Exploring the glassy behaviour of the Gaussian Core Model by random pinning

Vittoria Sposini
Faculty of Physics, University of Vienna, Austria
vittoria.sposini@univie.ac.at

Joint work with Manuel Camargo & Christos Likos

REWIRE
Reinforcing Women in Research

This project has received funding from the European Union's Horizon 2020 research and innovation programme under the Marie Skłodowska-Curie grant agreement No 847693

The Gaussian Core Model (GCM)

The GCM is a many-body system of point particles interacting via a Gaussian potential

$$V(r) = \epsilon \exp[-(r/\sigma)^2]$$

that was introduced by Frank Stillinger in the 1970's [1].

- MD simulations have shown that 1-component GCM vitrifies at high densities, $\rho \geq 1$ [2].
- A recent theoretical study based on the replica method has shown the emergence of a quantised glass at intermediate densities [3].

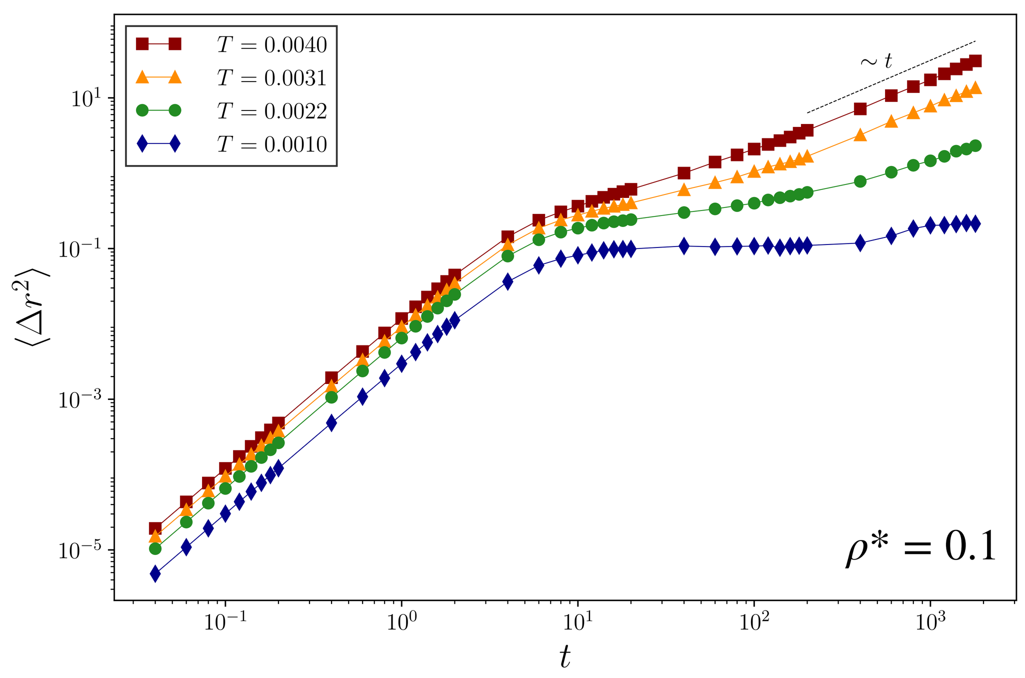
MD simulations with random pinning

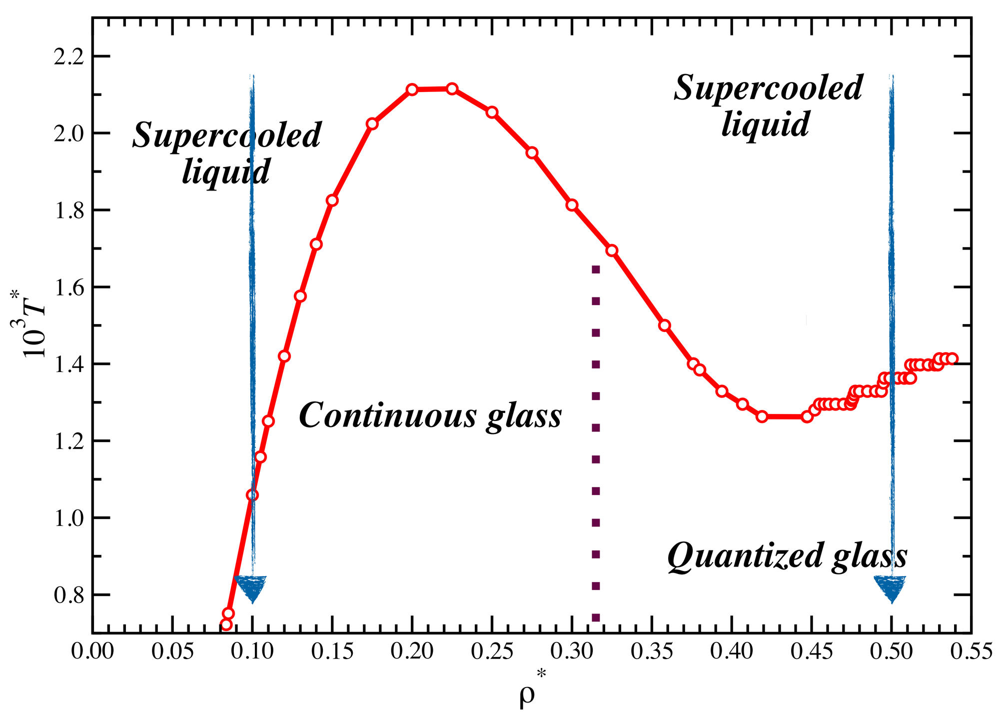
We perform MD simulations in LAMMPS to study a 1-component GCM system made of $N = 5000$ particles with periodic boundary conditions. We set $T^* = k_B T/\epsilon$ and $\rho^* = \rho\sigma^3$, such that $L = (N/\rho^*)^{1/3}$.

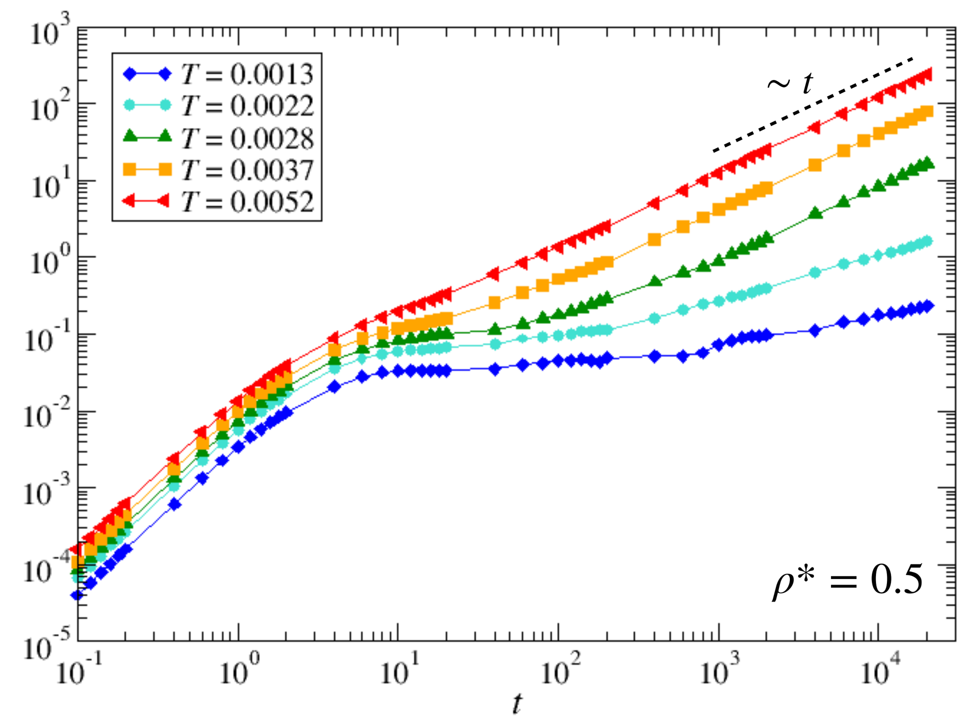
To avoid crystallisation we introduce random (bulk) pinning. In particular, for our study, we set a fraction of pinned particles $f_{\text{PIN}} = 10\,\%$.

