The transition probability can typically be written as

$$P(A \to B) = P^A_{\text{attempt}}(B) P^A_{\text{accept}}(B)$$

where the two factors have the following meaning:

$P^A_{\text{attempt}}(B)$ - The probability of selecting B as a candidate among a number of possible new configurations

$P^A_{\text{accept}}(B)$ - The probability of actually making the transition to B after the selection of B has been done

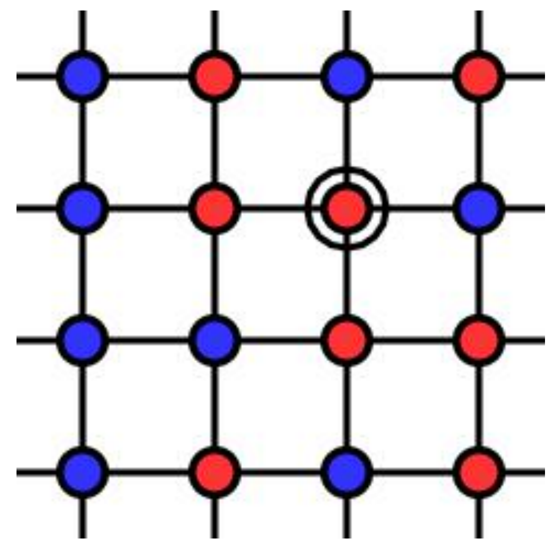
If B has been selected but is not accepted (rejected); stay with A

For an Ising model

➢ Select a spin at random as a candidate to be flipped (attempt)

➢ Actually flip the spin with a probability to be determined (accept)

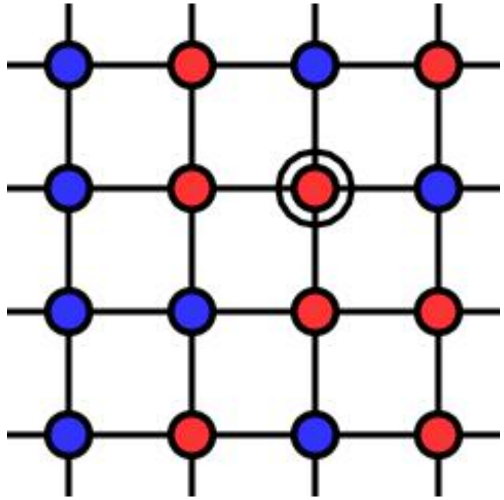
➢ Stay in the old configuration if the flip is not done (reject)



$P^A_{\text{attempt}}(B) = 1/N_{\text{spin}}$ uniform, independent of A, B

$P^A_{\text{accept}}(B)$ constructed to satisfy detailed balance condition

$$\frac{P^A_{\text{accept}}(B)}{P^B_{\text{accept}}(A)} = \frac{W(B)}{W(A)}$$



Two commonly used acceptance probabilities

Metropolis: $P^A_{\text{accept}}(B) = \min\left[\frac{W(B)}{W(A)}, 1\right]$

Heat bath: $P^A_{\text{accept}}(B) = \frac{W(B)}{W(A) + W(B)}$

Easy to see that these satisfy detailed balance

The ratios involve the change in energy when a spin has been flipped (or, more generally, when the state has been updated in some way)

Metropolis algorithm for the Ising model

$$E = J \sum_{\langle i,j \rangle} \sigma_i \sigma_j, \quad \sigma_i = \pm 1$$

Spin update

- Select a spin at random
- Calculate the change in energy if the spin is flipped
- Use the energy change to calculate the acceptance probability P
- Flip the spin with probability P; stay in old state with 1-P
- Repat from spin selection

Current configuration: S

Configuration after flipping spin j: $\tilde{S}_j$

Acceptance probability: $P(S \to \tilde{S}_j) = \min\left[\frac{W(\tilde{S}_j)}{W(S)}, 1\right]$

$$W(S) = \mathrm{e}^{-E(S)/T} = \mathrm{e}^{-\frac{J}{T}\sum \sigma_i \sigma_j} = \prod \mathrm{e}^{-\frac{J}{T}\sigma_i \sigma_j}$$

Only factors containing spin j survive in W-ratio

$$\frac{W(\tilde{S}_j)}{W(S)} = \exp\left[+\frac{2J}{T}\sigma_j \sum_{\delta(j)} \sigma_{\delta(j)}\right], \quad \delta(j) = \text{neighbor of } j$$

We want a simulation “time” unit which is normalized by the system size N (probability of a given spin having been selected after a time unit should be N independent).

