Computational Physics II | UCSD PHYS 142/242
Final Projects | Presentations due: Monday, March 11 - Friday, March 15, 2024
Report and code due: Friday, March 22, 2024, 8:00pm

Instructions

- You will be assigned to a group of 3–4 students and part of the project is to learn how to collaborate effectively. So, meet with your group members to discuss the project and divide the work.
- The project will be graded based on the quality of the report and code, the correctness of the results, and the depth of the analysis.
- The projects outlined here are designed to be open-ended, and give you the freedom to explore additional topics that we may not have covered in class.
- The presentation should be about 20 minutes and different group members should deliver different parts of it.
- The presentation/report should include an introduction to the problem, a description of the methods used (and why), and a discussion of the results.
- You should submit all code as a public GitHub repository with a README that explains how to run it. You are also encouraged to use GitHub to collaborate with your group members.
- The report should be about 4 pages, including figures and tables, but excluding references. It should be double column using the *Phys. Rev. Lett.* template.
- Please submit your report as a single .pdf file to Gradescope under "Final Project Report". The report should include a link to your public GitHub repository. The .zip file should contain all of your source code files.
- Fill out your project preferences here: https://forms.gle/exB5BEtVddbvmGDr7

2 2D Ising Model with MCMC

Consider the 2D Ising model in a square lattice Λ with 100×100 sites and periodic boundary conditions in the presence of an external magnetic field B. The energy of the system for a given spin configuration $\sigma = \{\sigma_i\}_{i\in\Lambda}$ is

$$E(\sigma) = -J \sum_{\langle ij \rangle} \sigma_i \sigma_j - B \sum_{i\in\Lambda} \sigma_i, \tag{5}$$

where $\langle ij \rangle$ denotes two adjacent sites (with no double counting), J is the spin-spin interaction, and $\sigma_i \in \{-1, +1\}$ is the spin at site i.

The magnetization of the system is

$$M(\sigma) = \frac{1}{|\Lambda|} \sum_{i\in\Lambda} \sigma_i. \tag{6}$$

Problem A: Use Markov chain Monte Carlo and the Metropolis-Hastings algorithm to simulate the 2D Ising model at different temperatures T and magnetic field strengths B. Discuss your strategy for determining the initial configuration, burn-in steps, total number of steps, and thinning (if any).

Problem B: Plot 1D scans of the magnetization M versus T for fixed B at three different values: $B < 0$, $B = 0$, and $B > 0$. Plot 1D scans of the magnetization M versus B for fixed T at three different values: $T < T_C$, $T = T_C$, and $T > T_C$, where $T_C = \frac{2}{\ln(1+\sqrt{2})} \approx 2.269$.

Problem C: Putting this all together, draw/describe the phase diagram in B versus T of the 2D Ising model, where the magnetization M is the order parameter. Consider discussing first-order phase transitions and critical exponents, hysteresis and metastable states, and/or specific heat and susceptibility. See Refs. [3, 4] for relevant discussions.