Problem set 9: Computational Molecular Physics and Methods of Molecular Simulations

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1. Metropolis Monte-Carlo (Thursday lectures)

(10 points)

With the Metropolis-Hastings Monte Carlo (MC) algorithm the configuration space of high-dimensional systems can be sampled. In contrast to molecular dynamics steps the MC moves do not need to follow a physically meaningful trajectory of a particle but can be arbitrary. However, there are a number of limitations for the choice of MC moves. For a simple double-well potential different possible moves are shown in Figure 1.

1. What is the acceptance criterion for MC moves in the Metropolis-Hastings algorithm?
2. Is the large MC move in Figure 1 (green) likely to be accepted?
3. For sampling an arbitrary system with an initially unknown potential energy landscape, is it better to choose large MC moves or smaller ones?

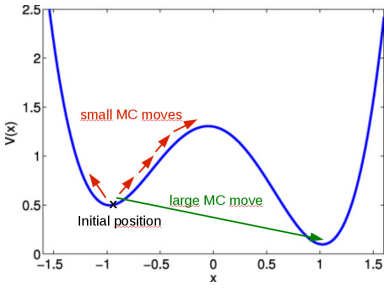

Figure 1: Different Monte Carlo moves for double-well potential

2. Metropolis versus Hybrid Monte-Carlo

(40 points)

1. Consider the asymmetic double well potential (in units of nm, kJ/mol)

$$V(x) = 100x^4 - 100x^2 - 10x \tag{1}$$

and plot Boltzmann distributions for three different temperatures where (1) the density is mainly confined to the lower well, (2) an intermediate case, and (3) where the density is essentially delocalized.

2. Set up a computer code for the standard (Metropolis) Monte-Carlo scheme. Try to sample the Boltzmann distributions for the three temperatures as efficiently as possible by varying the proposal step (see also task 1).

3. Set up a computer code for the hybrid Monte-Carlo scheme. Try to sample the Boltzmann distributions for the three temperatures as efficiently as possible by varying the proposal step, i. e., the lengths of the MD trajectories involved.

4. Are there any characteristic differences in the performance of the sampling by the two methods? And what do you expect in higher dimensions?

3. Langevin dynamics (Thursday lectures)

(10 points)

The temperature of molecular dynamics (MD) simulations can be controlled using different methods. One of these methods is Langevin dynamics.

1. Describe the basic concept of Langevin dynamics.

2. What are the main differences between Langevin dynamics and MD simulations in the NVE ensemble?

3. In Figure 2 schematic trajectories are shown for a system of two particles with an attractive potential between them. Describe qualitatively how the trajectories of these particles change when the simulation method is changed from MD simulations in the NVE ensemble to Langevin dynamics with high friction coefficients.

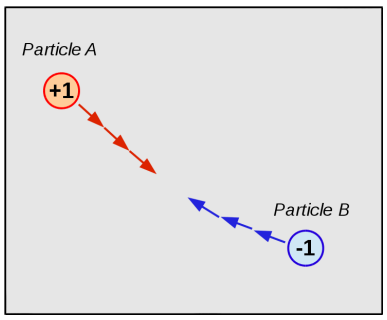

Figure 2: Schematic representation of the trajectories of two particles with opposite charges during a molecular dynamics simulation.