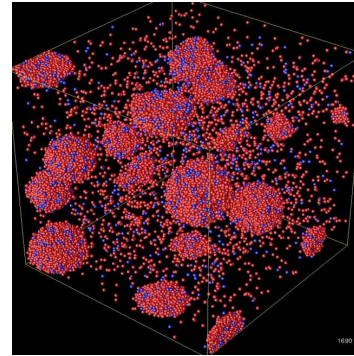
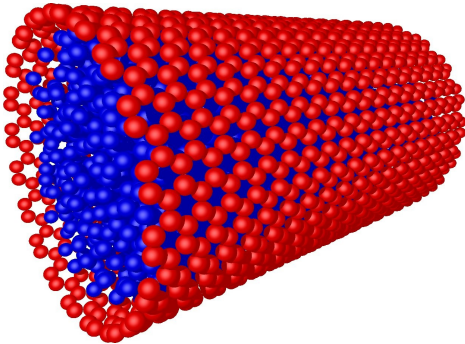


# Bachelor Thesis / Job Offer: Design and Implementation of a Scenario Generator

Ausschreibung: Stelle als Wissenschaftliche Hilfskraft / Bachelor Arbeit

In order to predict or analyse thermodynamic material properties like pressure or potential energy of a material, molecular dynamic simulations are getting more and more important. A typical example is the simulation of a mixture of two different gases with millions of molecules by studying the interaction of the single particles.



At the beginning of a timestep the positions and velocities of the molecules are given. From the positions, forces between the molecules can be determined, and the molecules are moved according to those forces.

Such a simulation programme called Is1/Mardyn has been realized over the last few years in a cooperation of the HLRS (Hochleistungsrechenzentrum Stuttgart), TU Kaiserslautern and our chair, facing the challenges of large amounts of data and high computational intensity necessitating the efficient use of supercomputers and clusters.

The software now supports a number of scenarios, and for every scenario there exists a separate commandline tool. As the usage of those tools is rather cumbersome, a flexible and extensible, unified scenario generator should be developed.

Basic requirements for the tool are

- easy-to-use graphical user interface, with preview functionality, making use of the Visualization ToolKit VTK ([www.vtk.org](http://www.vtk.org))
- flexible design of the generator core as a library, allowing new generators being implemented as plugins
- support of distributed generation of particle data, so that the core library can optionally be integrated with Is1/Mardyn (which is parallelized with MPI).

## Requirements for the candidate:

- knowledge in software engineering
- good programming skills, experience in c++-development in linux of advantage
- interest or knowledge distributed-memory programming in MPI of advantage
- interest in a challenging topic

## Contact:

Please send an informal application stating your previous experiences as well as your knowledge or skills to Wolfgang Eckhardt ([eckhardw@in.tum.de](mailto:eckhardw@in.tum.de)).