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

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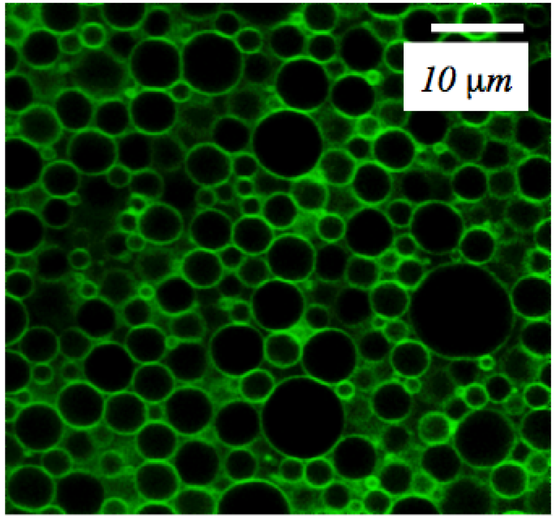
Purpose of the project



Dense assembly of emusion(cocecane 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 right figure). Our project is motivated by the recent developments of the mean-field theory for amorphous, glassy soft- matters in recent years [1] which produced interesting predictions on the rheological properties [2, 3, 4]. 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

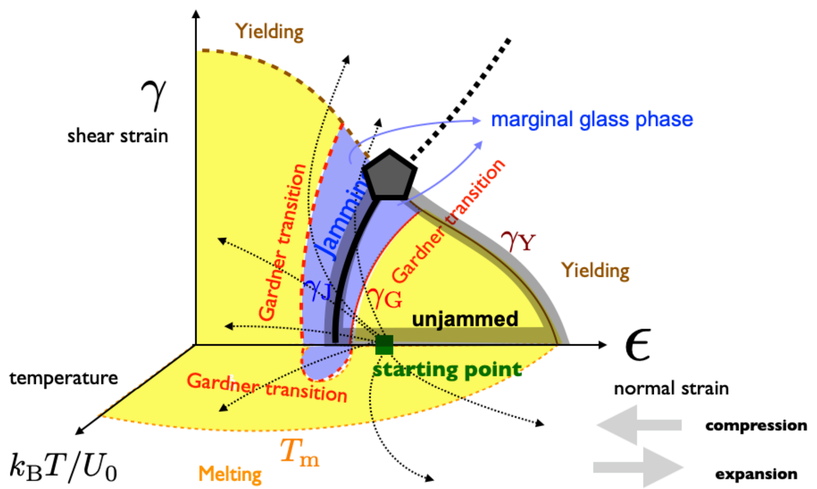
[1] Patrick Charbonneau, Jorge Kurchan, Giorgio Parisi, Pierfrancesco Urbani, and Francesco Zamponi. Nature communications, 5:3725, 2014.

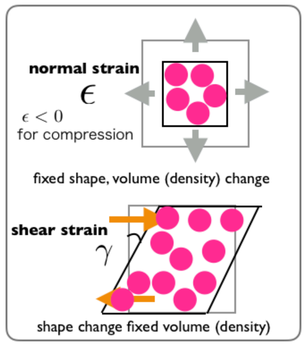
[2] Hajime Yoshino and Francesco Zamponi. Physical Review E, 90(2):022302, 2014.

[3] Corrado Rainone, Pierfrancesco Urbani, Hajime Yoshino and Francesco Zamponi, Phys. Rev. Lett. 114(1), 015701, 2015

[4] Pierfrancesco Urbani and Francesco Zamponi. Phys. Rev. Lett. , 118(3), 038001, 2017.

Development of parallelized rheology simulation schemes





Schematic stability-map of ultra-stable, emulsion glass upon deformations (normal/shear strain) and heating: the initial glass (marked by the green square) is prepared with the help of the swap-Monte Carlo method.
The region enclosed by the thick-gray line corresponds to the hard-sphere regime.

1. Preparation of ultra-stable glassy states at low temperatures/high densities. Such a state is represented as the 'starting point' - the green-square point - in the figure. This is a hard-sphere configuration in a glassy state.

2. Glass state following under quasi- static perturbations As shown in the figure, we explore the system under perturbations by applying the volume strain ε, shear-strain γ and temperature T . (k_B is the Boltzmann's constant.) Here U_0 is the energy scale for the deformation of spheres so that $U_0 \to \infty$ in the hard-spheres. With the hard-spheres, we are confined in the $k_B T/U_0 = 0$ plane. Starting from the initial configuration (green-square), we can bring the assembly of hard-spheres to each point in the region bounded by the thick-gray line. The hard-sphere glass state yields beyond the yielding line γ_Y and jamms approaching shear-jamming line γ_J.

