Exercise class 4

Maximilian Holst
Toni Heugel

Solution exercise sheet 3

ETH Eidgenössische Technische Hochschule Zürich
Swiss Federal Institute of Technology Zurich

Computational Statistical Physics
Exercise sheet 03

FS 2020
Oded Zilberberg

Exercise 1. Cluster algorithms

Goal: Cluster algorithms can be used to reduce the critical slowing down substantially. This week you have to simulate either the 3D Ising model or the Potts model with $q = 2$ using a cluster algorithm. You may choose either the Swendsen-Wang or the Wolff algorithm.

Task 1: Find the connection probability in the Ising model.

Hint: In the Potts model the probability for connecting sites in the same state is $p = 1 - \exp(-\beta J)$.

Task 2: Implement either the Swendsen-Wang or the Wolff algorithm. Check your code by plotting the binder cumulant or the magnetic susceptibility around T_c.

Task 3 (OPTIONAL): Implement the other algorithm as well.

Task 4: Compare the performance of the algorithms and show that in the cluster algorithms the critical slowing down is substantially reduced. Measure the runtime and compute the linear autocorrelation time τ (relative to the observable E or M) of the cluster algorithm and compare it to the Metropolis algorithm. Report a table with τ and the Monte Carlo speed defined as

$$\mathrm{MC}_{\mathrm{speed}} = \frac{\mathrm{sweeps}}{\mathrm{time}} \cdot \frac{1}{\tau}$$

for at least three temperature values, say T_c, $T_c + 1$, $T_c - 1$, and fixed size. Make another table with the temperature fixed at T_c and varying lattice size. Interpret the results.

Hint: Remember that you can extrapolate τ from the autocorrelation series

$$\rho_{XX}(\Delta t) = \frac{\left\langle (X_t - \bar{X})(X_{t+\Delta t} - \bar{X}) \right\rangle_t}{\sigma^2}.$$

Implementation

Connection probability Ising model: $p = 1 - e^{-2\beta J}$

Wolff:

- Main structure very similar to Metropolis code
- No subsweeps:
  - We flip ~N spins in 1 step
  - We want to find autocorrelation time
- Build cluster and flip it
  - start from randomly picked spin → flip it
  - Add next neighbors with probability p (if they have the same state) → flip them
  - No need to save the cluster
  - Recursive

Implementation

Metropolis:

- Use code from Ex. 1
- Number of subsweeps: $N=L^3$

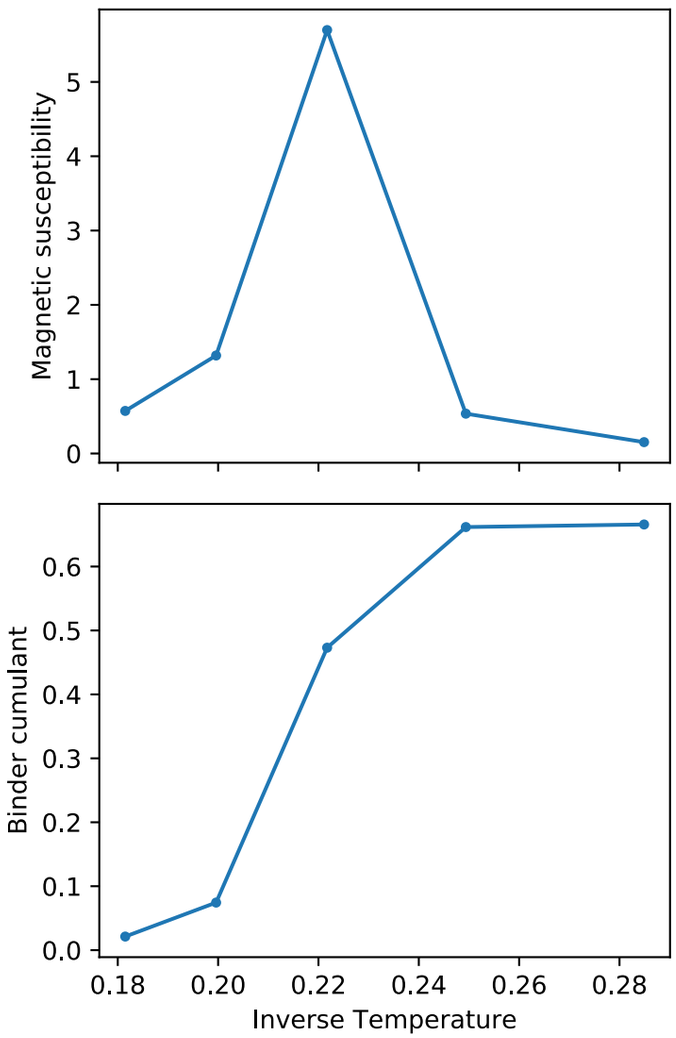
Autocorrelation time:

