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Problem set 6: Computational Molecular Physics

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Molecular dynamics (50 points)
Newtons equation of motion for a mass m connected to an ideal spring of spring constant k (1-d harmonic oscillator)is given by

$$\frac{d^2x(t)}{dt^2} = -\frac{k}{m}x(t) \tag{1}$$

Solve this linear differential equation numerically using:

a) Euler algorithm

b) Verlet algorithm

Consider time from 0 to 100 seconds , use $k = 0.1 newton/meter$, $m = 1kg$ and time step $\Delta t = 0.5 second$ with the following initial conditions:

$x(t = 0) = 0, v(t = 0) = 2$ meter/second

use $a = -k\frac{x}{m}\ meter/second^2$ to compute the acceleration.

c) Plot solutions as a function of time. Compare the numerical solutions with the analytical solution. Which algorithm produces better results?

d) Compute solutions for different time-steps ($\Delta t = 0.1, 0.2 \ldots 1s$) using both algorithms. Compare them, which time-step do you find satisfactory?

e) Compute and plot solution and energies (kinetic, potential and total energies) of the harmonic oscillator for the satisfactory time step found in part (d) using both Euler and Verlet algorithms. Discuss your results, which algorithm would you use suggest to use in molecular dynamics simulations? and why?

f) For a large molecule e.g. a protein in water a common trick is to fix some degrees of freedom such as the bonds to hydrogen atoms, or use heavier atoms (e.g D2O instead of H2O) . How will this effect the molecular dynamics simulation?

Use any of your favorite programming language to perform computations.