Computational Laboratory in Statistical Mechaics: Proposal

Sushrut Ghonge

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Why this course?

This course on *Computational Laboratory in Statistical Mechanics* builds on the foundation of computational problem solving that you acquired in the introductory level Computational Methods in Physics course.

In this course, you will initially familiarize yourself with the basics of statistical simulations. You will then learn the concepts of Monte Carlo simulations and use them to simulate physical systems. You will also learn the modern simulations done in industry and academics such as option pricing in finance and non-equilibrium systems in biophysics and chemical physics. Your computational explorations will give you a deeper, hands-on understanding of the concepts of applied statistics and statistical physics.

Learning objectives

Monte Carlo simulation is a technique for dealing with uncertainty, which is widely used in all sciences, engineering and many business operations. Monte Carlo simulations are based on generating random numbers according to a probability distribution, i.e. random variables. Therefore, this course starts with an introduction to random variables and their properties, including the famous central limit theorem.

Concepts of thermodynamics, such as equilibrium, work, heat and entropy all have their microscopic foundations in statistical mechanics. By hands-on computer programming, you will learn how macroscopic thermodynamics emerges from statistical mechanics.

The focus of this course will be to simulate various physical models and real-life systems. This will give you an experience of how statistical mechanics is applied in practice, even outside Physics. Doing this course will also improve your programming and scientific computing skills.

Prerequisites/Corequisites

Computational Methods in Physics, Thermal Physics.

Course structure

1. **Basic statistics**
   - Random number generators. Using random number generators to generate random variables according to a given probability distribution.
   - Sum of random variables. Probability distribution for functions of random variables.
   - Central limit theorem. *(Project 1)*
2. **Monte Carlo simulations**

- Understanding the meaning of equilibrium. Out-of-equilibrium states and non-equilibrium steady states. Detailed balance and entropy increase.
- The Metropolis algorithm, and why it works.
- Metropolis Monte Carlo simulations of 1D and 2D Ising models.
- Understanding the microscopic origins of work and heat through simulations.
- Phase transitions in the Ising model. *(Project 2)*

3. **Advanced applications**

   In order of increasing time requirement and difficulty:

   - Monte Carlo simulations in finance. Black-Scholes model. *(Project 3)*
     OR,
   - Non-equilibrium work and heat, Jarzynski equality and the fluctuation theorems. *(Project 3)*
     OR,
   - Renormalization group (RG). RG for the 1D and 2D Ising models. *(Project 3)*

4. **Simulating reaction-diffusion systems with networks**

   - Basics of networks: nodes and edges, adjacency matrix, degree distribution.
   - Diffusion processes on networks: modelling epidemics (OR) viral content on social media. *(Project 4)*

References

Any computational physics book of your choice will most probably have a chapter on random numbers and Monte Carlo simulations. For example:

1. Mark Newman, *Computational Physics*, 2012 (Chapter 10).
2. R.H. Landau, et. al., *Computational Physics: Problem Solving with Python* (Chapter 4, 17-18).

For advanced applications:

3. D. M. Chance: Teaching Note 96-03: Monte Carlo Simulation (PDF).
4. C. Jarzynski, *Nonequilibrium equality for free energy differences*, Phys. Rev. Lett., 78(14), 2690 (1997).
5. G. E. Crooks, *Entropy production fluctuation theorem and the nonequilibrium work relation for free energy differences*, Phys. Rev. E, 60(3), 2721 (1999).
6. H. Híjar and J. M. O. de Zárate, *Jarzynski's equality illustrated by simple examples*, European Journal of Physics, 31(5), 1097 (2010).

Networks:

7. D. J. Watts, and P. S. Dodds, ”Influentials, networks, and public opinion formation”, Journal of consumer research, 34.4, 441-458 (2007).