Computational Physics 2023

Sommersemester, 3th April, 2023 – 14th Juli, 2023

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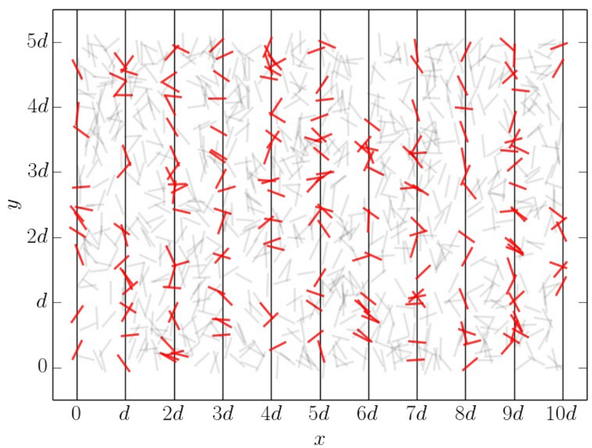
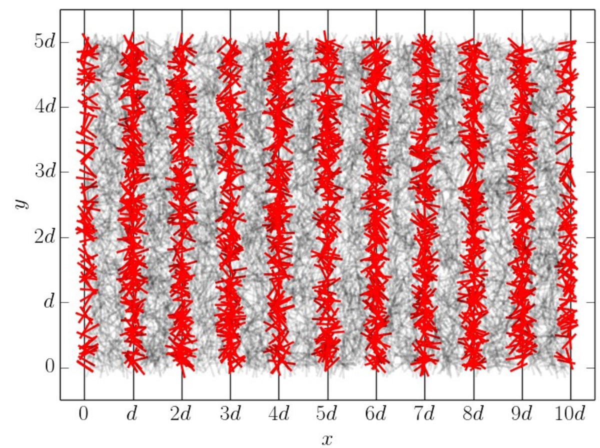
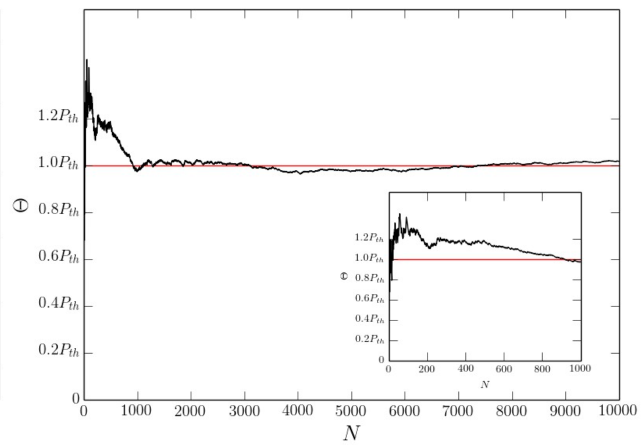
Buffon needle experiment:







MC Integration

Buffon's needle experiment [1] was originally used to provide π. Throwing a needle (see **Figure 1**) onto a flat plane with equally-spaced parallel lines, the probability that the needle touches the parallel line provides an estimate for π is

$$P = \frac{\int_0^{\pi} \frac{l}{2} \sin\theta d\theta}{\pi d/2} \tag{1}$$

and so

$$\pi = \frac{2l}{Pa} \tag{2}$$

where P is the probability, l the length of the needle and a the spacing with $l < a$.

