Computer Simulations of Packed Soft Colloids

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Overview

We apply the recently developed computational method Fluctuating Finite Element Analysis (FFEA) to highly packed soft colloids. We use this simulation method to probe the motion of colloidal particles and the corresponding rheological response.

Colloidal Glasses

- Transitions from fluids to disordered solids occur in many systems.
- Link between individual particle and collective suspension properties are not well understood.
- Existing computational approaches are often based on radially-symmetric soft sphere potentials
- Complex many-body interactions are important.
- This project considers thermal and flow-induced particle deformations using a mesoscale modelling method: Fluctuating Finite Element Analysis (FFEA).

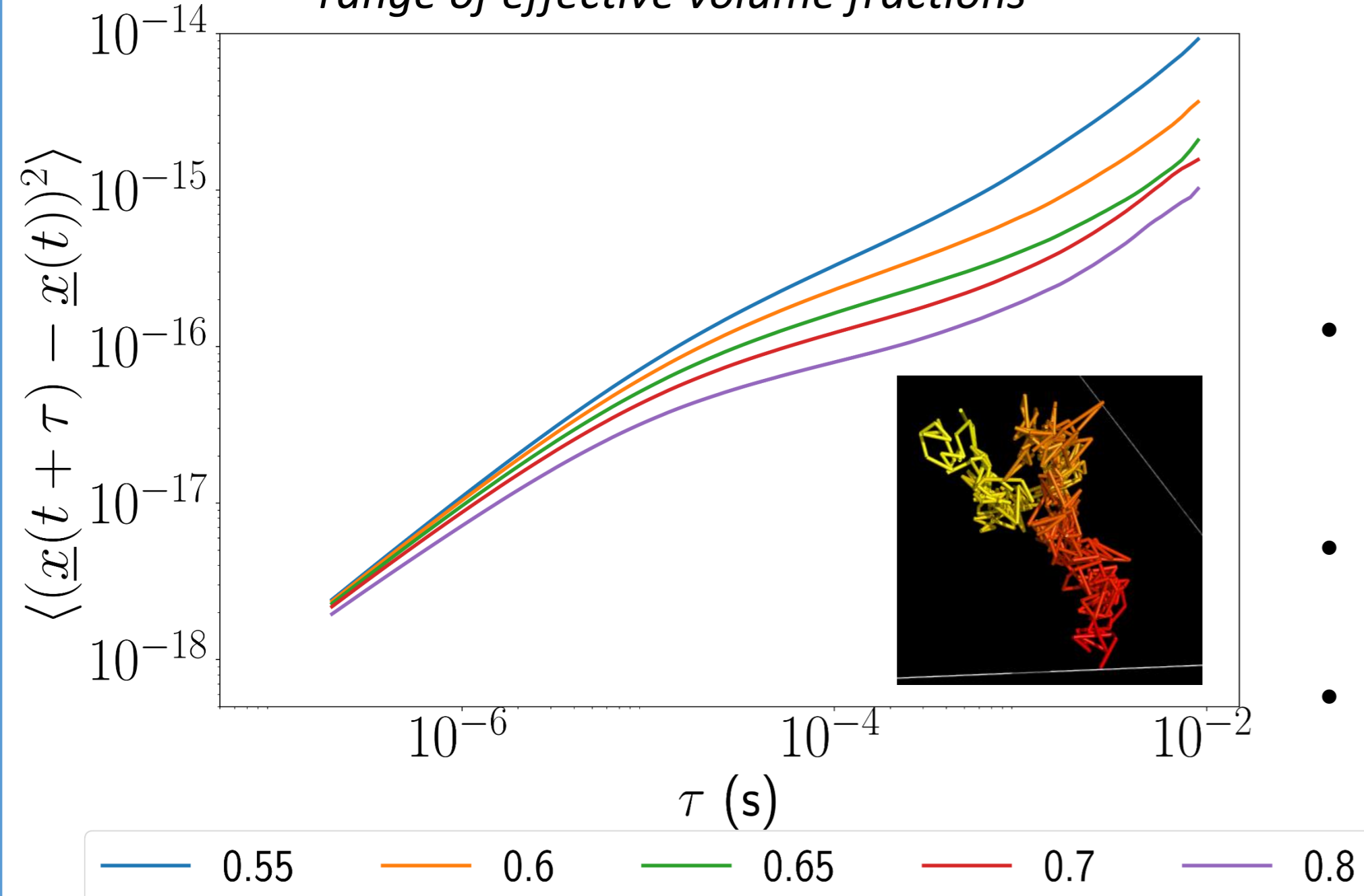

Pictured: Possible rearrangement in dense packings
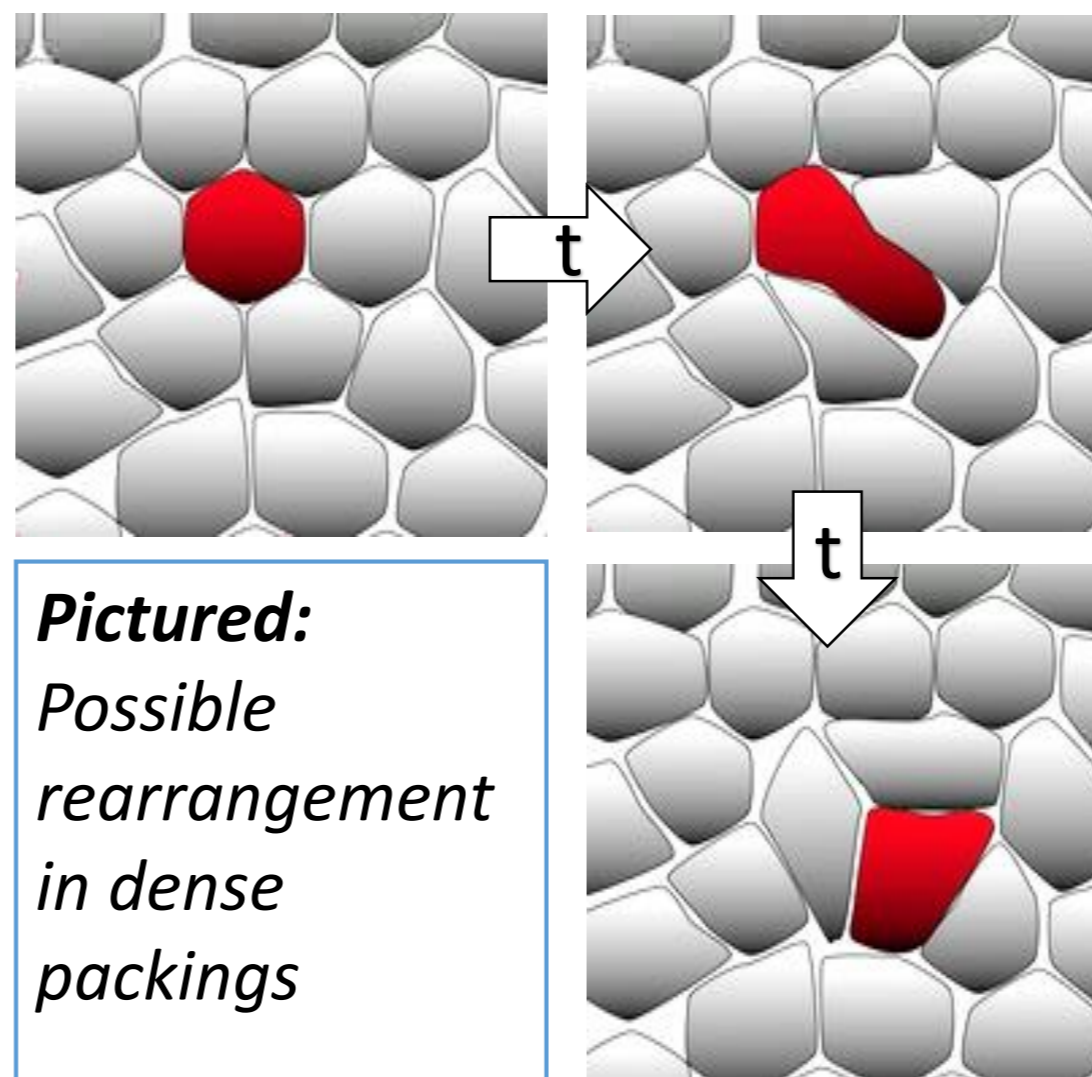
Fluctuating Finite Element Analysis
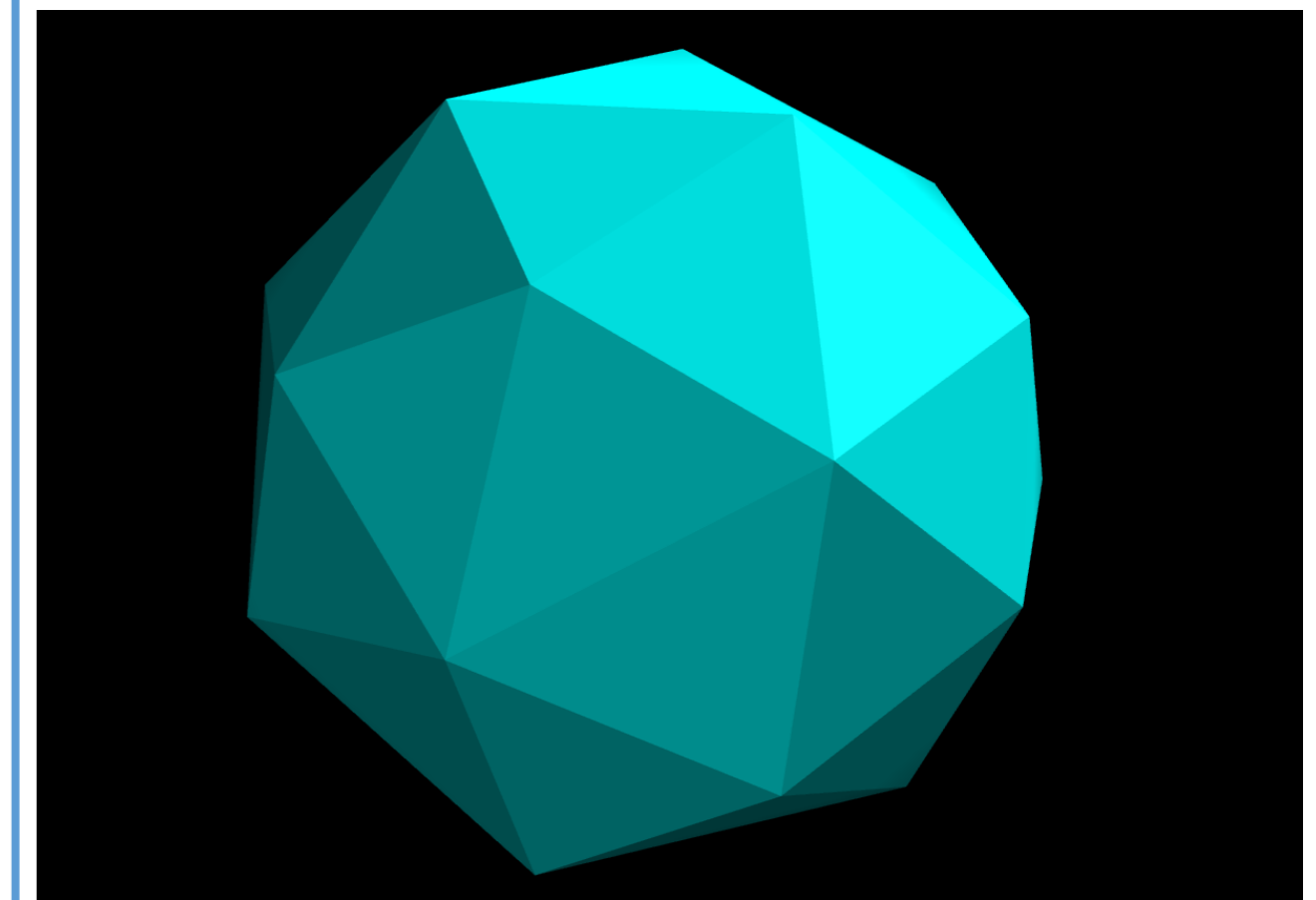
- Discrete finite element method developed in Leeds.
- Models mesoscale continuum objects subject to stochastic thermal forces and stresses.
- Models colloidal particles as interacting deformable objects suspended in a fluid and subjected to thermal fluctuations.
- Per-particle material properties can be varied, as well as total packing fraction of the system.
- Results presented use material parameters:
  - 100nm diameter,
  - 0.36 Poisson ratio,
  - 3.7/12.34 kPa Shear/bulk Modulus,
  - 8.8/2.47 mPa Shear/bulk Viscosity,
  - 1000kgm^{-3} Density.

