

# Problem set 5: Computational Molecular Physics

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(Please send the solution by e-mail to [tahereh.ghane@gmail.com](mailto:tahereh.ghane@gmail.com) by **Fri. 29.05 (4pm)** at the latest.)

## 1 Transition Matrix

(20 points) The files `data1.txt`, `data2.txt`, and `data3.txt` each contain a series of states, sampled by Markov Chain Monte Carlo, using the Metropolis algorithm.

1. Plot the histograms of the three series to visualize the distribution of the states. How do they differ for the three series?
2. Determine the transition matrices transitions between the states in the three series.
3. (a) Are the distributions, represented by the histograms (almost) invariant distributions for all of the three series?  
(b) If not, how would you explain this?