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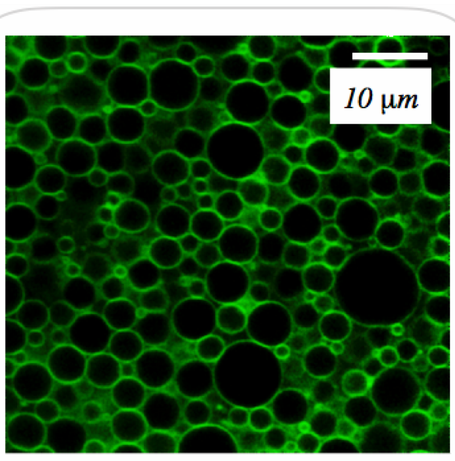
State following of amorphous soft condensed matters : developments of high-performance computational schemes

Research purpose



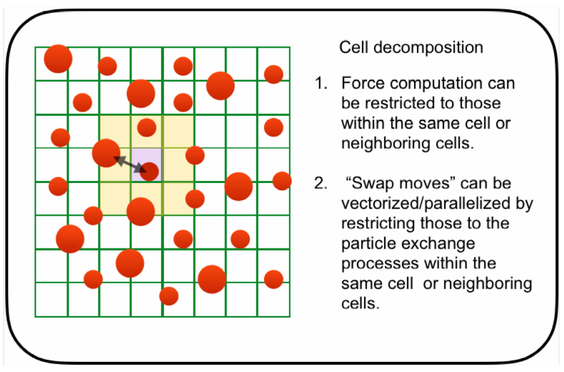
Dense assembly of emusion(cococane droplets Immerdesd in water+glycerol, confocal microscopic Image taken by ER Weels and C Hollonger)
(E. Weeks "Soft jammed materials" (2014))

The purpose of this project is to develop a set of high-performance computational schemes to study rheological properties of amorphous solid states of soft-matter such as dense assemblies of colloids and emulsions (see the figure). Our project is motivated by the recent developments of the mean-field theory for amorphous, glassy soft-matters in recent years [2] which produced interesting predictions on the rheological properties [3, 4, 6, 8]. However the mean-field theory is exact only in the large dimensional limit and its validity in the real three dimensional systems is a totally open question.
In the present project we will develop parallelized simulation schemes which enable

1. **Preparation of ultra-stable glassy states** at low temperatures/high densities
2. **Glass state following under quasi-static perturbations**

The core part of our project is **parallelization of the swap Monte Carlo (MC) method** [1] which enables preparation of "ultra-stable glasses", i.e. unprecedentedly stable glasses against decompression and shear deformations, by computer simulations. We then apply the scheme to elucidate rheological properties of dense assembly of emulsions.

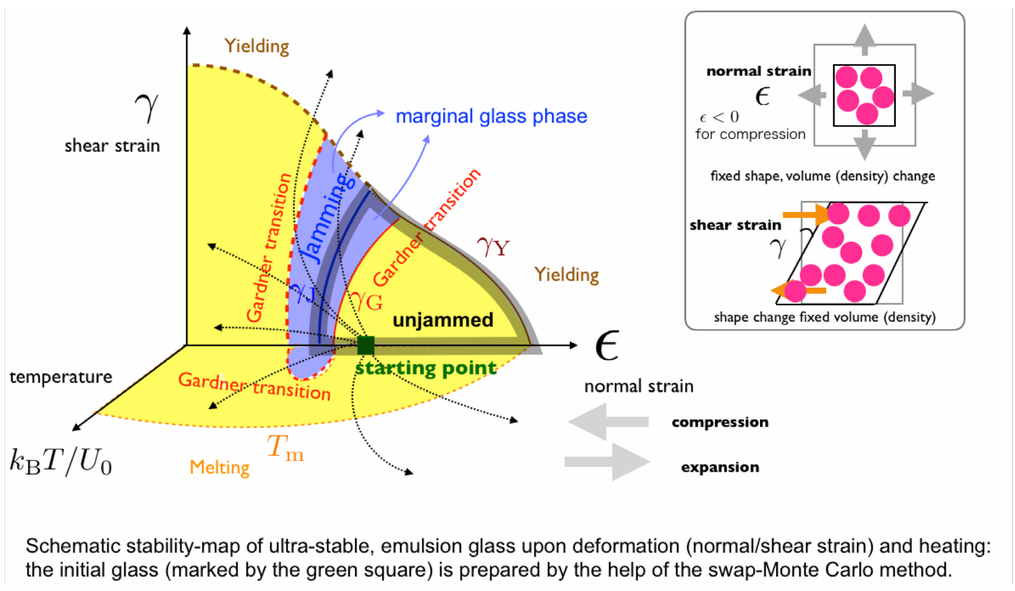
Methods



Glasses are born out of liquids. Unlike crystals, glasses emerge continuously in the liquid state as it becomes super-viscous by cooling or compression. To make clear-cut observations of salient features of rheological properties of glasse[5, 7, 9] , it is essential to prepare at first a high density, well equilibrated liquid. The swap Monte Calro metho [1] enables this task. However the swap Monte Carlo method has not been vectorized nor parallelized. In the present project, we will develop a parallelized version of the swap Monte Carlo method.

Research Plan

We consider dense assembly of poly-disperse emulsions as our physical target in the present project. Particles (i=1,2,...,N) are assumed to be spherical and characterized by diameters D_i with their centers of mass coordinates $\mathbf{r}_i = (x_i, y_i, z_i)$ and velocities $\mathbf{v}_i = (v_{x,i}, v_{y,i}, v_{z,i})$. We assume the continuous distribution of the diameters of particles used in [1, 7, 9]. (The use of poly-disperse particles also helps to avoid unwanted crystallization.) Particles interact with each other through a pair potential U(r)where r is the distance between the center of mass of the pair of the particles involved, normalized by the sum of their radii. In order to model emulsions we use the standard soft repulsive contact potential $U(r) = U_0(r-1)^2\theta(r-1)$ where $\theta(r)$is the Heaviside step function. (The hard-spheres used in [1, 7, 9] corresponds to $U_0 = \infty$.) Basically the particles move following the Newton's equation of motion which can be solved using standard molecular dynamics simulation schemes, which we fully parallelize in the present work. Note that particles move freely until they become in touch with each other. We chose the unit time of the MD simulation which is of the order of 1 collision.



Schematic stability-map of ultra-stable, emulsion glass upon deformation (normal/shear strain) and heating: the initial glass (marked by the green square) is prepared by the help of the swap-Monte Carlo method.

In the figure above we display an anticipated, schematic diagram of the emlusion glass. The initial glass state (marked by the green-square in the figure) is prepared by combining A) swap Monte Carlo and B) molecular dynamics. Having prepared a dense equilibrium liquid, we switch-off A) the swap moves being left with a piece of very stable, initial glass. Then we start to follow the evolution of the glass under mechanical perturbations: shear strain γ, normal strain ϵ and heating by increasing the normalized temperature k_BT/U_0 (here k_B is the Boltzmann's constant) by various trajectories as indicated by the dotted arrows in the figure. Various regimes of the system are investigated through physical quantities such as shear-stress and pressure.

Perspective

Our project on the simplest glass will be useful as a reference to explore rheological properties of a broader range of glass formers: repulsive soft spheres, sticky spheres, ellipsoids e. t. c.

References

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