Internships in GPU-based molecular dynamics simulations

August 2026

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 3 and end Friday August 28.

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. Simulations are performed using our package 'gamdpy' (GPU accelerated MD in Python, GitHub - ThomasBechSchroeder/gamdpy). 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.

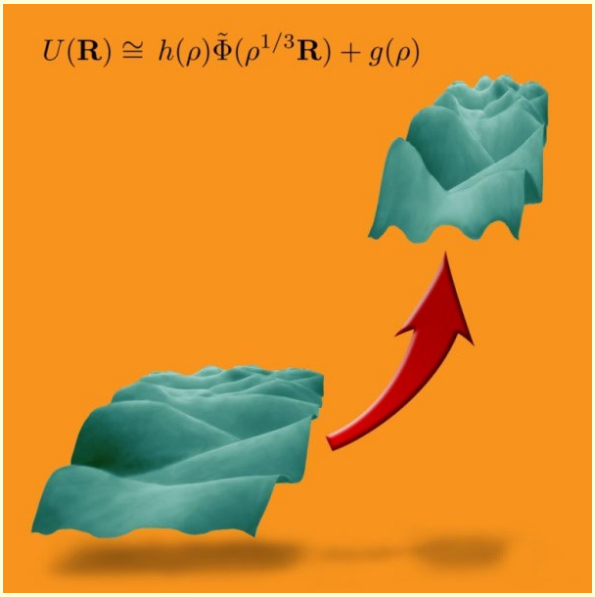
After the internship you will have gained skills in

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 April 1, consisting of:

1. A single page explaining your background and scholarly interests
2. A brief CV (including information on your gender and nationality)
3. 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.



Many liquids' and solids' potential-energy hypersurfaces undergo a simple affine deformation when density is changed, which forms the basis for isomorph theory.