1 Monte Carlo step (MC steps): N random spin-flip attempts

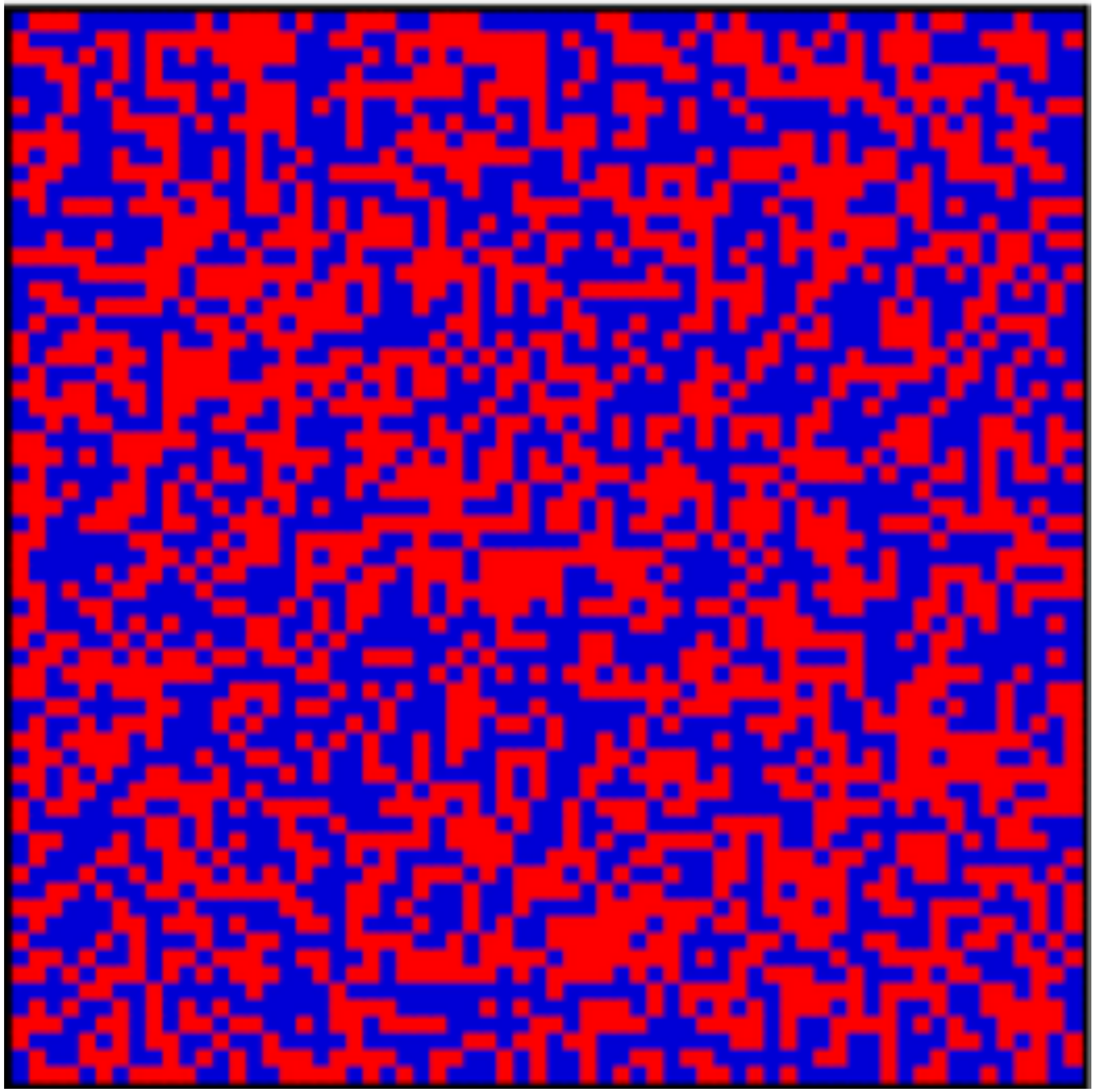
Measurements of physical observables done after **equilibration**
➢ the correct Boltzmann distribution is approached after some time that depends on the initial configuration

Binning: Accumulate data over bins consisting of M MC steps
➢ Averages and statistical errors calculated from bin averages

