SMCEF P1
Ferromagnetism
v0

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Contents

1 Introduction

The first SMCEF project is to implement the Ising model to a **3D** cubic grid and simulate for different reduced temperatures and external magnetic field.

The project is to be implemented by groups of 2 or 3 students, but notice that bigger groups are expected to deliver more and better work than groups of two students.

The objectives of the project are:

- Obtain an estimation for the Curie Temperature of the grid and compare with values of the 2D grid obtained in the classes
- Observe the Ferromagnetic - Paramagnetic hysteresis
- Analyze your code regarding to computational complexity
- Identify the critical code sections
- optimize your code to speed up the execution time

1.1 Grid and model specifications

The grid must has at least 10 length in each direction. This is a good starting point for testing and code improvement, the final project should use bigger grids, open to the students decision.

The grid is closed in all directions.

The minimum number of Monte Carlo (MC) cycles is 10.000, if feasible the students should use a higher number of MC cycles.

The number and ranges of temperature and magnetic field pairs should be chosen to ensure that the Curie Temperature and Ferromagnetic - Paramagnetic hysteresis are well observed in the obtained data. As per guidelines, the student should use at least 10 different magnetic fields, from strong negative to strong positive, and intermediate values including no magnetic field.

Regarding the temperature the students should use at least 5 different reduced

1.2 Physic quantities

The physical quantities to be measured from the simulation for each pair of reduced temperature and external magnetic field pairs are the same as the ones observed in classes, i.e. magnetic moment, average energy on grid point, magnetic susceptibility, and thermal capacity of the grid.

The magnetic moment is essential to observe the Ferromagnetic - Paramagnetic hysteresis, the magnetic susceptibility and thermal capacity to obtain estimations of Curie Temperature.

Use the results obtained in classes as a guideline to what it would be expected to obtained with your code.

1.3 Recommendations

The students are advised to start with a small grid ($10 \times 10 \times 10$ as an example), and eventually for lower MC cycle numbers.

Then increase the number of MC cycles and obtain better statistics on the several physical quantities.

Run the overall simulation, for some values of temperature and external magnetic field. Make a computer complexity of your code regarding the input parameters and try to identify the function with higher computer complexity.

Use a profiler tool to measure what are the critical code sections. Use that information to improve execution time, change the code, and or use parallelization.

When you consider the code as efficient as possible run the overall simulation for the best parameters and metaparametrs, like grid size, values of temperature, and magnetic field, number of MC cycles.

2 Deliverables

For this project each group must send a zip file containing:

- The non optimized code
- The final optimized code that was used to obtain the simulation results
- A group report on the work

All files must be named XXXXX-YYYYY(-ZZZZZ)-SMCEF-2024-P1-file_type, with:

- XXXXX, YYYYYY and eventually ZZZZZ the student numbers
- file_type as code-v0, code-v1, report

It does not represent the file extensions but please let them stay in the file names. The code files should be .py (not jupyter notebooks) and the report in pdf format.

The report should have a short introduction, about one page, reporting what is the objective of the simulation and what physical phenomena are we trying to simulate, with a concise description.

A section explaining the code structure, how it works (what information it needs and it's given to the code), and any decision or considerations you had to decide for the v0 code. Eventually, preliminary results obtained so far.

Another section with the computer complexity analysis and profiler measurements and what the group takes from that information.

A section explaining what were and why the optimization and or speed up improvements were implemented and how much did those code changes improve the execution time. Justify what parameters and metaparameters will be used in the final simulation

Finally a report of the results obtained with v1 code version for the more demanding input size, and compare them with the expected results.

In the conclusions besides analyzing the results, there should also be a short information on what were the main difficulties of the project, and what could eventually be improved.

3 Grading

The project grading is divided in different categories, namely:

- Codes v0 and v1 working and obtaining the expected results - 8 values
- Code readability and comments - 2 values
- Speed up implementations - 3 values
- Quality of final results - 2 values
- Report - 5 values divide as:
  - Readability and presentation of results - 1 values
  - Reasoning for the implementation decisions and speed up methods chosen - 3 values
  - Introduction and conclusions - 1 value

4 Project Deliver

The project should be sent by an email to ajw@fct.unl.pt, with subject "[SMCEF] P1 deliver of students (number of the students"), no later than 23:59 of May 13th.