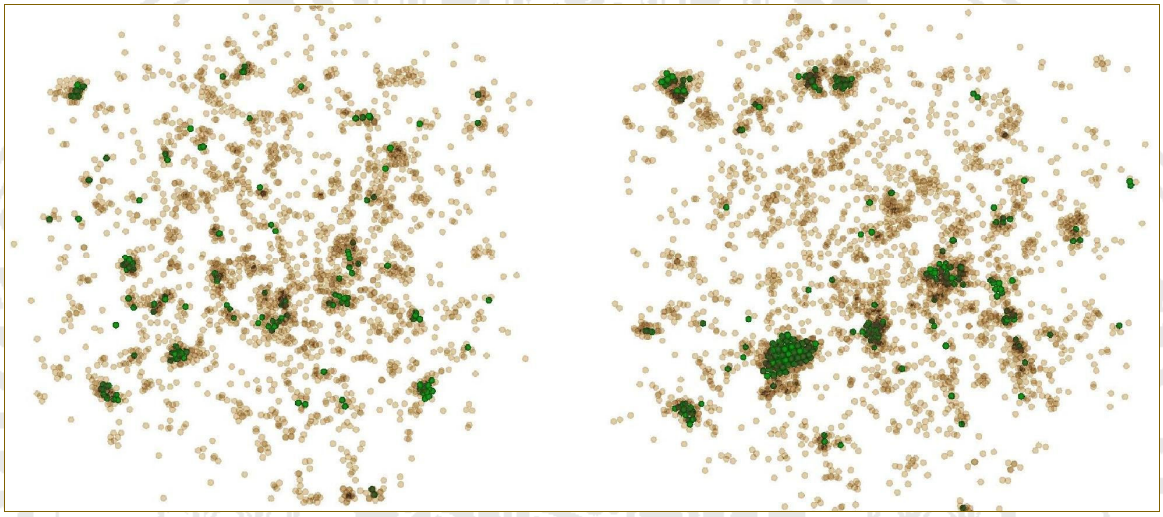
UNI FREIBURG
Fakultät für Mathematik und Physik
Albert-Ludwigs-Universität Freiburg
Physikalisches Institut

SONDERKOLLOQUIUM

AM 17. SEPTEMBER UM 13 UHR S.T.

IM HÖRSAAL II IM PHYSIKHOCHHAUS



Crystallization Revisited

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UNIVERSITE DU LUXEMBOURG

THEORY OF SOFT CONDENSED MATTER

Crystallization from the metastable fluid is a non-equilibrium process. Yet, it is usually discussed in terms of quasi-equilibrium concepts such as nucleation theory. Those approaches do not account for the fact that any irreversible process of finite duration is inevitably subject to dissipation, i.e. entropy production. In this talk we present a numerical approach to quantify dissipation for a system that crystallizes.

As a model, we have simulated hard spheres under compression at a constant rate. We interpret the dissipation as arising from the resistance of the system against phase transformation. An intrinsic compression rate is identified that separates a quasi-static regime from one of rapid crystallization. In the former, the dissipated heat grows linearly in the compression rate. In the latter regime the system crystallizes more easily, because new relaxation channels are opened, at the cost of forming a higher fraction of non-equilibrium crystal structures. We rationalize the change in crystallization mechanism by analogy with shear thinning, in terms of a kinetic competition rather than thermodynamic arguments.

We will use the talk also to introduce and discuss methods to determine equilibrium free energies of disordered systems and to simulate processes that occur with a small rate.