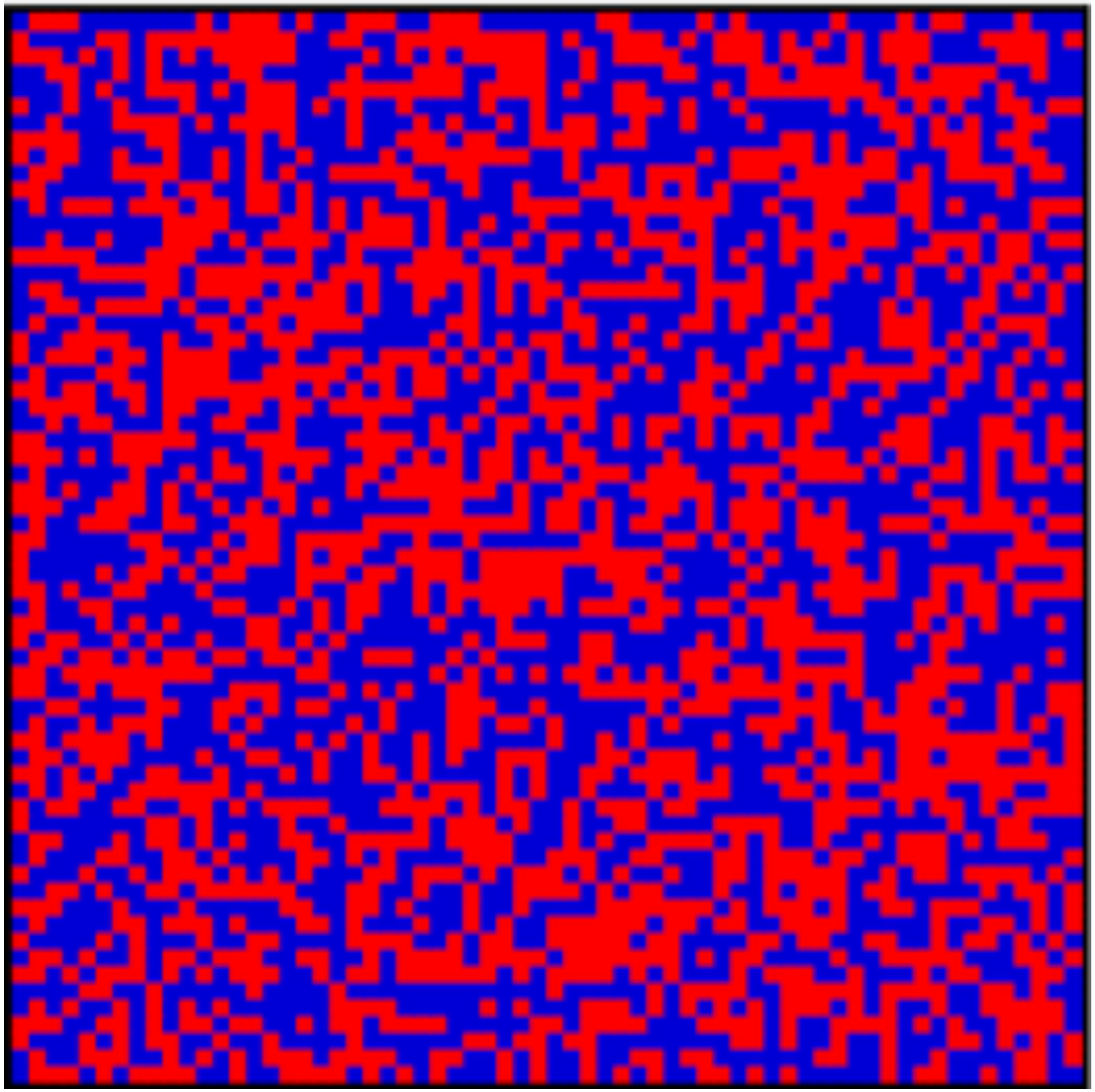
Flow of a complete simulation

- Generate arbitrary starting state
- Carry out a number of MC steps for equilibration
- Carry out a number of bins
  - each bin consists of M MC steps
  - measurements done after every (or every few) MC step
  - save bin averages in a file after each bin (or save internally in program)
- Calculate averages and statistical errors