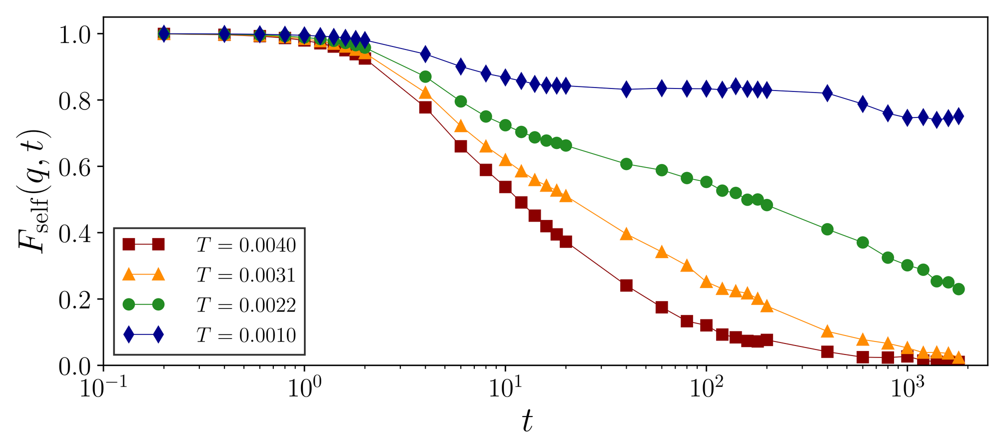
To prepare the system: We initialise it at a higher temperature, cool it down quickly to the desired temperature, pin a fraction f_{PIN} of particles and finally we let it equilibrate.

