Project 11

Replica exchange molecular dynamics simulation

Keywords: REMD, Markov chain Monte Carlo sampling, enhanced sampling
Deadline: Please, hand in your report by **Tuesday, 29 July 2014**

1 Introduction

The frequency with which a system will cross an energy barrier depends on the temperature. In molecular dynamics simulations of biomolecules at room temperature, the simulation tend to get stuck in local minima, and very long trajectory is needed to sample all relevant minima. In replica exchange MD simulations, the several simulations at different temperature are run in parallel. The algorithm then improves the sampling at a given temperature by attempting to exchange conformations between simulations at two different temperatures. The exchange is accepted based on a Markov-chain Mont Carlo criterion. The method is also referred to a as *parallel tempering*.

2 Outline of the project

1. Read and understand Ref. 1.
2. Why does the REMD method sample the correct Boltzmann distribution?
3. Implement and test the REMD using a suitable one-dimensional potential energy function. To sample these potential energy function, you can use the MCMC sampler which you implemented in exercise 7. (Strictly, this is then replica-exchange Monte Carlo, but the same principles apply.)
4. Document your results. Monitor how the replica wander through the different temperatures. Compare the sampling to a normal MCMC sampling.

3 Literature

3.1 Primary literature

1. Y. Sugita, Y. Okamoto, "Replica-exchange molecular dynamics method for protein folding", *Chem. Phys. Lett.*, **314**, p. 141-151 (1999).

3.2 Supporting literature

- Lecture notes and exercises.
- Chapters 3 and 13 in: D. Frenkel, B. Smit, "Understanding Molecular Simulation - From Algorithms to Applications", Academic Press, Elsevier (USA) 2002.
- Chapter 12 "Molecular dynamics: further topics" in T. Schlick, "Molecular Modeling and Simulation - an Interdisciplinary Guide", 2nd edition, Springer 2010.
- A. Mitsutake, Y. Sugita, Y. Okamoto, "Generalized-ensemble algorithms for molecular simulations of biopolymers.", *Biopolymers*, **60**, p. 96-123 (2001).

Project requirements

- Describe the results of the your project in a report of 5 to 12 pages (font size 11 pt).
- The report should also contain a short description of the theory and the methods. If you implement an algorithm, briefly describe the algorithm.
- Hand in your program along with the report.
- You will present the results of your project in a 20-minute presentation, after which we will have about 10 minutes time for discussion.
- Besides questions which are directly related to the results of the project, the discussion will also cover the theory of the project and the course content which is relevant to the project.
- If you run into problems during the project or have questions, please contact us
  - Bettina Keller, bettina.keller@fu-berlin.de
  - Francesca Vitalini, francesca.vitalini11@gmail.com
- During the lecture hours (Thu, 2.15 - 3.45 pm) one of us will be in the library to answer questions.