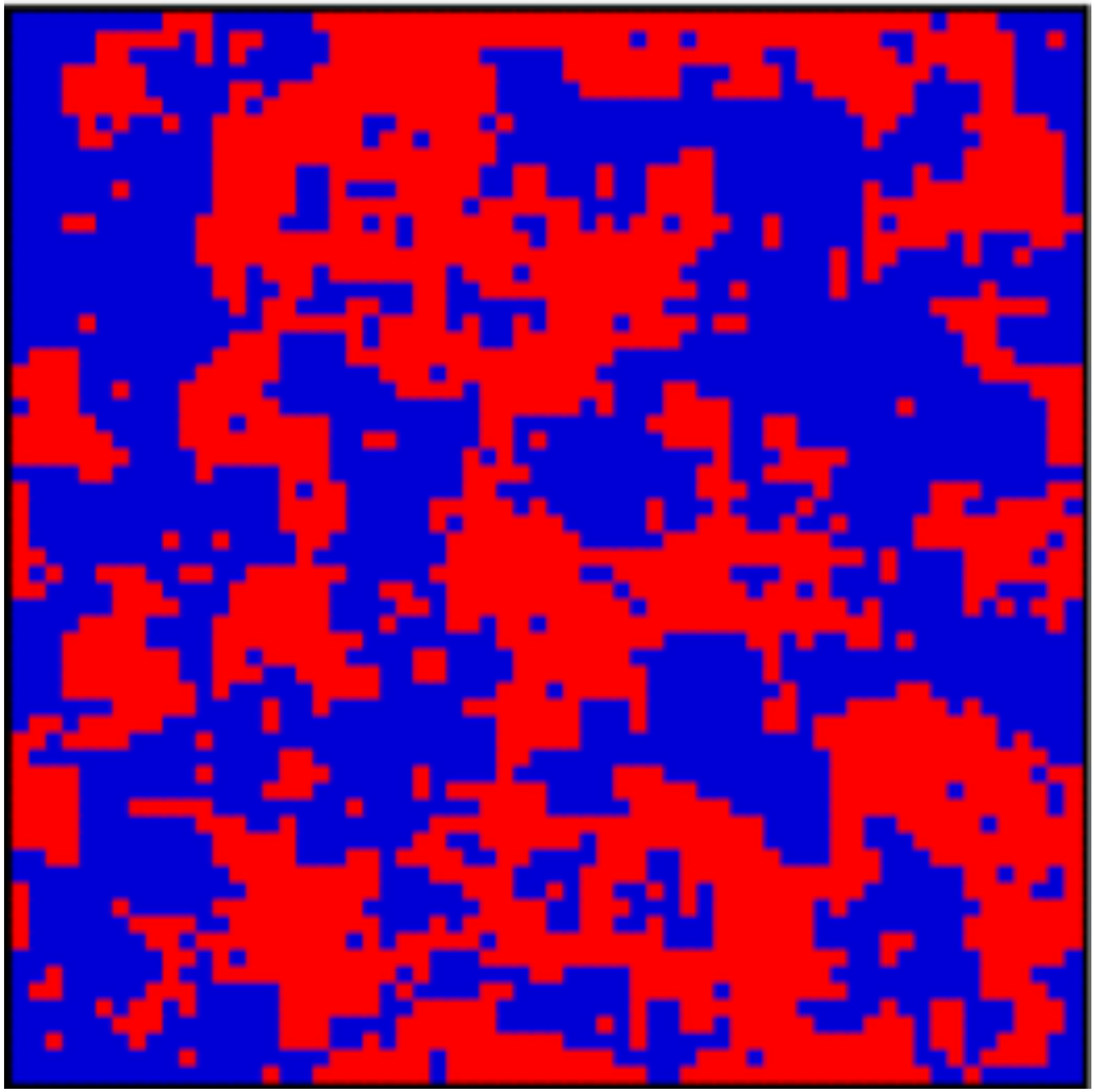
T = 4.00 1



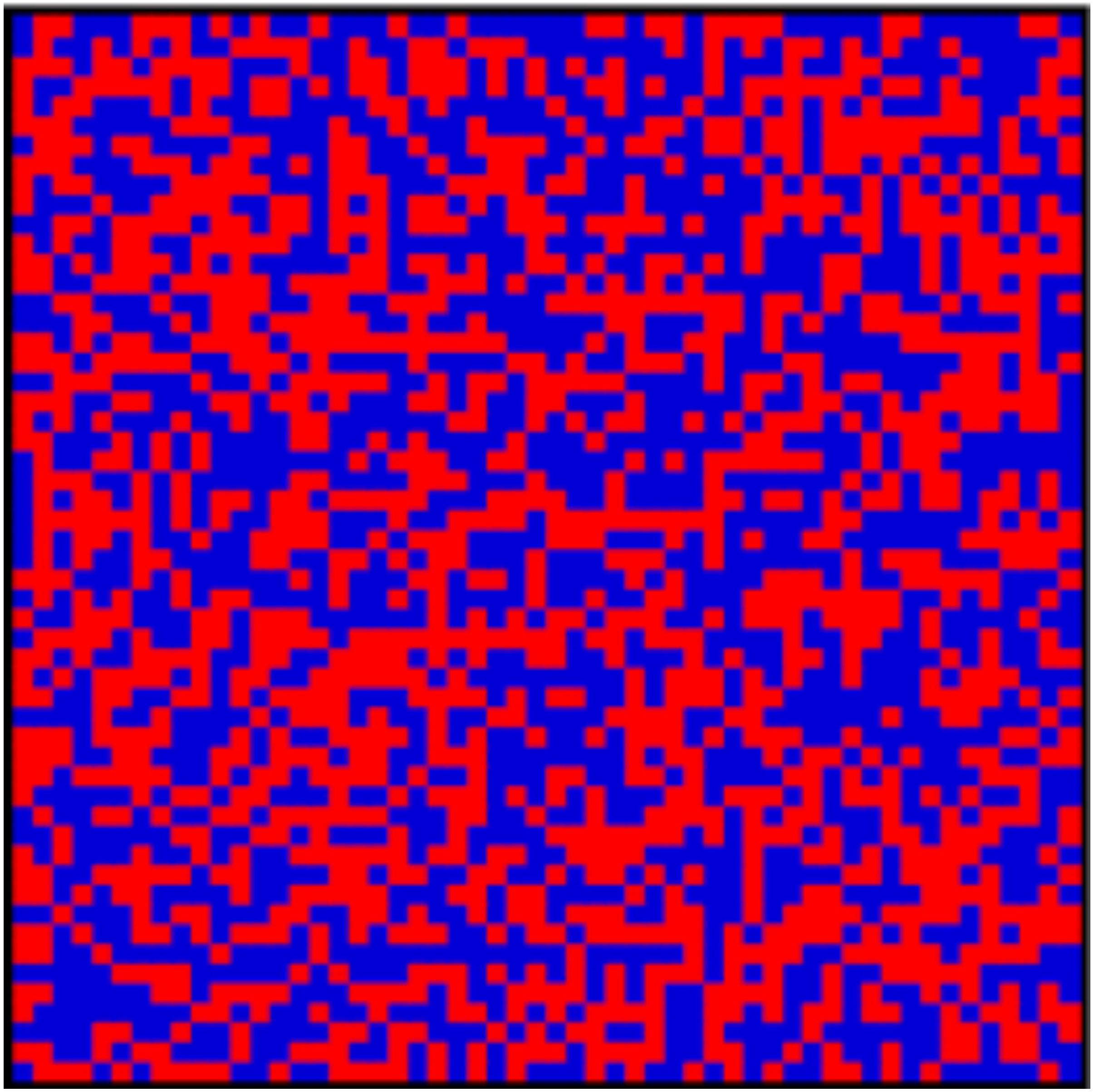
