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Problem set 8: Computational Molecular Physics

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1. Free energies and Ramachandran plot (15 points)

The txt files provided for problem set 4 psiA dihedrals and phiL dihedrals contain trajectories (time series) of dihedral angle coordinates from a simulation of Alanine-Leucine. The first column is the time step, the second is the dihedral angle.

Plot a Ramachandran plot (phiL vs psiA) in terms of free energy. First builds a 2D-histogram of psiA and phiL and then compute the relative free energy of each bin i using

$$A_i = -k_B T ln \frac{z_i}{z_0} \tag{1}$$

where z_i is the number of counts in bin i and z_0, the maximal number of counts in a bin. Use value of $k_B T = 1.0$

What assumptions are made w.r.t. the trajectory that allow the calculation of relative free energies in this way, i.e. by counting ?

2. Langevin dynamics (20 points)

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

a) Describe the basic concept of Langevin dynamics.

b) What are the main differences between Langevin dynamics and Newtonian ("normal") Molecular Dynamics simulations?

c) Given numerically perfect integrators, would Langevin dynamics be a good approach to simulate Juno's trajectory from Earth to Jupiter? In which aspects are trajectories in molecular simulations a different matter?

d) Where does the temperature enter in the Metropolis Markov Chain Monte-Carlo method and in the Hybrid Monte-Carlo method?

3. (Bonus) Brownian dynamics (25 points)

Brownian dynamics can be considered a limiting (overdamped) case of Langevin dynamics where the viscous force is much larger than the inertia term. The equations of motion than simplify to

$$\dot{q}(t) = \left[-\frac{dW}{dq} + R(t) \right] \cdot \frac{1}{\zeta} \tag{2}$$

where q is the position, $W(q) = V(q) - b \cdot q^2$ is the effective potential with b a scaling parameter due to the heat bath, R is a random force an ζ is the friction term.

A numerical integration scheme with time step Δt than looks like

$$q(t + \Delta t) = q(t) + \left[-\frac{dW}{dq} + R(t) \right] \cdot \frac{1}{\zeta} \cdot \Delta t \tag{3}$$

which can be rewritten as

$$q(t + \Delta t) = q(t) + F_{eff}\left(q(t)\right) \cdot D\Delta t \cdot \beta + R(t) \cdot \Delta t \cdot \beta \tag{4}$$

where β is the inverse temperature and $D = \beta\zeta$. The second, random force term, is normal distributed with zero mean and width $\sigma(t) = \sqrt{Dt}$.

Implement Brownian dynamics (use $\beta = 1.0$, $b = 0.01$, and $D\Delta t = 0.001$) and perform 100 simulations of 100 steps for a particle of unit mass

a) freely moving (no potential ($W = 0$), starting at $q(0) = 0.0$. Plot a histogram of the final positions.

b) moving in a quadratic potential $V(q) = 0.5(q - 3)^2$.

   (a) starting at $q(0) = 0.0$

   (b) starting at $q(0) = q_{min}$

   Plot histograms of the positions and momenta, respectively, as obtained from the trajectories.

You can use your favorite programming language.