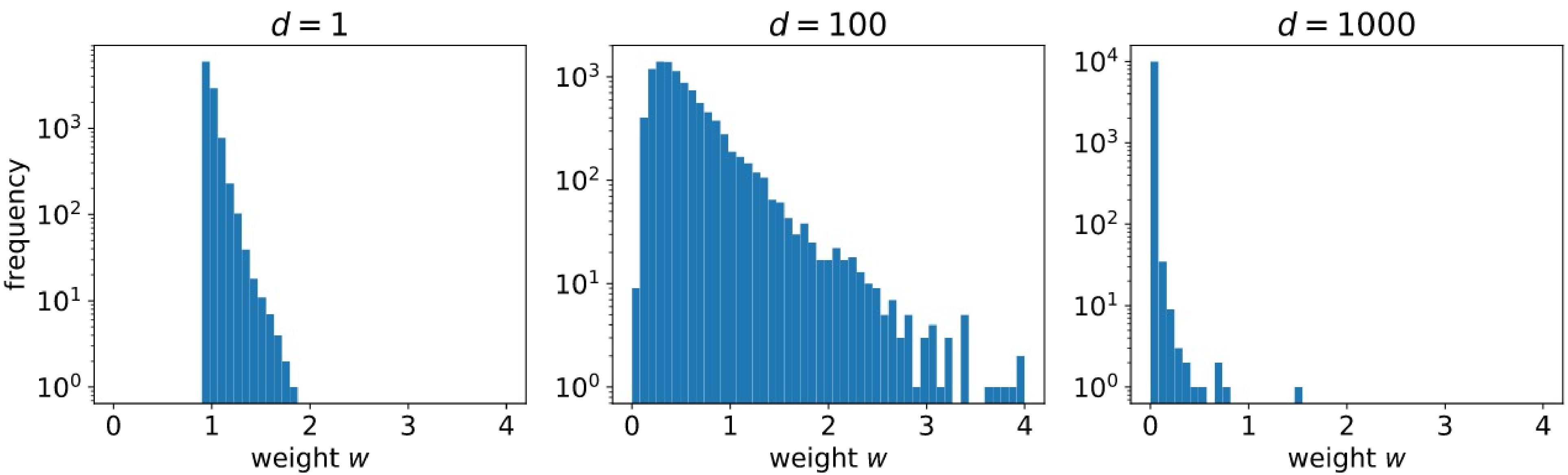
MC Integration (High dimensions)

$$\int p_{\mathrm{real}}(R)A(R)dR \approx \frac{1}{N}\sum_{i=1}^{N} w(R_i)A(R_i)$$

$$p(R_1,\ldots,R_d) = (2\pi\sigma)^{d/2} e^{-\frac{\sum_{k=1}^{d} R_k^2}{2\sigma}}$$

$$\sigma_{real} = 1 \qquad \sigma_{sample} = 0.9$$

N=10000

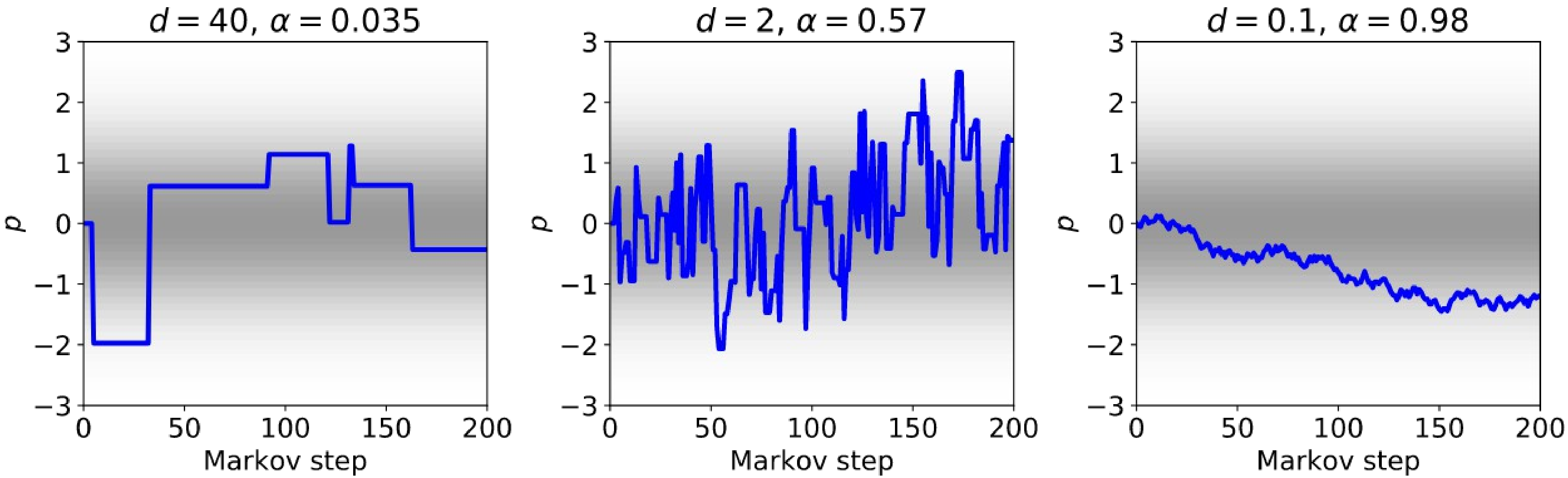


MC Integration

$$x' = x + d \times \text{random number between -1 and 1}$$

$$p(x) = (2\pi\sigma)^{1/2} e^{-x^2/2\sigma} \qquad A_{xx'} = \begin{cases} 1 & \text{if } p(x') > p(x) \\ \frac{p(x)}{p(x')} & \text{if } p(x') < p(x) \end{cases}$$

