

PHYSICS 104B, WINTER 2010
ASSIGNMENT ONE

Due Thursday, January 14.

Your homework solution should include a hardcopy of the code, answers to the questions, and the indicated figures. Commenting your code is strongly encouraged.

[1a.] Write a molecular dynamics (MD) code to solve the simple harmonic oscillator using the Euler algorithm. Run your code for the initial conditions $x_0 = 3.$, $v_0 = 0.$, and for spring constant and mass $k = 2.$, $m = 7.$ Use a range of time steps and time intervals, for example ($N = 1000, dt = 0.05$) and ($N = 5000, dt = 0.01$). Plot $x(t)$ and $E(t)$.

[1b.] Discuss your results. What is the analytic solution? Does the accuracy improve as dt decreases? Do you get the correct period? Is energy conserved?

[2.] Repeat problems [1a] and [1b] using the leapfrog algorithm. How do your results differ from Euler?

[3.] Choose some set of values for $k, x(0), v(0), m$, and γ . Plot your MD $x(t)$ for the damped case along with the analytic solution and show they agree.

[4.] Add a anharmonic term so the spring force is $F = -kx - ax^3$. Run your code for different amplitudes of motion, but all other parameters fixed. Is the guess made in class that the period now depends on the amplitude correct?

[*] Extra credit: Analyze the energy errors in the “leapfrog” version of MD.

[5a.] Write a molecular dynamics program to solve the Kepler problem for one planet orbiting the sun. You may assume the sun is sufficiently massive that it is stationary at the origin. Use the leapfrog algorithm to update positions and velocities.

[5b.] Verify you get circular orbits of the correct period when you start out the planet with $GM_{\text{sun}}/r^2 = v^2/r$. Generate the orbit for a velocity which is twice this value. Generate the orbit for a velocity which is half this value. Make a figure showing all three orbits on the same plot. Are the orbits what you expect?

[5c.] Check angular momentum is conserved. What is the percent variation for various time steps?