Computational Physics P452
Term paper project

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Topic: Wolff Cluster Algorithm

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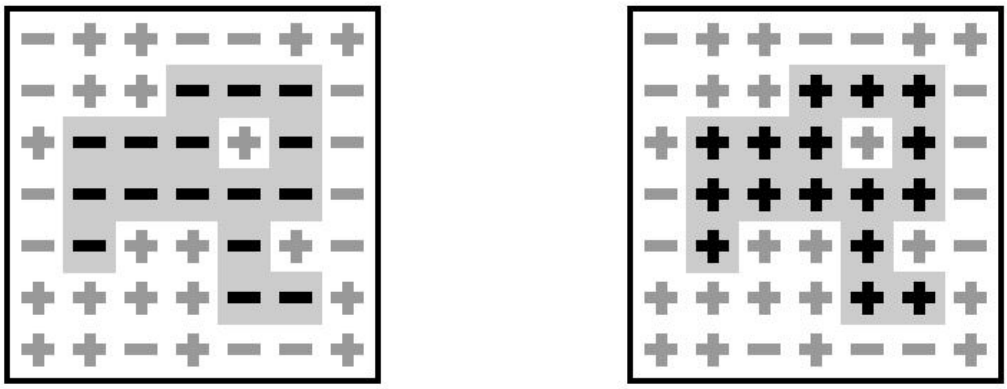

Krauth (2003)

Ising Model

Let us begin with a quick introduction on Ising model. It is a model used to simulate magnetic systems in statistical mechanics. It can be considered as a lattice with discrete values. I used -1 and +1 values which represent up spin and down spin at that specific site. The Hamiltonian of the system is given by:

$$H = -\sum_{<i,j>} J_{ij}\sigma_i\sigma_j - B\sum_j \sigma_j$$

where σ_i, σ_j are spins of neighbouring sites (the long range interactions are ignored), J_{ij} is the interaction term between spins and B is external magnetic field. In absence of external magnetic field, the Hamiltonian becomes,

$$H = -\sum_{<i,j>} J_{ij}\sigma_i\sigma_j$$

Energy, Magnetisation, Specific heat and Susceptibility

We use 2D Ising model for square periodic lattice. After using the algorithms to simulate the model for a particular temperature and reach a particular configuration (equilibrium). Using this we can study its properties over a range of temperature, like calculating its energy, magnetisation and specific heat.
Average energy is given by,

$$E =< \sum_{<i,j>} H_{ij} >= \frac{1}{2} < \sum_{i,j} H_{ij} >$$

The 1/2 term comes from counting pair of spins twice.
Average magnetisation is given by,

$$< M >= \frac{1}{N^2}\sum_{(i,j)} \sigma_{ij}$$

The specific heat capacity Cv is given by,

$$C_V = \frac{\partial < E >}{\partial T} = \frac{\beta}{T}\left(< E^2 > - < E >^2\right)$$

The susceptibility χ is given by,

$$\chi = \frac{\partial < M >}{\partial H} = \beta \left(< M^2 > - < M >^2 \right)$$

where $\beta = (k_B T)^{-1}$.
I have implemented Wolff Cluster algorithm and compared it with Metropolis algorithm, both performed on periodic square lattice. So first, let us discuss Metropolis algorithm.

Metropolis algorithm

It is implemented by the following procedure:

1. Initially, take a N X N lattice with random configuration, basically a N X N matrix with randomly assigned +1 and -1 values.

2. Choose a site in the matrix.

3. Flip the spin at that chosen site. Now we calculate the change in the energy ΔE in the configuration due to change in the spin.

4. If $\Delta E<0$, the spin flip is favourable and hence the changed configuration is the final configuration. If $\Delta E>0$, then we compare $\exp(-\Delta E/k_B T)$ with a randomly generated number between 0 and 1. If $\exp(-\Delta E/k_B T)$ is greater, then the spin is favourable else it return to its original configuration.

5. Repeat from step (2).

After equilibrating, all the observables (Energy, Magnetisation, Specific heat, Susceptibility) are calculated and averaged over a number of steps.

Plots

No. of steps for equilibration = 256
No. of steps for average calculation = 512
Calculated for 32 temperature points between 1.53 and 3.28 J/Kb.

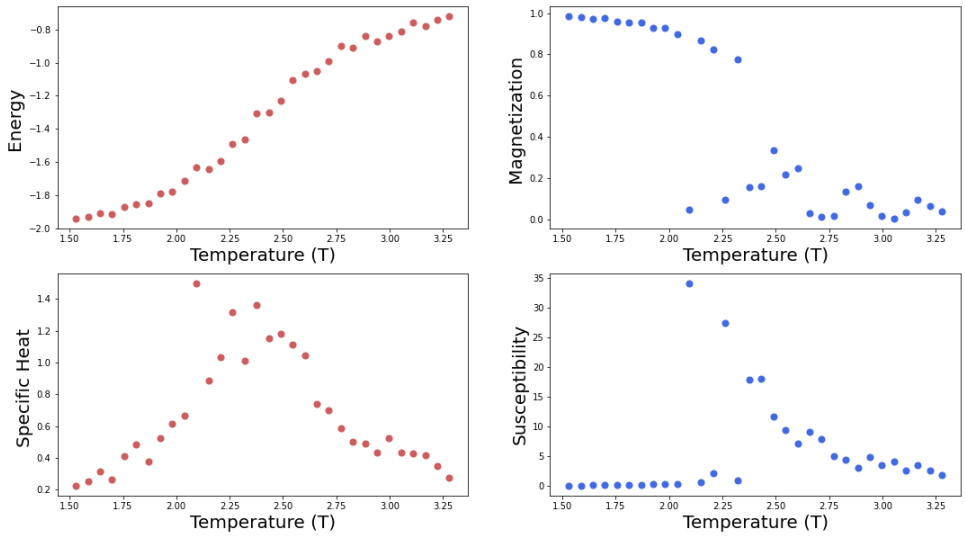

Figure 1: The observables for J=1, N X N= 10 X 10, (Bennett (2016))