Models and Methods

Assembly of N hard/soft spheres in a box with volume V

Polydisperse spheres with pdf of diameter D $P(D) \sim D^{-3}$

Event driven molecular dynamics

To simulate hard-spheres, even-driven MD code is developed

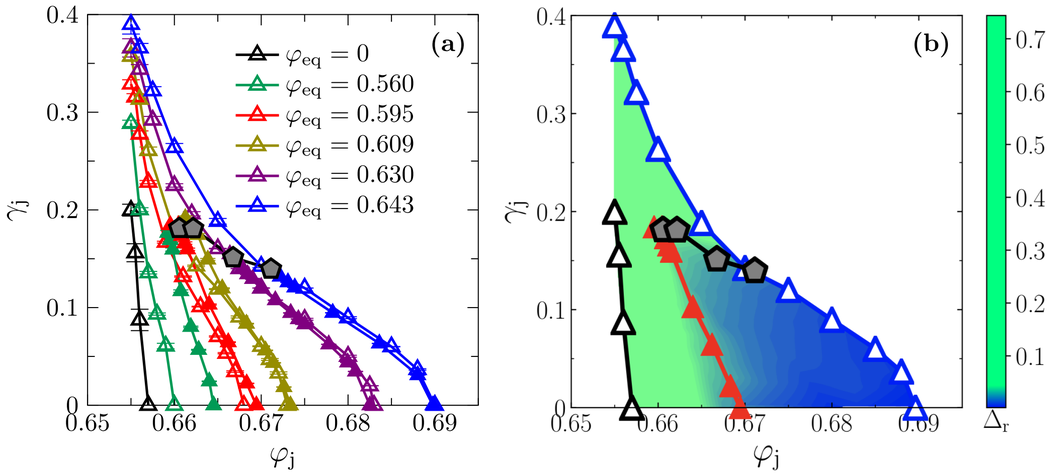
SWAP algorithm

To enhance equilibration of the initial hard-sphere configurations, the position of spheres with different radii are exchanged (GPU parallelization in progress)

FIRE algorithm

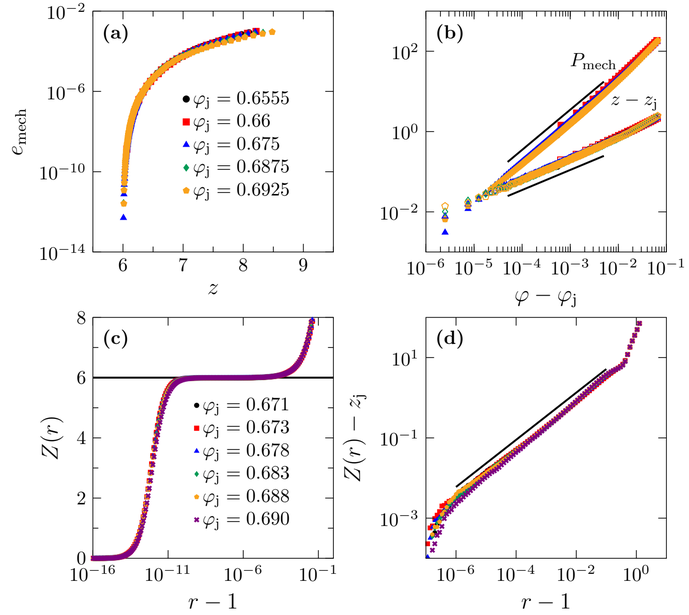
Energy minimization scheme used to remove overlaps between soft-spheres (GPU parallelization, done)

Analysis of jamming via compression/shear



(a) shear-jamming (SJ) line starting from different initial density with hard-spheres (filled symbol) and soft-spheres (empty symbols) . (b) the region explored by the hard-spheres is “reversible” characterized by very small mean-squared displacement before/after cycling up to jamming from the initial states.

Yuliang Jin, Hajime Yoshino, ‘A Jamming Plane of sphere packings’, submitted (preprint: arXiv:2003.10814)

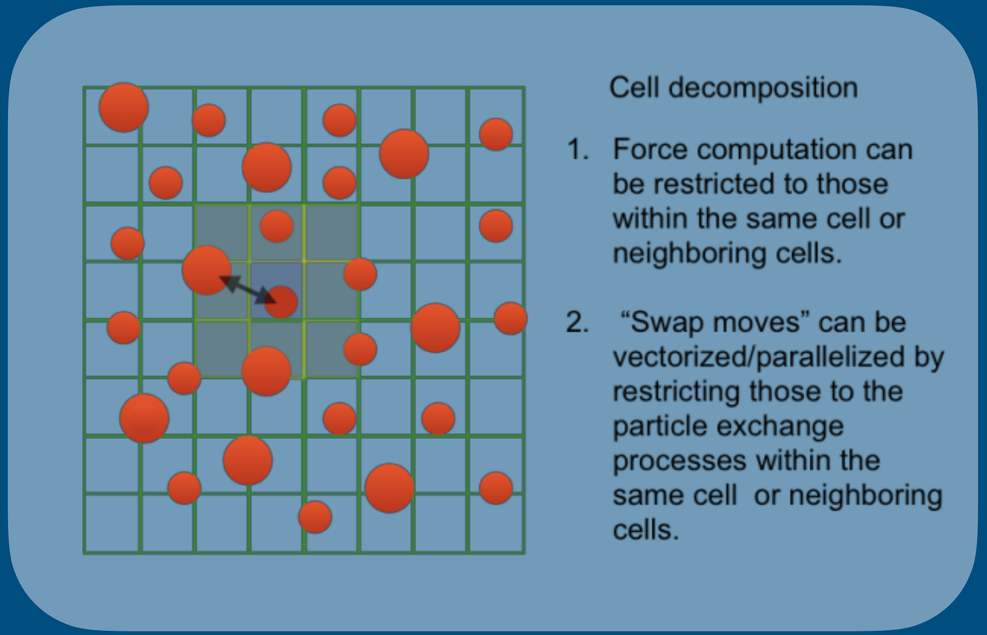


3 Isostaticity and universality of jamming. We show scalings (a-b) above jamming $\varphi > \varphi_j$ in athermal SSs, and (c-d) below jamming $\varphi < \varphi_j$ in thermal HSs, for $\varphi_{eq} = 0.643$ and $N = 8000$. Data in (a-b) are obtained from athermal compressions of SS packings from φ_j to φ, for a few different φ_j along the SJ-line. (a) Energy density e_{mech} versus coordination number z. (b) Mechanical pressure P_{mech} and the excess coordination number $z - z_j$ as functions of $\varphi - \varphi_j$.

Perspective

GPU parallelization of the SWAP algorithm

(in progress)



Further exploration of the non-linear rheology beyond jamming via soft-core potential model