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Problem set 7: Computational Molecular Physics

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by 4 July 2016, 12pm

1. Molecular dynamics (10 points)

Extend your code for verlet algorithm (previous problme set) to two particles connected by a spring $F = k(x_2 - x_1 - x_0)$; where $\Delta x = x_2 - x_1$ is the distance between particles and x_0 is the equilibrium length of the spring.

Using the harmonic oscillator model of the $C - C$ bond whose vibrational wavenumber is $\omega/2\pi c \approx 1000cm^{-1}$. (Wavenumber is the number of waves per length, i.e. the inverse of the wave length. c is the speed of light.)

a) Convert the value of wavenumber into frequencies[Hz] and vibrational periods [s].

b) Calculate the reduced mass $\mu = \frac{m_1 \cdot m_2}{m_1 + m_2}$ and the force constant k.

c) Use a short time step (1/1000 of the vibrational period), propagate 50 periods for (realistically chosen) initial conditions and plot results.

2.Metropolis versus Hybrid Monte-Carlo (40 points)

Consider the asymmetric double well potential (in units of nm, kJ/mol)

$$V(x) = 100x^4 - 100x^2 - 10x \tag{1}$$

a) Set up a computer code for the Markov Chain Monte-Carlo (Metropolis acceptance criterion) scheme. Try to efficiently sample the Boltzmann distributions for $300K$ temperature by varying the proposal step.

b) Set up a computer code for the hybrid Monte-Carlo scheme. Try to efficiently sample the Boltzmann distributions for $300K$ by varying the proposal step, i. e., the lengths of the MD trajectories involved.

Use verlet integrator for MD steps.

c) Are there any characteristic differences in the performance of the sampling by the two methods?