$$\alpha = \frac{\text{number of accepted moves}}{\text{number of total moves}}$$



"Critical slowing down"

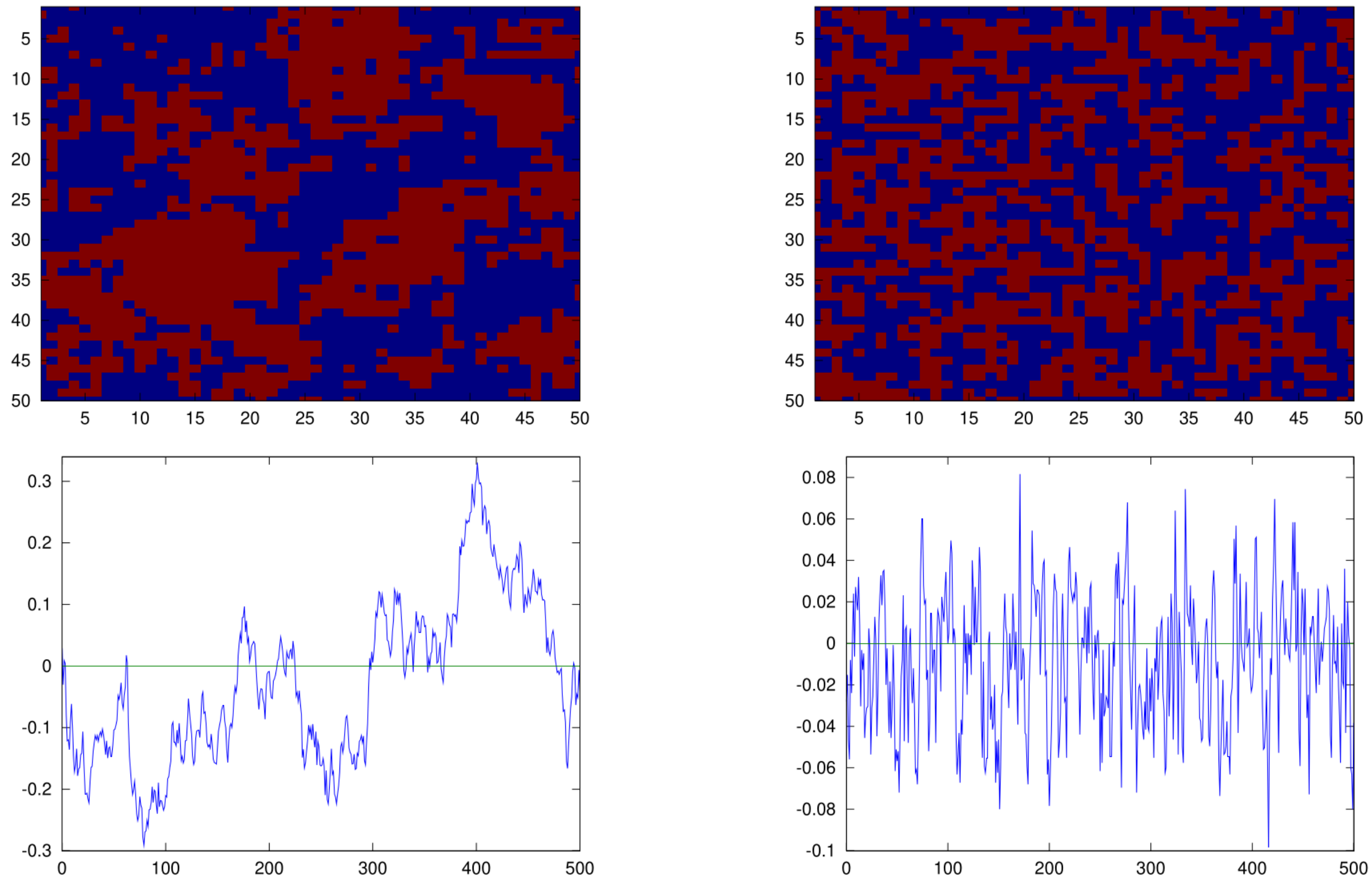
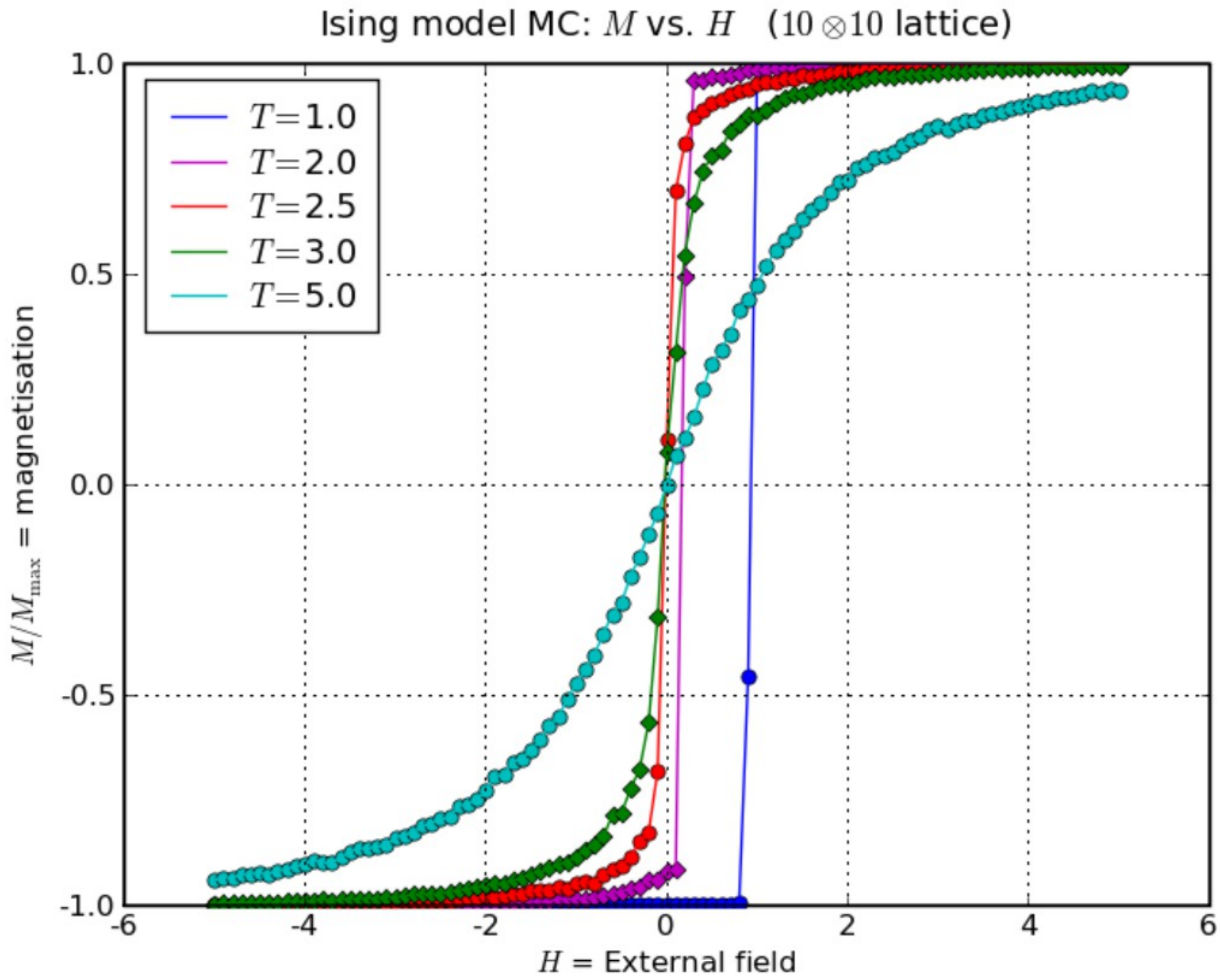
