Syllabus

Statistical Mechanics: Algorithms and Computations

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1. Course Description

a. Pre-requisites

The Course is to be based on the acquisition of the following Courses:

- Mathematical analysis;
- Linear algebra.

b. Abstract

In this course you will learn a whole lot of modern physics (classical and quantum) from basic computer programs that you will download, generalize, or write from scratch, discuss, and then hand in. We will learn a lot of about algorithms, and about the deep insights into science that you can obtain by the algorithmic approach.

c. Course Type

Blended learning

2. Learning Objectives

The objective of this course is to form a foundation of Statistical Mechanics.

3. Learning Outcomes

On completion of the course, the student should know the basic models of Statistical Mechanics and corresponding computer algorithm.

4. Course Plan

Topic 1. Monte Carlo algorithms (Direct sampling, Markov-chain sampling).

We will learn about algorithms by playing with a pebble: we will use the 3x3 pebble game to understand the essential concepts of Monte Carlo techniques (detailed balance, irreducibility, and a-periodicity), and meet the celebrated Metropolis algorithm. Finally, we will let you understand some useful aspects of Markov-chain Monte Carlo, related to convergence and error estimations.

Topic 2. Hard disks: From Classical Mechanics to Statistical Mechanics.

We will get in touch with the hard-disk model, which was first simulated by Molecular Dynamics in the 1950's. We will describe the difference between direct sampling and Markov-chain sampling, and also study the connection of Monte Carlo and Molecular Dynamics algorithms, that is, the interface between Newtonian mechanics and statistical mechanics. Also we will see classical concepts from statistical physics (partition function, virial expansion, ...), and will show that the equiprobability principle might be more subtle than expected.

Topic 3. Entropic interactions and phase transitions.

We switch from the hard-disc to clothe-pins aligned on a washing line. This is a great model to learn about the entropic interactions, coming only from statistical-mechanics considerations. You will see an example of a typical situation: Having an exact solution often corresponds to finding a perfect algorithm to sample configurations. Finally, we will go back to hard disks, and get a simple evidence of the transition between a liquid and a solid, for a two-dimensional system.

Topic 4. Sampling and integration.

We will deepen our understanding of sampling, and its connection with integration, and this will allow us to introduce another pillar of statistical mechanics (after the equiprobability principle): the Maxwell and Boltzmann distributions of velocities and energies. Also we will push the limits of sampling until we can compute the integral of a sphere in 200 dimensions.

Topic 5. Density matrices and Path integrals (Quantum Statistical mechanics 1/3).

Start to learn about quantum statistical mechanics. We will start by learning about density matrices and path integrals, fascinating tools to study quantum systems. In many cases, the Trotter approximation will be useful to consider non-trivial systems, and also to follow the time evolution of a system. All these topics, including the matrix-squaring technique, will be reviewed during this topic, where you will also study the anharmonic potential.

Topic 6. Lévy Quantum Paths (Quantum Statistical mechanics 2/3).

We will introduce the properties of bosons, indistinguishable particles with peculiar statistics. At the same time, we will also go further by learning a powerful sampling algorithm, the Lévy construction, and you will thoroughly compare it with standard sampling techniques.

Topic 7. Bose-Einstein condensation (Quantum Statistical mechanics 3/3).

We discuss the Bose-Einstein condensation phenomenon, theoretically predicted in the 1920's and observed in the 1990's in experiments with ultracold atoms. In the path-integral framework, an elegant description of this phenomenon is in term of permutation cycles, which will also lead to a great sampling algorithm, to be discussed in the homework session.

Topic 8. Ising model - Enumerations and Monte Carlo algorithms.

We come back to classical physics, and in particular to the Ising model, which captures the essential physics of a set of magnetic spins. This is also a fundamental model for the development of sampling algorithms, and we will see different approaches at work: A local algorithm, the very efficient cluster algorithms, the heat-bath algorithm and its connection with coupling. All of these will be revisited in the homework session, where you will get a precise control over the transition between ordered and disordered states.

Topic 9. Dynamic Monte Carlo, simulated annealing.

We start by learning about a dynamic Monte Carlo algorithm which runs faster than the clock. This is easily devised for a single-spin system, and can also be generalized to the full Ising model from previous topic. We move towards the simulated-annealing technique, a physics-inspired optimization method with a very broad applicability.

Topic 10. The Alpha and the Omega of Monte Carlo.

We repeat the experiment of Buffon's needle, already performed in the 18th century, and then we touch the sophisticated theory of Lévy stable distributions, and their connection with the central limit theorem.

5. Reading List

All materials in https://www.coursera.org/learn/statistical-mechanics

6. Grading System

The student's final assessment consists of the assessment of the exam A_{exam} and the accumulated assessment A_{acc} obtained on the platform https://www.coursera.org/learn/statistical-mechanics as follows: $A_{final} = (A_{acc} + A_{exam})/2$.

7. Examination Type

Oral examination. Control elements are not blocking.

8. Methods of Instruction

The course is being studied on the online platform https://www.coursera.org/learn/statistical-mechanics

9. Special Equipment and Software Support (if required)

Not required