Exploring the glassy dynamics

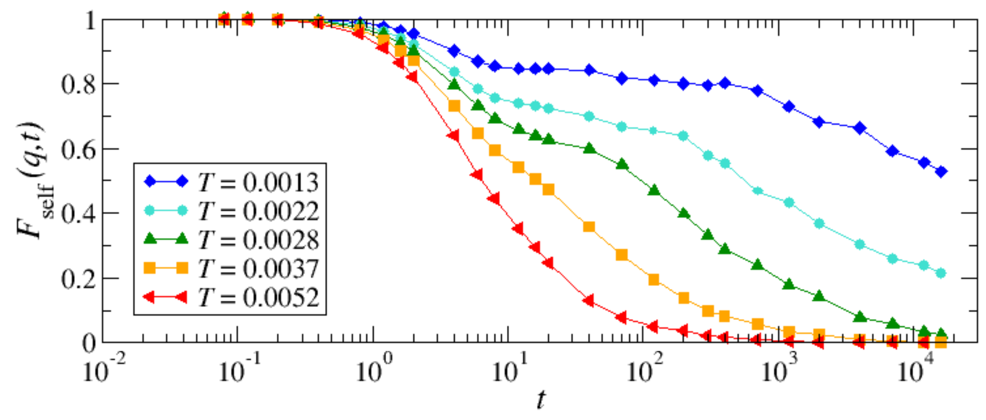




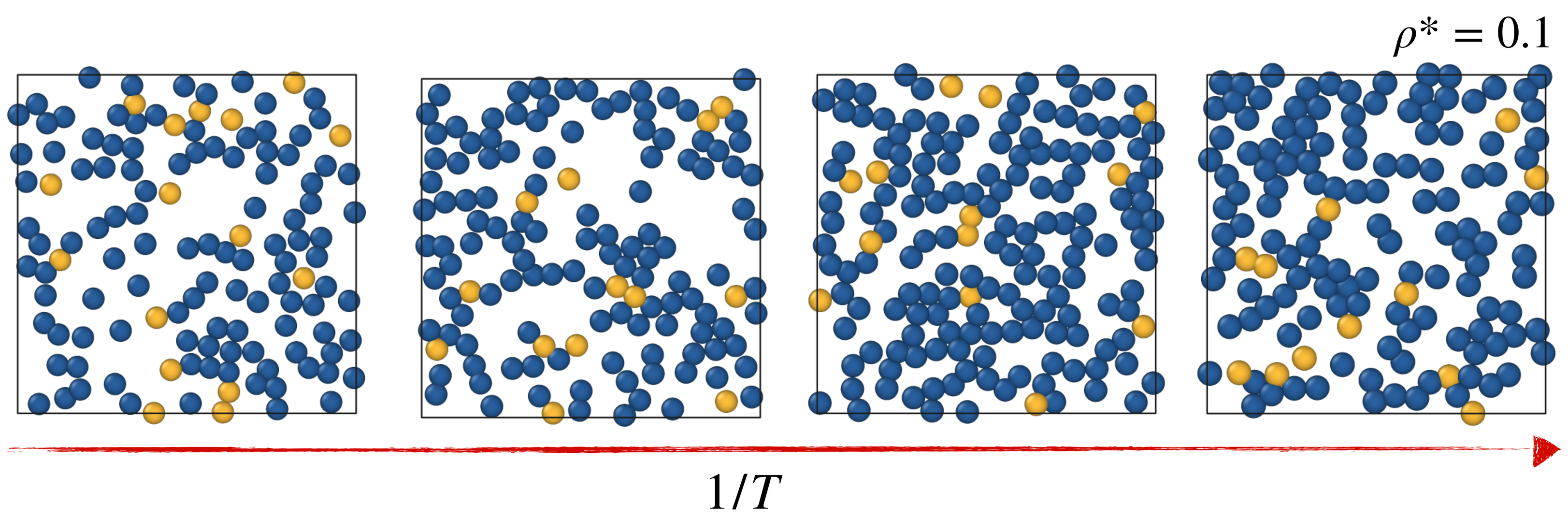


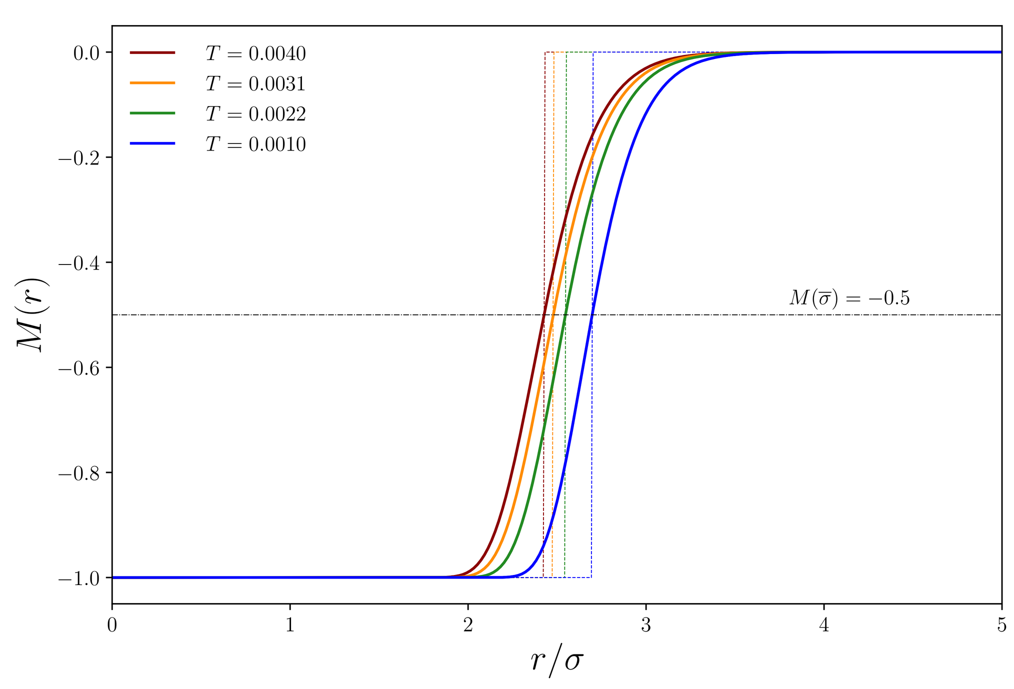


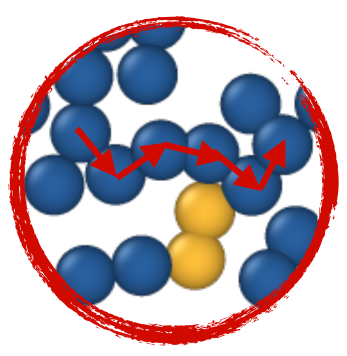
- Upon quenching, the mean square displacement $\langle \Delta r^2 \rangle$ shows a weak localisation followed by a subdiffusive regime (SD);
- The intermediate scattering function $F_{\text{self}}(q,t)$ shows an intermediate logarithmic decay before the development of a plateau, characteristic of a 2-step relaxation (B-type glass).