- Calculate autocorrelation series from sampled magnetization or energy
- Find cutoff
- Use $\sim e^{-t/\tau}$ to find the autocorrelation time τ

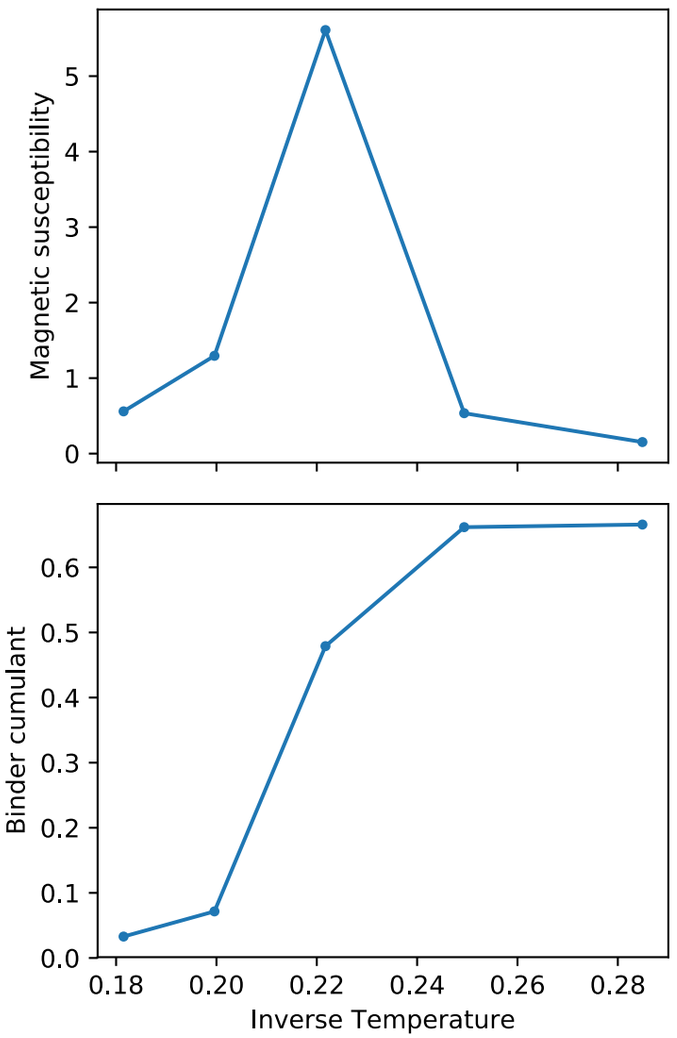
Measure runtime of sampling

Code

Results



Metropolis



Wolff

Results

β	L	runtime	τ	MC_{speed}
0.28	10	141.3	2.4	294
0.25	10	125. 2	5.9	163
0.22	10	171. 0	30.4	19
0.20	10	161.2	7.2	86
0.18	10	160.5	3.3	188

β	L	runtime	τ	MC_{speed}
0.28	10	102.6	0.96	1017
0.25	10	74.2	1.74	777
0.22	10	17.6	5.61	1016
0.20	10	2.3	4.81	8855
0.18	10	1.2	7.57	10721

Table 1: Runtime, autocrorrelation time and $\mathrm{MC}_{\mathrm{speed}}$ of M as a function of temperature for Metropolis (left) and Wolff algorithm (right).