T = 2.30 1



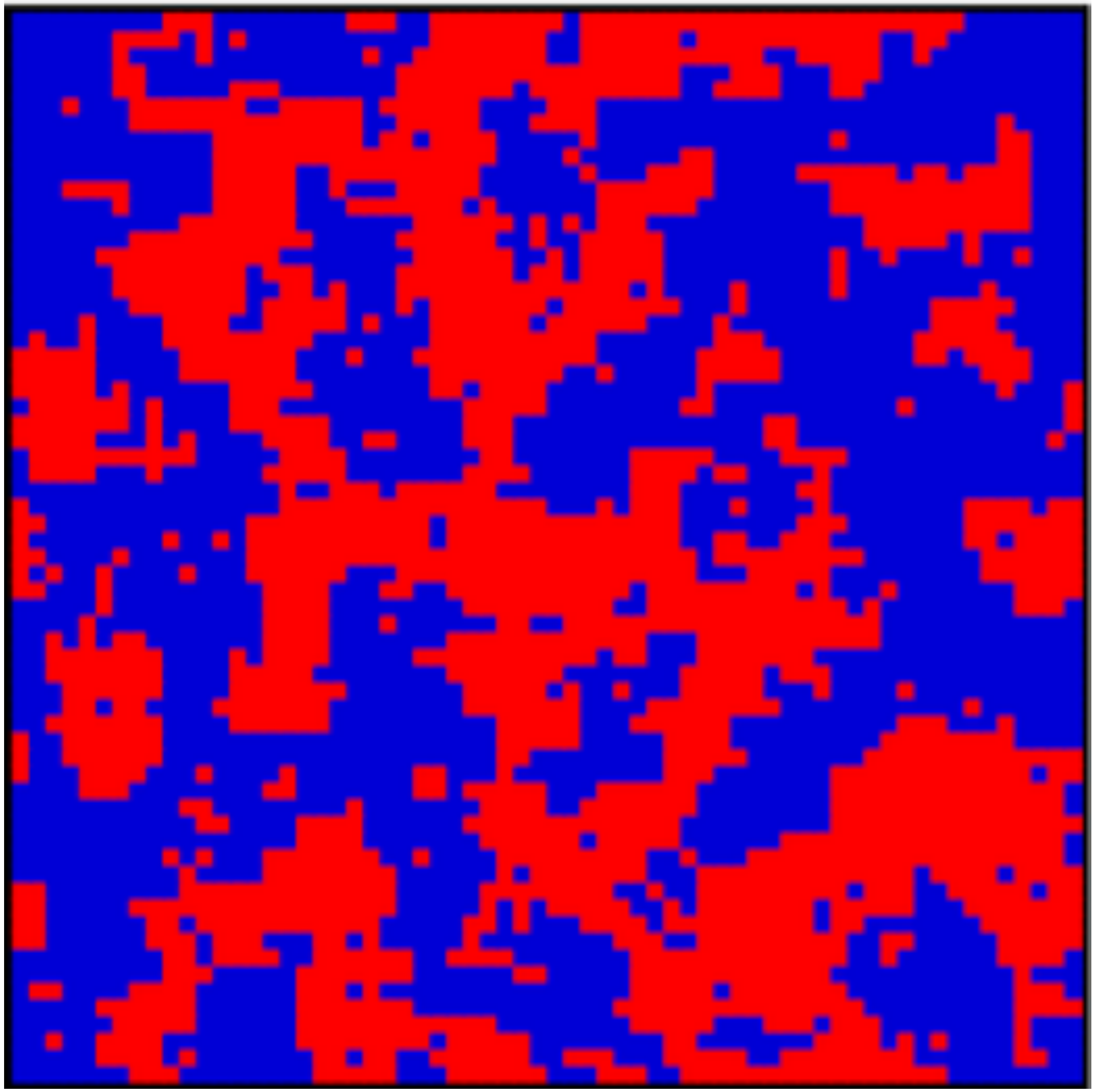
T = 2.30 10



