Computational Simulations I

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Number of Lectures

12 Lectures (Wednesday 11 a.m, Room 210):

- October: 16, 23, 30
- November: 6, 13, 27
- December: 4, 11, 18
- January: 8, 15, 22

12 Exercise classes (Friday 13.30 pm, Room 114):

- October: 25
- November: 1, 8, 15, 22, 29
- December: 6, 13, 20
- January: 10, 17, 24

Exam Date: 29th January 2020 (11 a.m)

Important points to note

- Admission to Exam will be based on your performance in homeworks: score $\geq 50\%$
- There will be 11 homeworks
- Submit hard copy of your homeworks (email submission is not encouraged)
- Exercise classes will be taken by MSc. Stanislav Kazmin

Contents of the Course

- Brief Overview of Statisical Mechanics
- The Ising Model in $d = 1$
- Random and Self Avoiding Walk
- Random Numbers
- Monte Carlo Simulations: Basics with the Ising model as example in $d = 1, 2$
- Histogram reweighting
- Error Analysis, Autocorrelation time
- Simulations of Nonequilbrium phenomenon of Coarsening
- Basic Molecular Dynamics: Concept of thermostats, calculating Diffusion constant

Prerequisite

- Very basic knowledge of programming in any language: fortran, C, C++, julia, python
- Knowledge of any plotting software: gnuplot, origin, matplot (python), etc.
- Even if you are not familiar with any of them ..this is a good chance

References

- *Monte Carlo Methods in Statistical Physics* by M.E.J Newmann and G.T. Barkema
- W. Janke, *Monte Carlo Simulations in Statistical Physics - From Basic Principles to Advanced Applications*, invited Ising Lectures, Lviv, Ukraine, in: *Order, Disorder and Criticality: Advanced Problems of Phase Transition Theory*, Vol. 3, edited by Y. Holovatch (World Scientific, Singapore, 2012), pp. 93 - 166.
- *A Guide to Monte Carlo Simulations in Statistical Physics* by D. Landau and K. Binder
- *Understanding Molecular Simulations: From Algorithms to Applications* by D. Frenkel and B. Smit