

Problem set 7: Computational Molecular Physics

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June 16, 2015

(Please send the solution by e-mail to tahereh.ghane@gmail.com by **Fri. 26.06 (4pm)** at the latest.)

1 lag-time

(40 points) The .txt file attached to this set contains trajectory for Brownian simulation. The first column is the time step, the second and third are x and y components.

- Plot the data and cluster the xy plane into small boxes of size 3.0×3.0 .
- Find the count matrix C and transition probability matrix between different clusters.
- Choose lag-time (τ) such that Markov property maintains.
- Repeat (a)-(c) by clustering the data into the boxes of 1.5×1.5 and 2.0×2.0 and discuss the results.

2 Hybrid MC

(40 points)

- Write a routine which fills a vector of length n with double precision Gaussian random numbers distributed according to $\exp(-x^2/2)$. Test this routine by filling 10 such vectors and histogramming. Does the distribution match your expectation?
- Now introduce momentum P and fill it with normally distributed random numbers. Write a routine which, given a position and momentum and time step 2 fs, computes the Hamiltonian molecular dynamics for an ideal case. For simplicity use the harmonic oscillator hamiltonian and the mass equal to 1.
- Plot position and total energy during the time
- Repeat part (b) and (c) with 3 different time steps. How do you explain the effect of changing the time step?