

## Jacobson problem set: Molecular dynamics

This problem set supplements the lectures by stepping you through a molecular dynamics simulation for a simple one dimensional potential. This problem set was adapted and simplified from a problem designed by Biophysics student John Chodera for my advanced course, Biophysics 206.

You may use Matlab or any programming language you like to complete the problem set. However, I designed the problem set so that it can be completed in Excel or any other spreadsheet/graphics program. I generated my own results in Excel.

The potential energy function you will use is the following “double well” potential:

$$V(x) = (x-1)^2(x+1)^2 + 0.3x$$

1. Plot this function over the range  $-1.8 < x < 1.8$ .
2. Compute analytically the gradient of the potential. Plot the gradient over the same range.
3. There are many different ways of integrating Newton's equations of motion using finite difference methods. The derivation of these was described briefly in lecture and can also be found in various textbooks such as Leach, “Molecular Modelling: Principles and Applications”. The basic idea is to expand the position, velocity, and acceleration in Taylor series so that the state of the system at time  $t + \Delta t$  can be estimated from the state of the system at time  $t$ . For example, in one dimension, the Taylor series expansion for the position is

$$x(t + \Delta t) = x(t) + \Delta t \cdot v(t) + \frac{1}{2} \Delta t^2 \cdot a(t) + \dots$$

where  $v$  is velocity and  $a$  is acceleration. The particular variant we will use here is the velocity Verlet algorithm (Swope WC, Andersen HC, Berens PH, and Wilson KR. J. Chem. Phys. 76 (1982) 637). The integrator uses the above expression plus the following expression to update the velocities:

$$v(t + \Delta t) = v(t) + \Delta t \cdot \frac{1}{2} [a(t) + a(t + \Delta t)]$$

For this example, use the following initial conditions:  $x(0) = -1.5$ ,  $v(0) = 0$ . The acceleration at time zero (and any other time) can be computed using Newton's second law,  $F=ma$ , where the force is the negative of the gradient. We will arbitrarily choose the mass of the object to be  $m=1$ . Integrate the motion for (at least) 4000 time steps, using  $\Delta t = 0.01$ . Plot the position versus time, and also the total energy (potential plus kinetic energy) versus time.

4. Now switch the time step to  $\Delta t = 0.3$ . What happens? Why?
5. Bonus problem: Sample this potential with a Monte Carlo algorithm, and compare results with molecular dynamics.