β	L	runtime	τ	MC_{speed}
0.22	8	77.3	19.1	68
0.22	10	171.0	30.4	19
0.22	12	217.6	41.6	11
0.22	16	534.5	74.4	2

β	L	runtime	τ	MC_{speed}
0.22	8	14.0	4.57	1558
0.22	10	17.6	5.61	1016
0.22	12	25.6	6.48	603
0.22	16	53.5	8.78	215

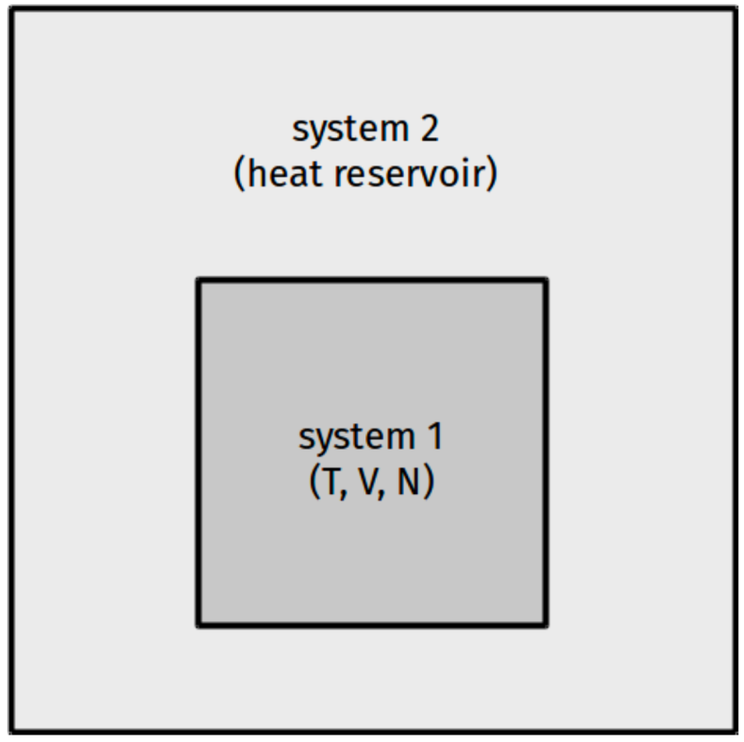
Table 2: Runtime, autocrorrelation time and $\mathrm{MC}_{\mathrm{speed}}$ of M as a function of system size at T_c for metropolis (left) and Wolff algorithm (right).

Exercise sheet 4

Canonical ensemble

System connected to temperature bath

- Constant number of particles
- Constant volume
- Constant temperature



Probability of phase space configuration X:

$$\rho(X) = \frac{1}{Z_c} \exp(-E(X)/k_B T)$$

Partition function:

$$Z_{mc} = \sum_X \exp(-E(X)/k_B T)$$

→ Metropolis, Wolff, Swendsen-Wang

Microcanonical ensemle

Isolated system:

- Constant number of particles
- Constant volume
- **Constant energy**

Probability of phase space configuration X:

$$\rho(X) = \frac{1}{Z_{mc}}\delta(H(X) - E)$$

Partition function:

$$Z_{mc} = \sum_{X} \delta(H(X) - E)$$

Creutz algorithm

- Condition of energy conservation slightly relaxed
- Energy fluctuations allowed
- Idea:
  - Introduce *demon*
  - Small reservoir of energy E_D
  - Can store maximum energy E_{max}

Creutz Algorithm

- Choose a site,
- Compute ΔE for the spin flip,
- Accept the change if $E_{\max} \geq E_D - \Delta E \geq 0$.

