Molecular Biophysics
Computational Techniques HW #2
Due April 12th

For the harmonic oscillator approximation of a carbon-hydrogen bond, calculate the position, velocity, and acceleration for the hydrogen atom bonded to a carbon with fixed position from 0 to 10 fs, at 1 fs timesteps.

Start the calculation with $v(0) = 0$, $x(0) = 0.5$ Å

First, calculate the position, velocity, and acceleration analytically.

Next, use the poor equations of motion from lecture on 3/31 to calculate position, velocity, and acceleration:
$x(t+\Delta t) = x(t) + v(t)\times\Delta t + (1/2) \times a(t) \times (\Delta t)^2$
$v(t+\Delta t) = [x(t+\Delta t) - x(t)]/\Delta t$

Finally, calculate position, velocity, and acceleration using the Verlet algorithm:
$x(t+\Delta t) = 2x(t) - x(t-\Delta t) + a(t) \times (\Delta t)^2$
$v(t) = [x(t+\Delta t)-x(t-\Delta t)]/2\Delta t$
Use the analytic solution of $x(-\Delta t)$ to seed the first step.

Note that the Verlet algorithm is a better approximation of the analytic solution (as advertised).