"Monte Carlo Method for Problems in Mathematics, Physics, and Biology"

9/16-27/2019

Instructor*:*   **Dr. Andriy Baumketner, Institute of Condense Matter Physics**
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The lectures*:*   This lecture series will introduce Monte Carlo simulation method to solve problems in math, physics and biology. The goal is to cover both basic algorithms as well as advanced topics. Emphasis will be placed on problems in condensed matter and biological systems*. Requirements: math and physics at undergraduate level*

Lecture	*Topics*
1	What is Monte Carlo. Historical perspective.
2	Review of probability
3	Intro to Stat Mechanics: ensembles, simple thermodynamic averages. Ergodicity. Fluctuations.
4	Markov chain Monte Carlo.
5	Importance sampling. Metropolis method.
6	MC for Bayesian inference.
7	MC for simulation of condensed matter.
8	Isothermal-isobaric ensemble. Grand canonical ensemble. Gibbs ensemble. Hamiltonian MC.
9	Methods of enhanced conformational sampling.
10	Multicanonical ensemble.
11	Replica-exchange method. Multiple-histogram methods.

Reading materials*:*

Textbooks: A. Leach "*Molecular modeling: Principles and applications*"
         M. P. Allen and D. J. Tildesley "*Computer simulations of   liquids*"
          D. Frenkel and B. Smith "*Understanding Molecular Simulation*"
Review papers: P. Diaconis, "*The Markov chain Monte Carlo revolution*", Bull. Am.
          Math. Soc., 46 (2009) 179
Lecture notes: ph.icmp.lviv.ua/~andrij/dallas2019

Time: Week 1: **Mon**. 9/16, 5pm; **Tue**. 9/17, 3:30pm; **Wed**. 9/18, 5pm;
           Thur. 9/19, 5pm; **Fri**. 9/20 3:30pm
       Week 2: **Mon**. 9/23, 5pm; **Tue**. 9/24, 3:30pm; **Wed**. 9/25, 5pm;
           Thur. 9/26, 3:30pm; **Fri**.9/27 3:30pm
       Each lecture lasts one hour, lab sessions will be arranged

Place*:* Clements 126