Self-Diffusion

Averaged Self Diffusion over 1000 colloids for a range of effective volume fractions


- Effective volume fraction $\zeta = \frac{N V_0}{V_{Sys}}$ varied; N: number of blobs; V_0: equib. particle volume; V_{Sys}: system volume.
- Mean-square displacement calculated using multi-tau correlator[1].
- 3 dynamic regimes; intermittency.
- Simulations performed with both 100 and 1000 particle - finite size effects observed for 100 particle simulations.

0.55   0.6   0.65   0.7   0.8

1. J Ramírez et al. J Chem Phys 133 (15)

Shear-Response

Time evolution of elastic response to range of shear rates at $\zeta = 0.8$

Shear rate
67s^{-1} 268s^{-1} 1340s^{-1}
201s^{-1} 670s^{-1}
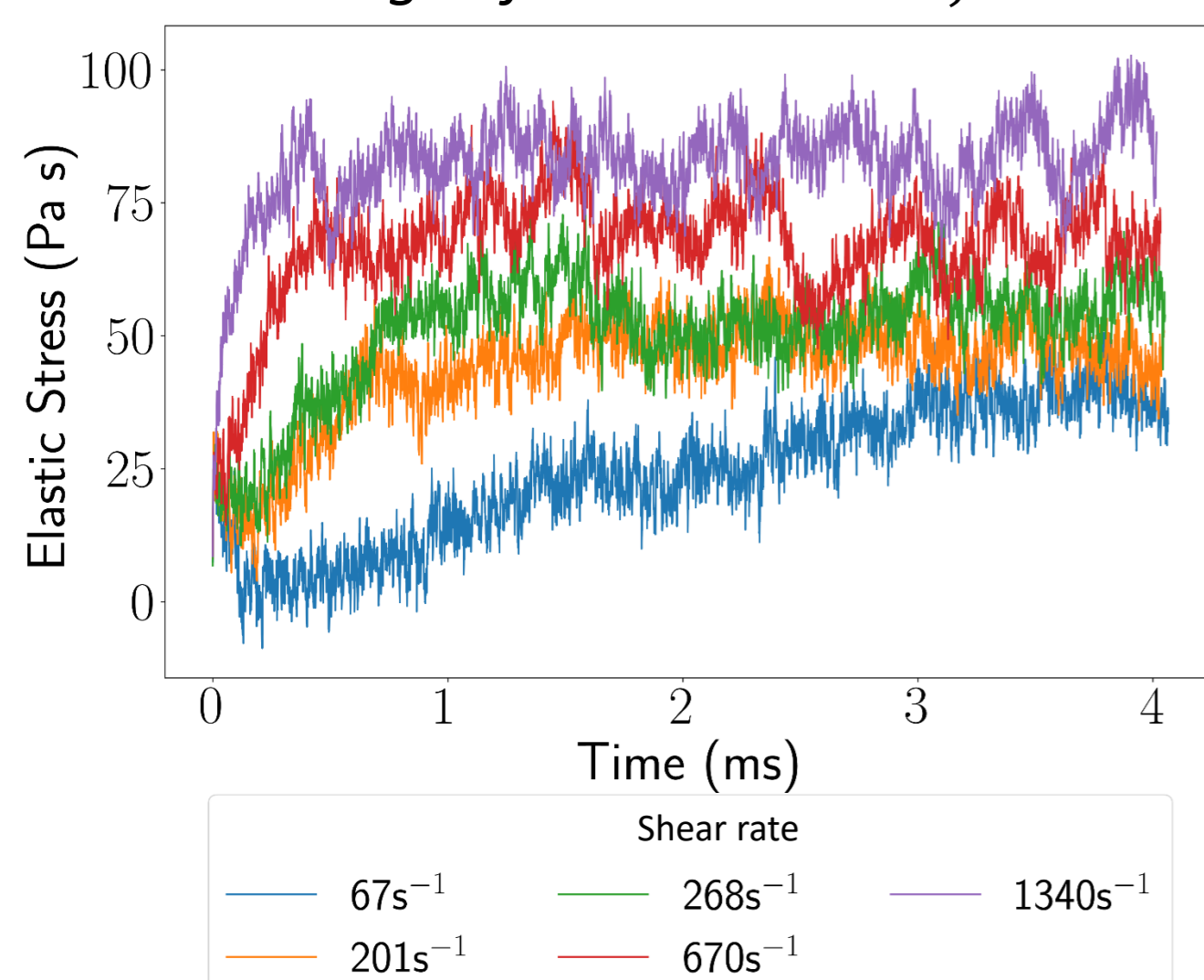
- Linear shear applied through sheared solvent and Lees-Edward's boundary conditions.
- Passes transient behaviour quickly, but soft systems can have lengthy and complicated transient behaviour.
- Indications of intermittent behaviour for higher shear rates.

Average post-transient elastic response to range of shear rates at $\zeta = 0.8$