

Computational Physics II

WiSe 2014/15

Problem 2: Molecular dynamics with a Lennard-Jones potential

Date: November 20, 2014

Deadline: December 11, 2014

Write a molecular dynamics program for argon atoms in a cube and make animations illustrating the atom motion in

1. a gas phase,
2. a liquid phase, and
3. a “solid” phase.

The atoms interact with a Lennard-Jones potential. You can find parameters for the potential and phases in my lecture notes. Use either hard walls, elastic walls, or periodic boundaries for the cube. You may need to add an external potential to stabilize the “solid” phase.