Cluster formation

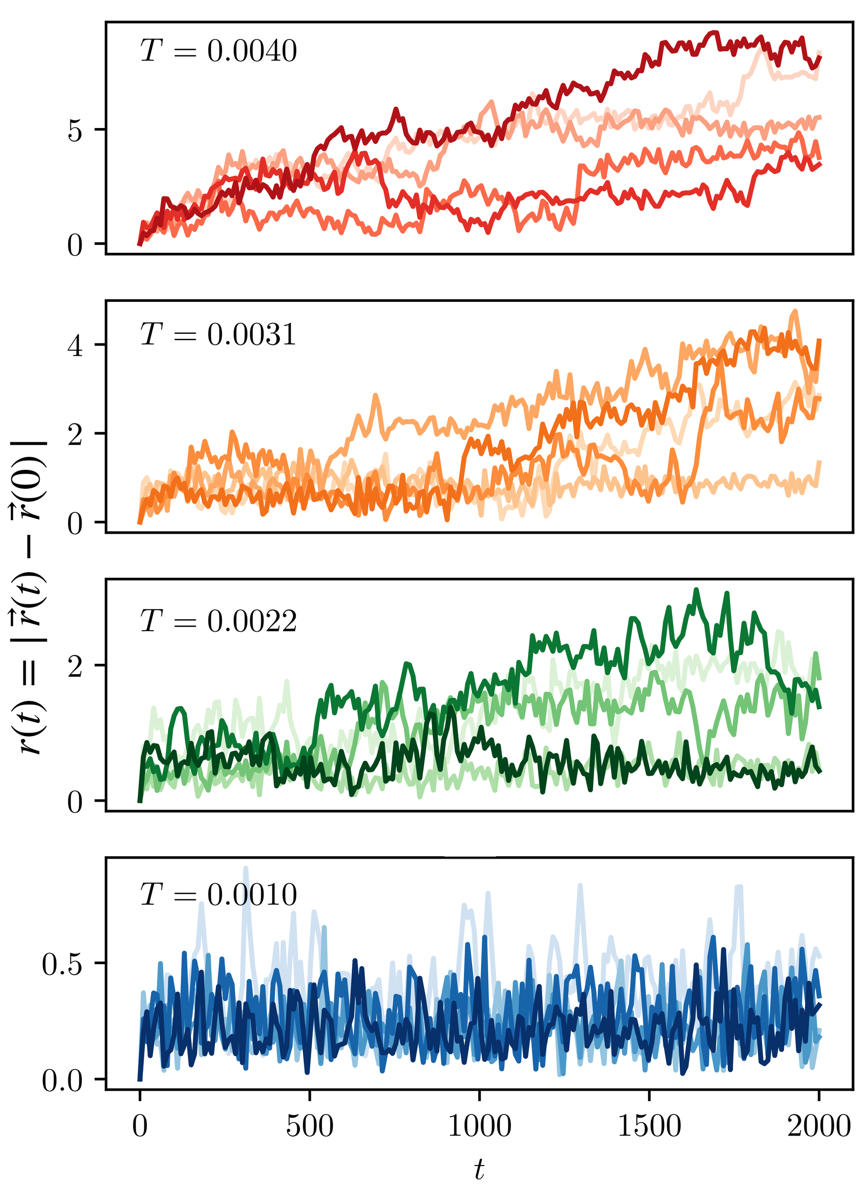


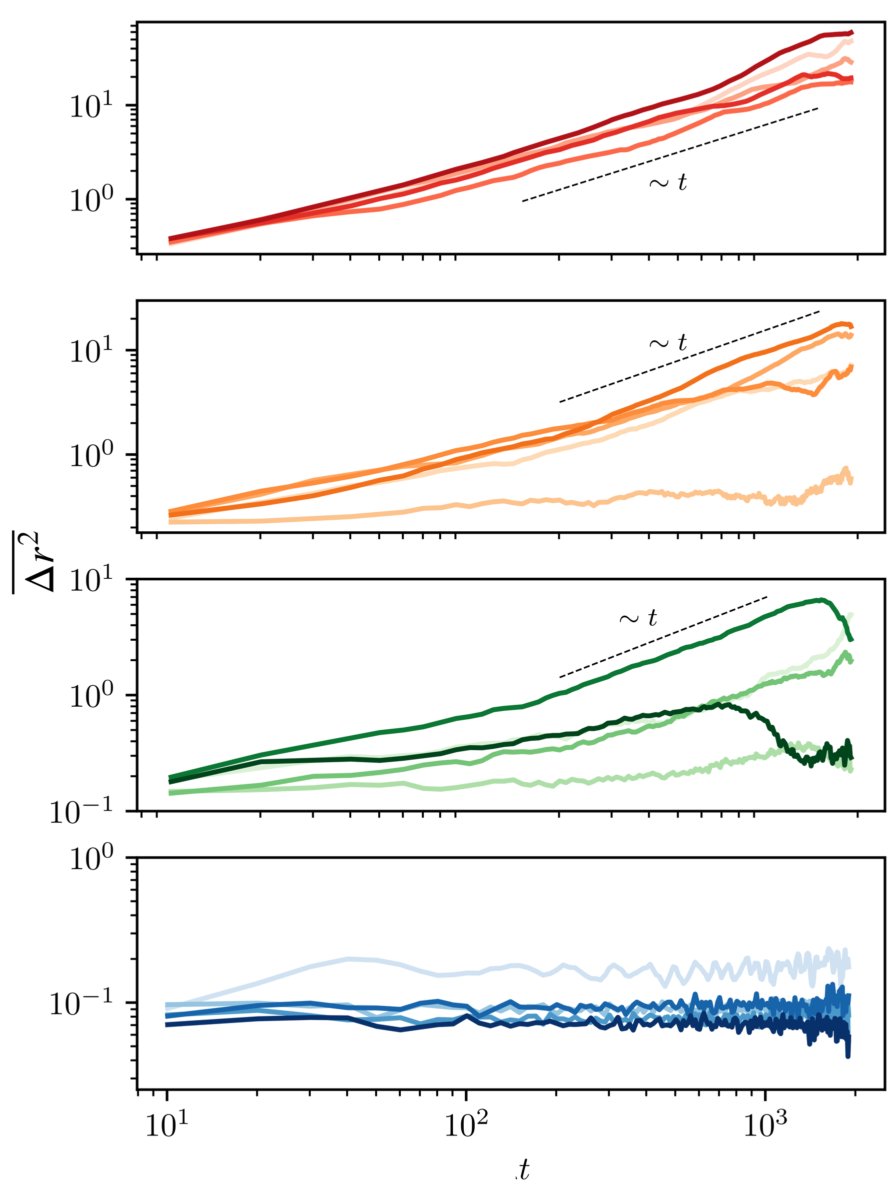




Working hypothesis: particle hopping within clusters

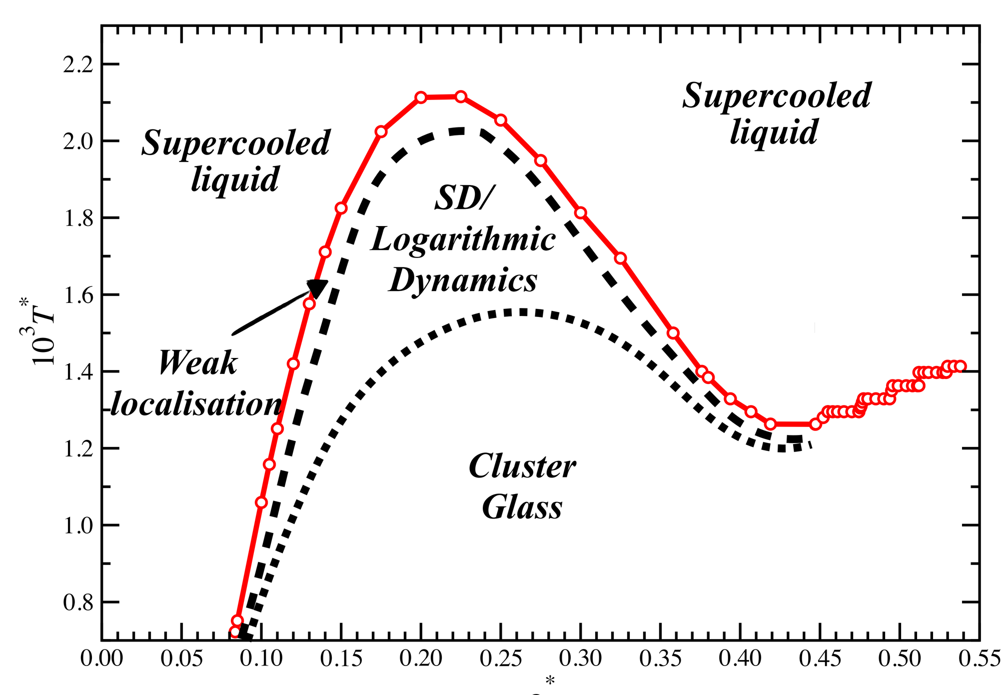
Single-particle dynamics





Conclusions and Outlook

- The random pinning procedure helps in exploring the glassy behaviour of the GCM at low and intermediate densities. The results are reliable at length scales that are larger than the average distance between the pinned particles.
- The logarithmic decay of the intermediate scattering function indicates a competition between different arrest mechanisms: (i) single-particle localisation, (ii) cluster glass.
- The subdiffusive trend of the mean square displacement suggests the presence of fractal patterns (created by the clusters) along which the particle can move.
- The glassy behaviour of the GCM is dominated by cluster formation, which in this system represents a non-equilibrium phenomenon.



References:

[1] F. H. Stillinger, *J. Chem. Phys.* **65**, 3968 (1976). [2] A. Ikeda & K. Miyazaki, *Phys. Rev. Lett.* **106**, 015701 (2011). [3] J-M. Bomont, C. Likos, & J-P. Hansen, *Phys. Rev. E* **105**, 024607 (2022).