Wolff cluster flipping method

Unlike Metropolis or 'single spin flip' algorithm, Wolff cluster algorithm involves formation of a single cluster and flipping all the spins in the cluster. Hence it converges faster towards equilibrium than single spin flip algorithms.

Algorithm

1. Take a N X N lattice with randomly assigned +1 and -1 values.
2. We choose a site randomly, say i.
3. Now we will form a bond from i to the nearest neighbour with same spin (say j) and probability of $p = 1 - \exp[-2J\beta]$. This will form a cluster, if the bond is formed.
4. Now j will form bond with nearest neighbour with same spin (say k), and with probability p. The cluster is updated if the bond is formed.
5. Repeat step (3) until no new bonds are formed.
6. All the spins in the cluster are flipped.

7. Repeat from step (1)

Pseudo-code/Implementation (Krauth (2003))

```
i := random particle;    # pick a site
C := {i};
Cold := {i};
while Cold != {}
    Cnew := {};
    for all i in Cold
        for all j neighbor of i with Si = Sj , j not in C
            if ran[0, 1] < p then
                Cnew := Cnew + {j};
                C := C + {j};
    Cold := Cnew;
for all i in C           # spin flip
    Si := -Si;
```

Plots

J=1
N = 10
No. of steps for equilibration = 128
No. of steps for average calculation = 128
Calculated for 32 temperature points between 1 and 5 J/Kb.

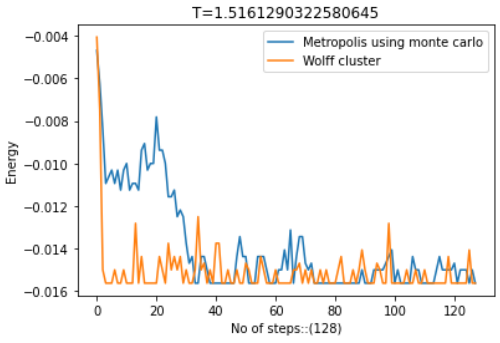

Figure 2: Comparision between Wolff and Metropolis at T = 1.516 J/Kb

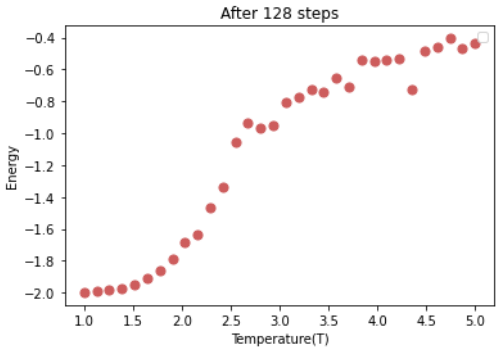

Figure 3: Energy vs T

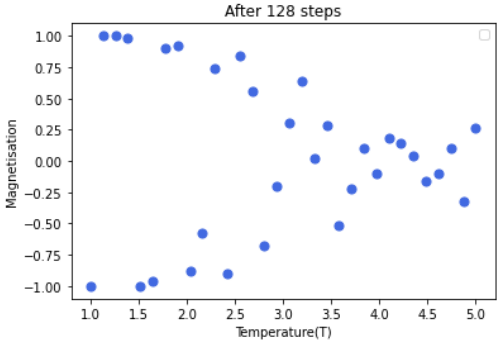

Figure 4: Magnetisation vs T

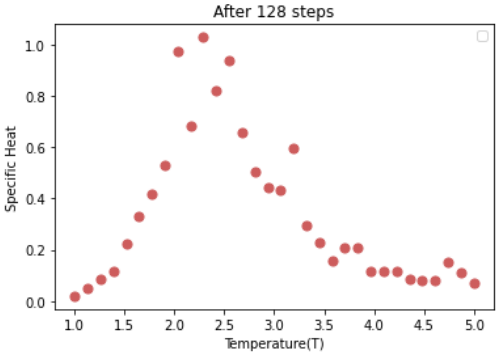

Figure 5: Specific heat vs T

Conclusion

In figure 2, from the plot we can verify that in case of Wolff cluster it equilibrates in less number of steps. For the rest of the observables, the plots came as expected. In figure 4, from the magnetisation plot we can see how it changes from ferromagnetism to paramagnetism as temperature increase. Temperature increase leads to increase in energy, thus figure 3. In case of specific heat plot (figure 5) we see a discontinuity around Curie temperature (temperature during transition from ferromagnetic to paramagnetic).

References

Bennett, D. (2016). Numerical solutions to the ising model using the metropolis algorithm. *JS TP*, 13323448.

Krauth, W. (2003). Cluster monte carlo algorithms. *arXiv preprint cond-mat/0311623*.

The code is uploaded here on Github.