

Exam Computational Physics

2020

Thorvald M. Ballestad

May 7, 2020

Abstract

Metropolis Monte Carlo simulation of 2D Ising model, using the Mon-Jasnow and extended Mon-Jasnow algorithm. This report is not intended as a scientific report, but as an answer to the exam. The goal of this report is to give a brief overview of how I have solved the problem, and then go into the parts of the solution that I think are the most interesting. Thus, this report consists of a brief documentation of the code and then explanations and thought on the interesting aspects of the solution.

1 Overview of the code

The simulation is written in Julia and the plots are generated in Python. As the Python code is just simple plotting, I will not give it much focus here. The code is separated into files, the main part being in `utils.jl`. Nothing should be run directly from `utils.jl`, it contains the machinery that can be used from other designated scripts. For each type of “operation” that we want to execute, there should exist a file, that extends `utils.jl`, for example `task1.jl` and `investigate_error.jl`.

Metropolis: select at random - i attempt flip

Interesting solutions: - Indexes for neighbor points - Very modul based code.
— i Was very easy to implement new types of index vectors - Does not really need energy, only the energy difference, which can be calculated explicitly every sweep - Exponent lookup - δ_{H_s} *wee allocated outside loop*

2 Results

3 Findings related to performance

During the development process, several benchmarks were made, and I discovered some small changes that had huge impact on performance. Especially pices

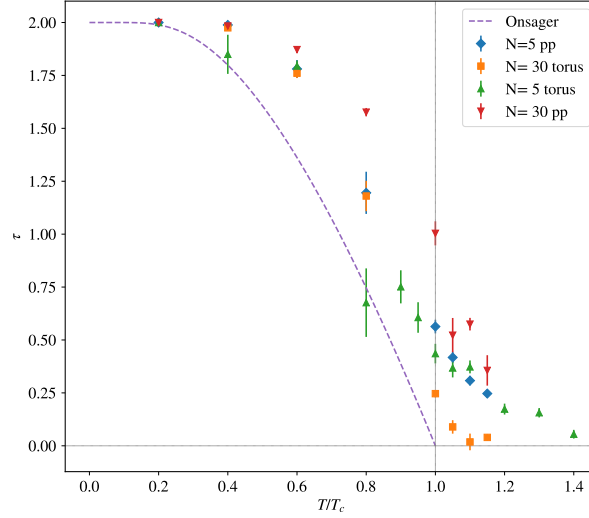


Figure 1: τ as a function of T .

of code that are involved in the very core of the simulation loop, the flipping, are vital to streamline as they are executed several million times.

- Index vectors, not having to create the tuples at the expense of using some more memory.
- UInt8 -> Integer, possibly some silent conversions that I did not find.
- Structs - Optimizing neighbor function failed.
- > If one is able to optimize it, very advantageous.

References

- [1] M. E. J. Newman and G. T. Barkema, *Monte Carlo Methods in Statistical Physics* chap. 3, Oxford University Press, Oxford, 1999.
- [2] L. Onsager, *Crystal statistics. I. A two-dimensional model with an order-disorder transition*, Phys. Rev. 65, 117 (1944).
- [3] K.K. Mon and D. Jasnow, *Direct calculation of interfacial tension for lattice models by the Monte Carlo method*, Phys. Rev. A 30, 670 (1984).

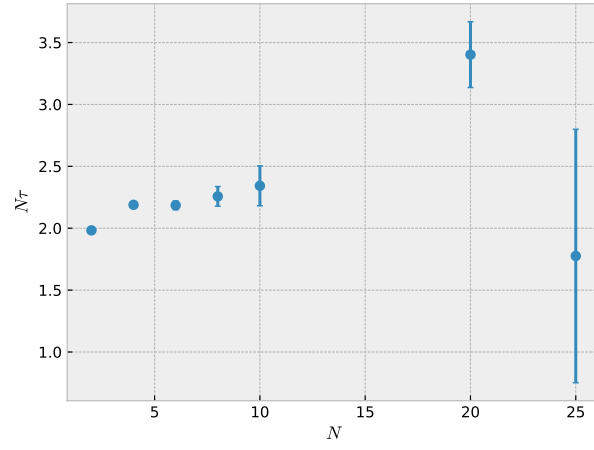


Figure 2: $N\tau$ as a function of N for $T = T_c$.

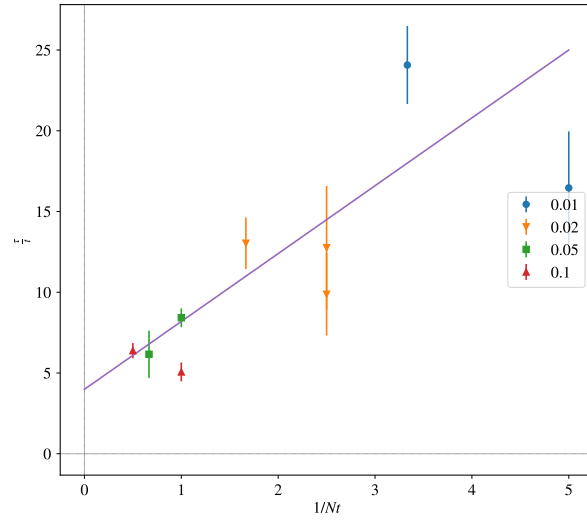


Figure 3: τ/t as a function of $\frac{1}{Nt}$.