Problem set 8: Computational Molecular Physics and Methods of Molecular Simulations

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Please hand in by: 1st July, 2014 (4pm)

1 Numeric integration

(40 points) Using the harmonic oscillator model of the C-H bond given on the previous exercise sheet, set up computer codes for the Euler scheme and the original Verlet scheme of numerical integration of Newton's equations of motion.

- Using a rather short time step (1/100 of the vibrational period), propagate 5 periods and compare the analytic solution with the numeric solution of the **coordinate** (both Euler and Verlet) for three different (realistically chosen) initial conditions. Represent the results as curve plots.
- Using three different time steps (1/1000, 1/100, 1/10 of the vibrational period), propagate 50 periods and compare the analytic solution with the numeric solution of the **energy** (both Euler and Verlet) for one initial condition. Represent the results as curve plots.
- Use linear regression to quantify the drift and fluctuation of the energy versus time and discuss the quality of the two propagators.

2 Integrators in HMC

(10 points) Despite of being area-preserving and conserving the mean energy, the original Veret scheme is NOT directly suitable for use in hybrid-MC simulations. What is the problem (hint: calculation of $H = H(q, p)$) and what variant of the Verlet scheme is used to overcome this problem?