

Internships in GPU-based molecular dynamics simulations

August 2024

The *Glass and Time* center at Roskilde University invites students at the graduate or undergraduate levels to apply for summer internships. The internships begin Monday August 5 and end Friday August 30.

After an introduction to GPU-based molecular dynamics, you will perform a molecular-dynamics study of a well-defined, fundamental scientific question in liquid-state theory or beyond. *Glass and Time* has exclusive access to a GPU-cluster with more than 1,000 TFLOP peak performance. Each student helps formulate a scientific problem to be simulated and is assigned a supervisor.

Shared-room accommodation is provided free of charge in central Roskilde. Moreover, travel costs are supported by up to 2,000 DKK for European participants and up to 5,000 DKK for flights from outside Europe.

After the internship you will have gained skills in

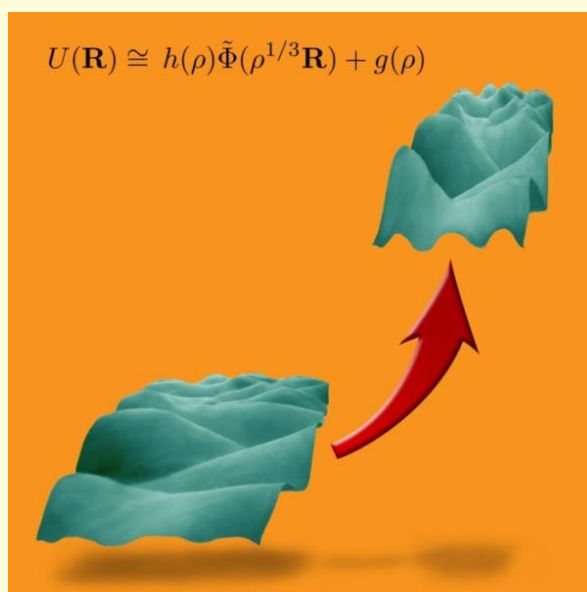
1. Setting up a molecular-dynamics simulation
2. Analyzing simulation data
3. Performing simulations on high-performance GPU-based supercomputers

Interested applicants are invited to submit an application before May 31, consisting of:

1. A single page explaining your background and scholarly interests
2. A brief CV
3. Exam documentation of your highest academic degree

Applications are sent to Prof. Jesper Schmidt Hansen, jschmidt@ruc.dk, who can also be contacted for more information.

The internships are financed by the VILLUM-funded *Matter* project directed by Prof. Jeppe Dyre.



Many liquids' and solids' potential-energy hypersurfaces undergo a simple affine deformation when density is changed. *Matter* explores this fact's consequences for material properties via the isomorph theory.