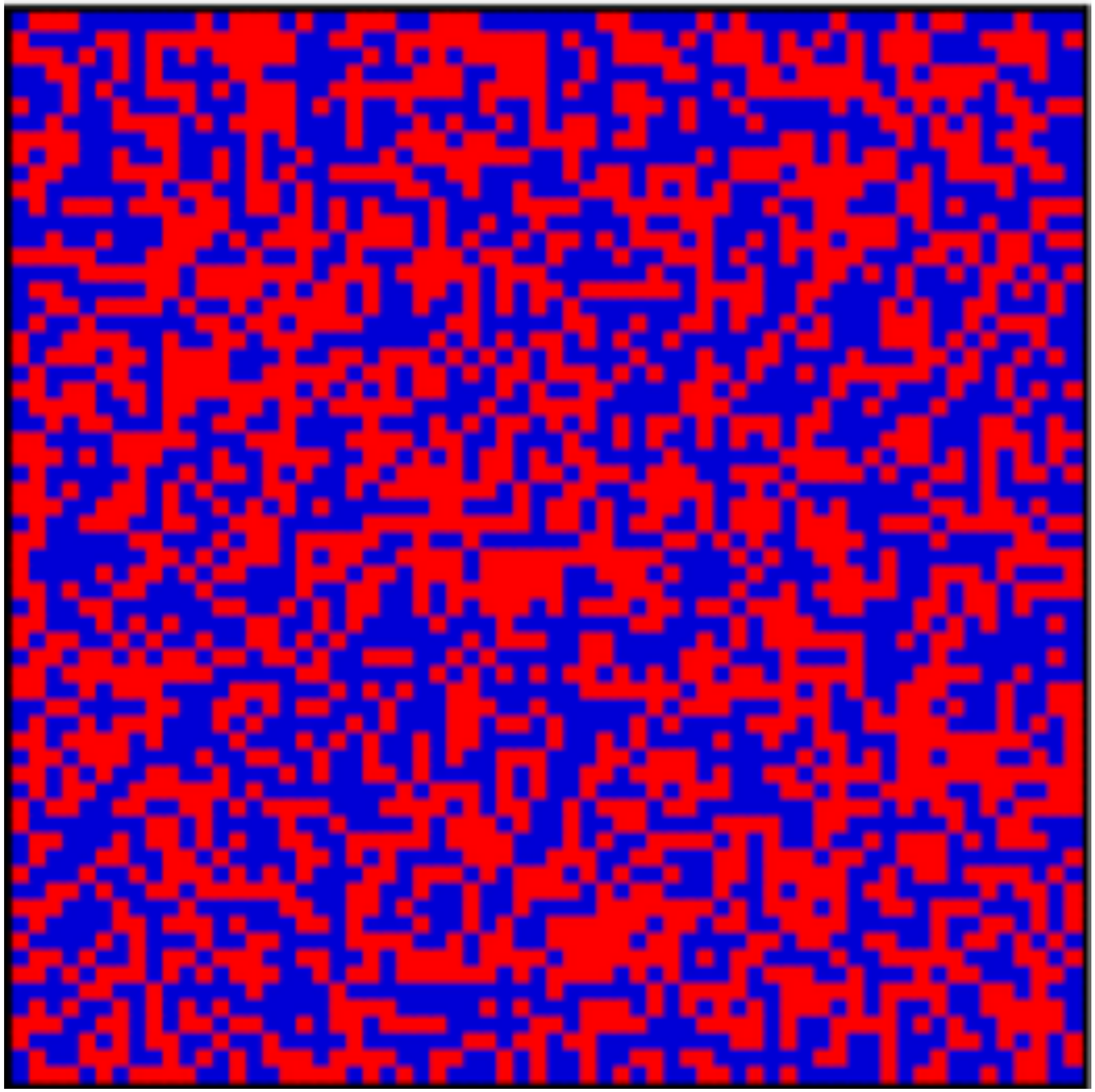
T = 2.00 1



T = 2.00 10



T = 1.00 1



T = 1.00 10

