Internships in GPU-based molecular dynamics simulations

August 2025

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 4 and end Friday August 29.

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.

After the internship you will have gained skills in

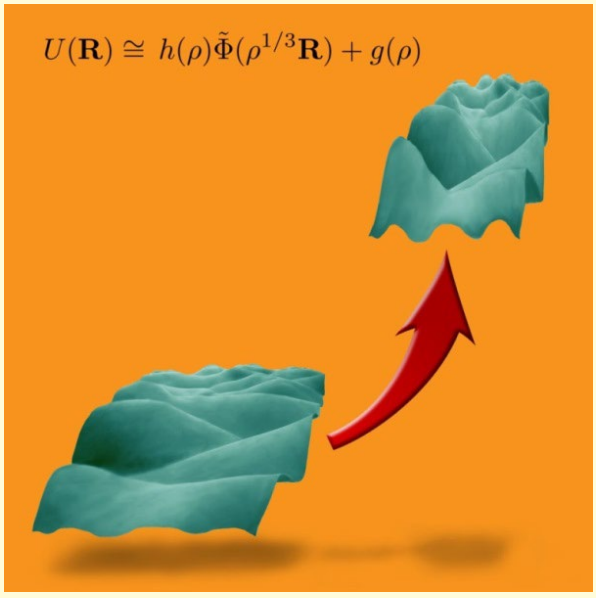
1. Setting up a molecular-dynamics simulation
2. Analyzing simulation data
3. Performing simulations on high-performance GPU-based supercomputers

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

- A single page explaining your background and scholarly interests
- A brief CV (including information on your gender and nationality)
- Exam documentation of your highest academic degree

Applications are sent as a single pdf file 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.