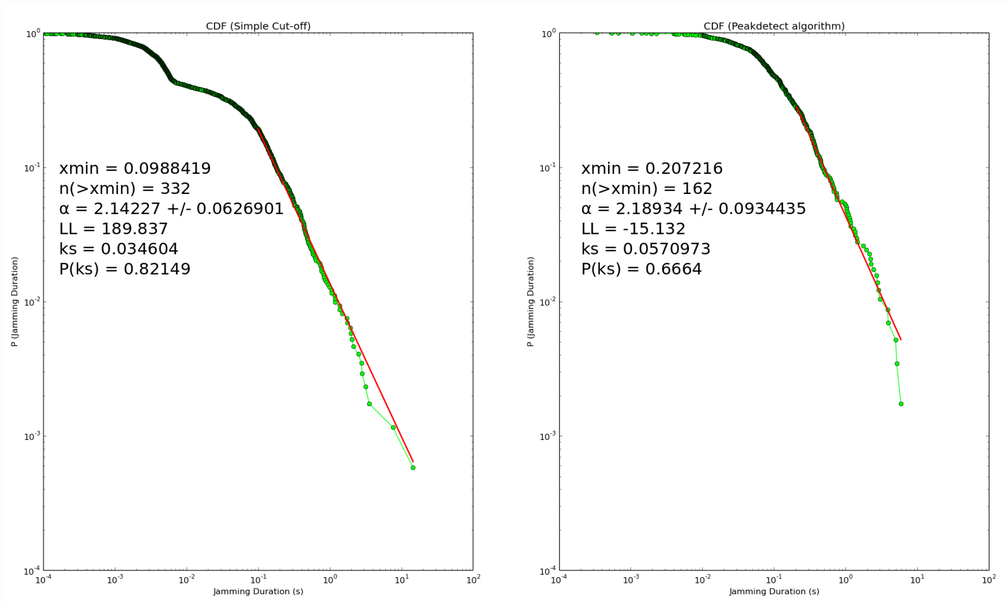
Benchmarking code

- Comparison of thermostats with Lue et al. [1]





CDFs and Power Laws



- Noise removed from data and time between remaining peaks obtained.
- Time between peaks analogous to jamming duration.
- Power law algorithms[2] implemented to temporal statistics

Conclusions

- Temporal statistics of force fluctuations show jamming durations follow a power law behaviour.
- Successful Molecular Dynamics simulations for both kinetic and configurational thermostats.
- Regions of shear thickening with configurational thermostat currently being explored.

1. *"Configurational Thermostats for Molecular systems"*, L. Lue at al, Mol Phys 100 (14), 2002.
2. *Power-law distributions in empirical data"*, A. Clauset, C.R. Shalizi, and M.E.J. Newman, "SIAM Review 51(4), 661-703 (2009).