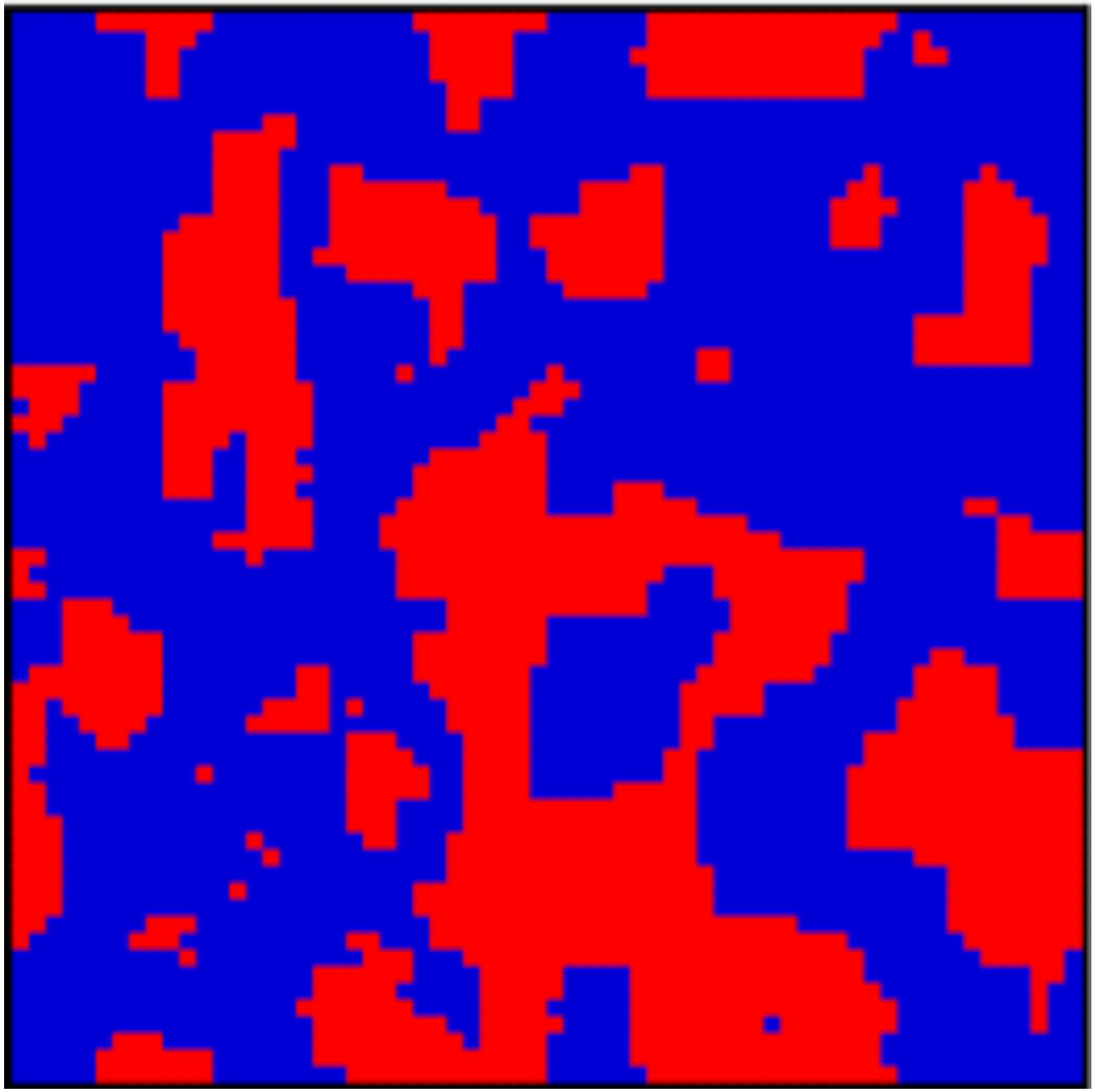
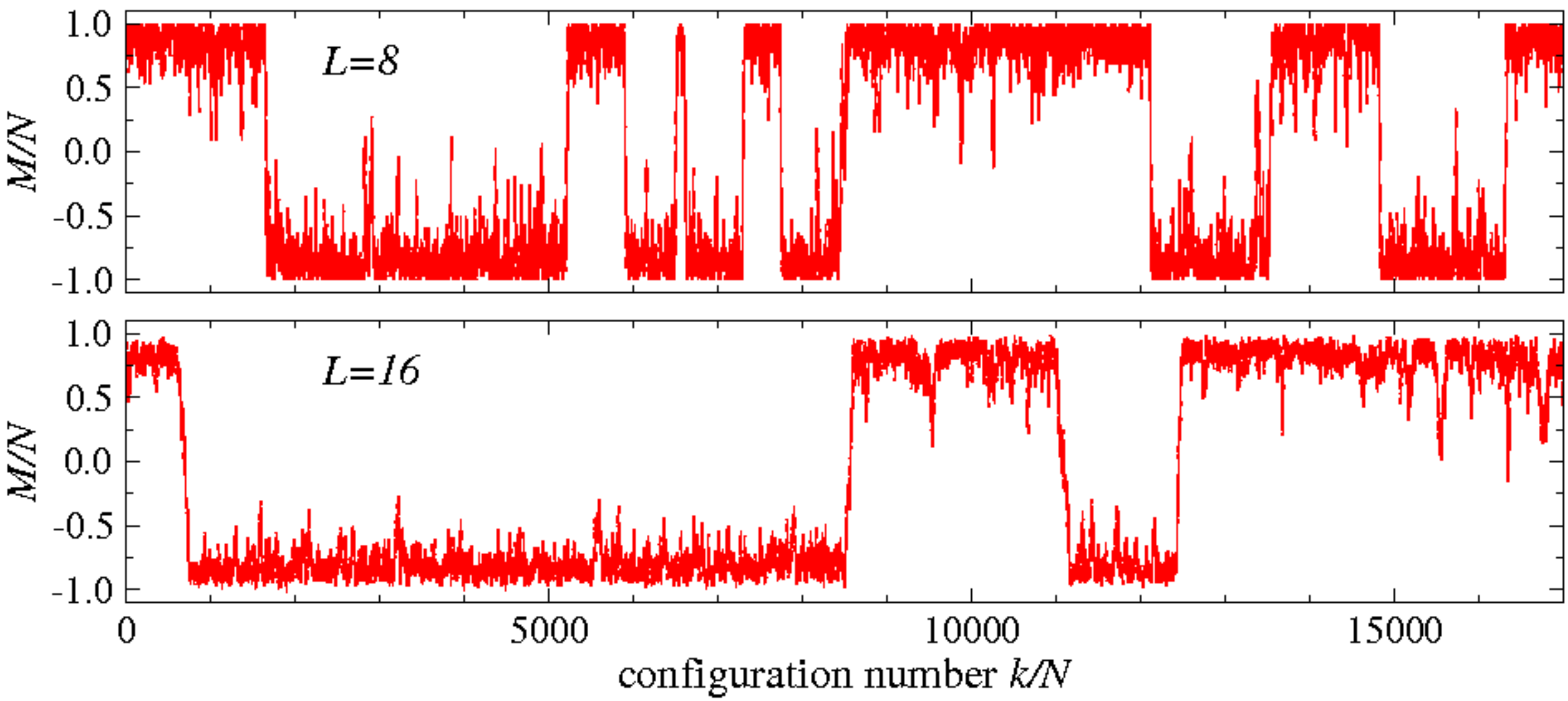


