# Chemistry 5850 Fall 2005 Assignment 7

Due: Monday, Nov. 7.

Weight of this assignment: 29 marks

1. Hamilton's equations of motion are not symmetric with respect to $x_i$ and $p_i$. Is it possible to use a different Hamiltonian such that the signs are reversed? [2 marks]

2. The ideas used to treat Hamiltonian systems extend very naturally to any system with an appropriate number of first integrals. For instance, the Lotka-Volterra equations are a very simple model of predator-prey dynamics. In dimensionless form, they can be written

$$\begin{aligned} \dot{x} &= x(1-y), \\ \dot{y} &= \mu y(x-1). \end{aligned}$$

   (a) Show that $F = \mu x + y - \mu \ln x - \ln y$ is a constant of the motion. [3 marks]

   (b) Draw the trajectories of the Lotka-Volterra model using an exact technique (i.e. not by numerical integration). [4 marks]

   Bonus: With a suitable change of variables, the Lotka-Volterra system can actually be written in Hamiltonian form. Find this change of variables and the transformed Hamiltonian.

3. The symplectic integrator we studied in class can fairly easily be implemented in Maple for a planar system:

```
symplecticstep := proc(h) global x,p; local xnext, pnext;
assign(fsolve({(xnext-x)/h = (H(x,pnext)-H(x,p))/(pnext-p), (pnext-p)/h
= -(H(xnext,pnext)-H(x,pnext))/(xnext-x)}, {xnext=x,pnext=p}));
x:=xnext; p:=pnext;
<x,p>; end;
```

   The code is mostly straightforward: Given a function $H(x,p)$ and the current values of $x$ and $p$, the relevant equations are solved and the result assigned back to $x$ and $p$. The last statement before the end of the procedure just prints the current state vector $(x,p)$ to the screen. The parameter $h$ is the step size ($\Delta t$).

   Use this integrator to obtain trajectories of the anharmonic oscillator with Hamiltonian

$$H = \frac{p^2}{2m} + \frac{1}{2}kx^2 + \frac{1}{6}\gamma x^3$$

   for $k = 1$, $m = 1$, $\gamma = 0.1$ and initial conditions such that closed trajectories are obtained. Is the value of the Hamiltonian exactly conserved for very long runs (millions of periods of the oscillator)?[1] How sensitive are the results to the value of $h$?

   Obtain Hamilton's equations of motion for this system and use the Runge-Kutta integrator in `xppaut`. Use an auxilliary declaration to keep track of the value of $H$. How does this integrator behave for this problem? [20 marks]

[1] Obviously, I'm assuming that it's reasonable to ask for runs of this length. Start with shorter runs and see how it goes.