Optical trapping is an experimental method, in which objects with a size ranging from a subatomic to nanometer scale are localised with a laser due to a gradient force. In this thesis, we use methods from the field of computational physics to simulate the behaviour of a nano particle in a laser trap and its interactions with the laser and the surrounding gas.
Gieseler et al. performed such an Optical Tweezer experiment to investigate the fluctiation theorem. In their experiment they use a Langevin equation to model the dynamics of a silica nanosphere in a laser trap, where the temperature of the heat bath is used to describe the stochastic force acting on the nano particle. Millen et al. conducted a similar experiment and raised the point, that there are four different temperatures present during this experiment: the temperature of the impinging gas particles, the emerging gas particles, the center of mass and the surface of the nano particle. With these temperature regimes in mind, the experiment is simulated using molecular dynamics in order to determine the influence of the laser power and the temperature of the surrounding gas on the center of mass temperature.
To simulate the experiment, each part needs to be modeled appropriately. The nano sphere is represented by a set of atoms that interact with each other via a Lennard-Jones potential. The gradient force of the laser, which localizes the nano particle, is approximated by a harmonic potential. Since the laser energy is absorbed by the nano particle, the internal temperature of the nano particle increses, which is achieved by applying the eHEX algorithm to the nano particle. The surrounding gas acts as a barostat and a thermostat and will be represented by an algorithm that uses an ideal gas as pressure medium.