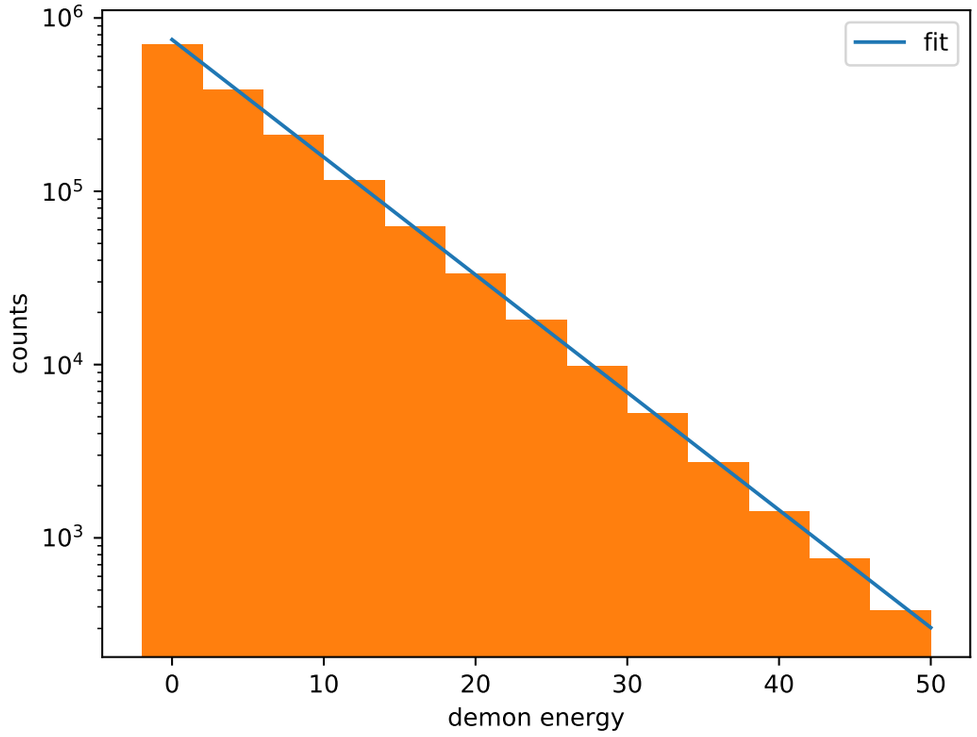
Creutz algorithm

Creutz Algorithm

- Choose a site,
- Compute ΔE for the spin flip,
- Accept the change if $E_{\max} \geq E_D - \Delta E \geq 0$.

Temperature?

- Plot histogram of E_D
  - $P(E_D) \propto \exp(-E_D/k_B T)$
  - Fit



Exercise sheet 4

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Computational Statistical Physics
Exercise sheet 04

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Exercise 1. Microcanonical Monte Carlo

Goal: So far, we treated the Ising model in the canonical ensemble (fixed temperature) where the samples were drawn according to the Boltzmann distribution. In this week's exercise we are going to perform a microcanonical Monte Carlo simulation of the 3D Ising model according to the Creutz algorithm (M. Creutz, Phys. Rev. Lett., 50, 1411, (1983)).

The Creutz algorithm is defined in the following way:

1. Start with an initial spin configuration x of a given energy E and define a container energy E_d (demon energy) such that $E_{max} \geq E_d \geq 0$.
2. Choose a spin at random and flip it to obtain the configuration y.
3. Calculate the energy diffference ΔE between the configurations x and y.
4. If $E_{max} \geq E_d - \Delta E \geq 0$ choose a new spin and repeat the process. If not revert the spin flip and choose a new spin.

Task 1: Modify your program of the first exercise to simulate a microcanonical Ising system using the Creutz algorithm.

Task 2: Determine the corresponding temperature T using

$$P(E_d) \sim e^{-\frac{E_d}{k_B T}}.$$

Task 3: Compute T for different E. Plot energy and magnetization as a function of temperature and compare your results to the results obtained with the Metropolis algorithm.

Task 4: Repeat the above tasks for different system sizes and compare your results.

Task 5 (OPTIONAL): What happens in the case $E_{max} = 0$ (Q2R algorithm)? Discuss the issue of ergodicity.

Instructions

Structure for simulation at energy E:

1. Initialize a configuration with all spins in the state +1
2. Increase the energy until E is reached
   - Randomly flip spins that increase the energy
3. Sampling using the Creutz algorithm
   - Start with $E_D = 0$
   - Accept spin flips with $0 \leq E_D - \Delta E \leq E_{max}$
   - Update E_D
4. Find the temperature using the distribution of E_D
   - $P(E_D) \propto \exp(-E_D/k_B T)$