Project 05

Energy minimization and simulated annealing

Keywords: Markov chain Monte Carlo, energy minimization, simulated annealing
Deadline: Please, hand in your report by **Tuesday, 29 July 2014**

1 Introduction

In this project, you will explore different methods to find minima in the potential energy surface. These methods can be broadly divided into methods which yield the nearest local minimum (steepest descent, conjugate gradient, ...) and methods which aim at finding the local maximum (simulated annealing). While first class of methods the positions are updated according the local gradient and Hessian of the potential, simulated annealing annealing and related techniques allow for sampling of the potential energy surface

2 Outline of the project

1. Read and understand Chapter 14 of Ref. 2. (In particular, 14.1 to 14.4 and 14.7)
2. For a suitable two-dimensional potential, implement and compare energy-minimization algorithms which find the nearest local maximum
   - steepest descent
   - conjugate gradient
   - Newton Raphson
3. Extend the Markov chain Monte Carlo (MCMC) sampling algorithm from exercise 7, such that it can sample a two-dimensional potential
4. Use this MCMC algorithm to implement a simulated annealing algorithm. Test the algorithm and compare its results to the local minimization algorithms.

3 Literature

1. Lecture notes and exercises.
2. F. Jensen “Introduction to Computational Chemistry”, John Wiley & Sons Ltd (1996)
3. Chapter 12 in: T. Schlick, “Molecular Modeling and Simulation - an Interdisciplinary Guide”, 2nd edition, Springer 2010.
4. Chapters 3 and 4 in: D. Frenkel, B. Smit, "Understanding Molecular Simulation - From Algorithms to Applications", Academic Press, Elsevier (USA) 2002.

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.