**Summary**

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* Implemented a shearing DPD simulation with equations and dynamics from Pryamitsyn
  + Viscosity is calculated with a Lees-Edwards system, shear stress is computed and then the integral of this stress autocorrelation function is computed.
* Investigated variation of viscosity with:
  + Shear rate
    - No major dependence of viscosity on shear rate as long as temperature is maintained near 1. This happens for shear rate .
  + Number of particles
    - Increasing trend that rises rapidly near . Trend is largely exponential, doesn’t really obey the empirical relation.
  + Particle Size:
    - Viscosity was *slightly* decreased when particle size was reduced from 2.5 to 2 with particle number correspondingly increased to maintain the same value of .
    - **Inconclusive results.**
  + **Simulation time [0 shear]**
    - **Increased viscosity since we are integrating over a longer period of time.**
  + Colloid-colloid repulsion parameter [0 shear]
    - Increased viscosity as well, peaks more sharply near
  + Packing/Jamming state
    - Visually, it is observed that the particles gradually transition from an open and loose configuration to a tight configuration that appears closer to the close packing configurations
    - To quantify the “tightness”, coordination number is measured and found to increase linearly with for .
    - To quantify the order, the “bond angles” were plotted and peaks were found near and .
    - **Shear Rate and Particle Size could be varied**
  + Nonhomogeneous particle sizes -- Similar to how the supercooled water has varying sizes of "solid" water
    - Viscosity measurements as a function of size/stdev
    - Take pictures of state

Possible Areas for Investigation

* Investigating the onset of order/disorder as a function of packing fraction and shear rate
* Varying models of colloid-colloid interactions 🡪 Hertzian contact etc

**Previous Issues**

* Implementing the Lees-Edwards BC + SLLOD does not give reasonable results for the viscosity.
  + Is the stress computed wrongly?
  + Are the SLLOD modifications to the EoM necessary? With the first modification that relates position to velocity, is there still a need for the velocity jump at boundaries?
* Is the viscosity formula correct?
  + It does not appear to conform to the **empirical formula** even though Pryamitsyn and Pan have shown that it works.
  + Why is it that the viscosity function **does not rise significantly at**  and only doing so near 0.9?
  + In fact, the particles appear to be compressed significantly, causing to be possible. Because of this, **will viscosity even diverge**? It seems like it will just keep packing closer and closer. Is it no longer meaningful to investigate once there is **significant overlap**?
* Is the current **integration time** sufficient?
  + Integrating with 10x the duration indicates up to 50% increase in viscosity at and up to 2 to 3x viscosity at
* Is there a need to modify the number of water particles as we increase the number of colloidal particles to **keep pressure constant**?
  + The pressure appears to be increasing smoothly as a function of water particles / density of water particles, as is summarised in the equation of state:
* Is there a way to check and see if the old GK results are correct/compatible with the new LE results?
  + Main discrepancy seems to arise from the divide by 3, differences in MOI, and differences in the interaction distance (4.45 vs 0.9 \* 5, 2.45 vs 0.8 \* 3)
  + It seems that they \*are\* compatible. The 0 particle case gives ~1.4 for the old GK results and ~4.2 for the LE results, and obviously .