Illustration of simulation

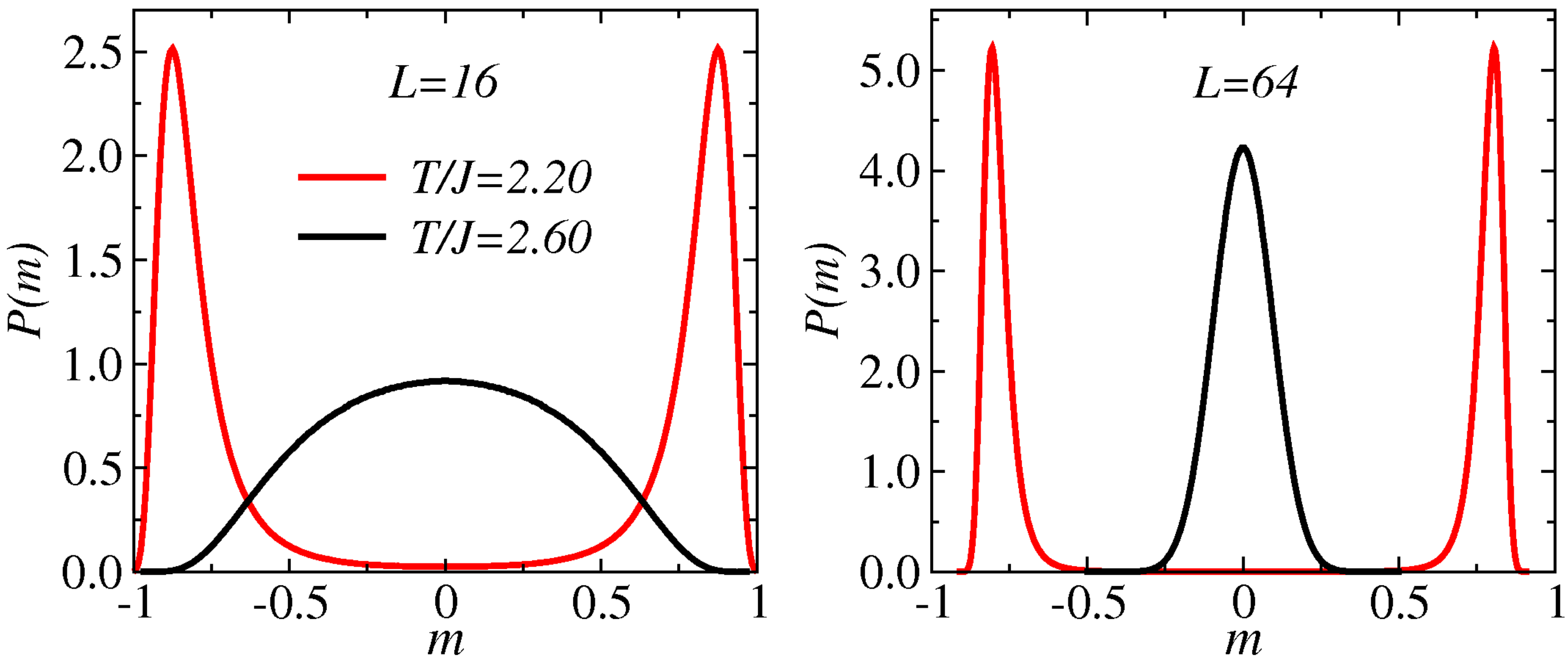
Evolution of the magnetization, 2D Ising model, T/J=2.2 (below Tc)

- <M>=0, but time scale for M-reversal increases with L
- Symmetry-breaking occurs in practice for large L



Magnetization distribution P(m)

The distribution depends on T and L
- single peak around m=0 for T>Tc
- double peak around +<m> and-<m> for T<Tc



Symmetry breaking (sampling of only m>0 or m<0 states) occurs in practice for large L
- because extremely small probability to go between them