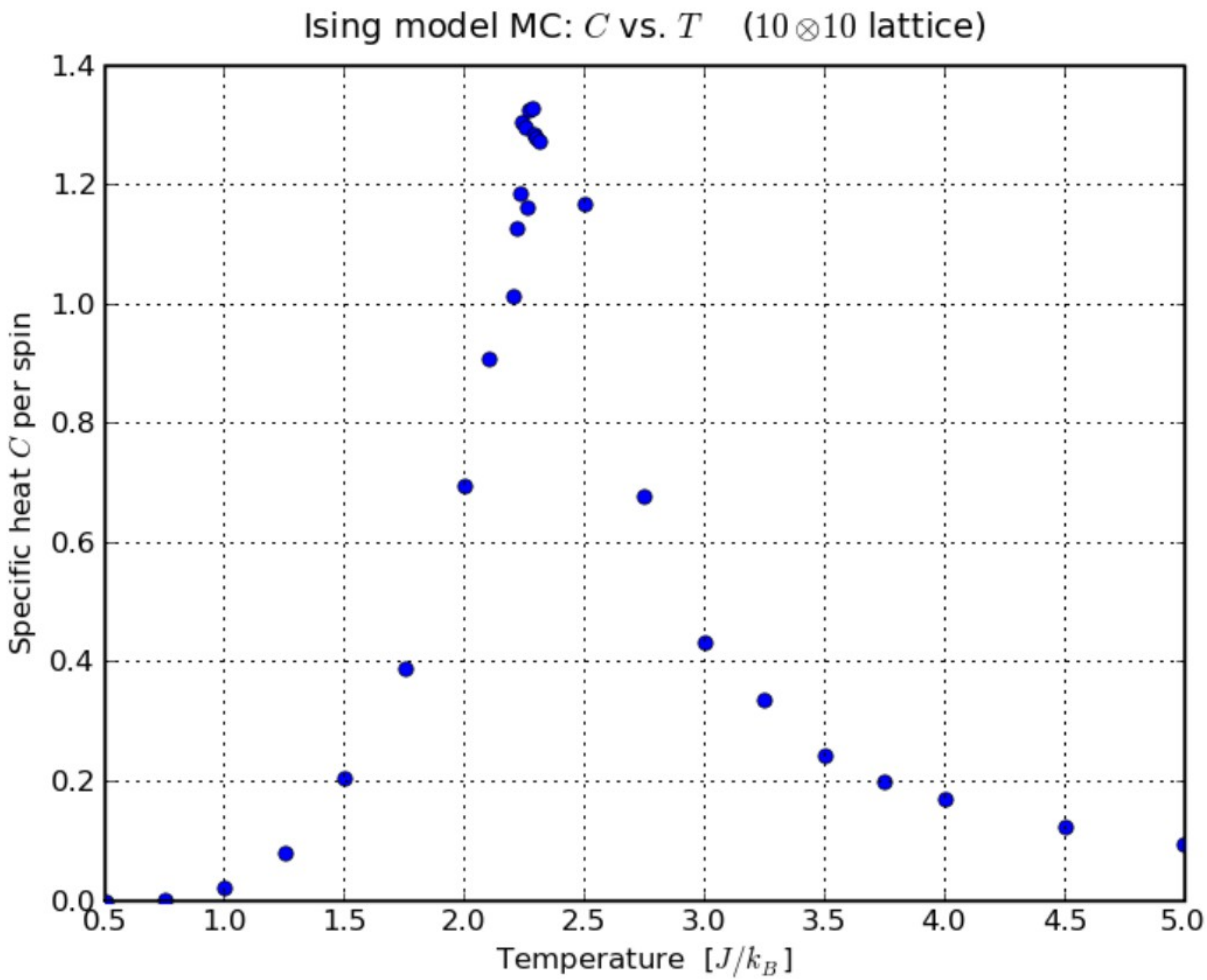


Figure 4: Typical spin configurations (top) and magnetization vs. time plots (bottom) for the Metropolis algorithm for the Ising model. Left: $T = 2.5$, Right: $T = 5$. Spins arrange in clusters which are bigger close to the critical temperature $T_c \approx 2.26$. Note also an increase of the autocorrelation time in the vicinity of T_c.

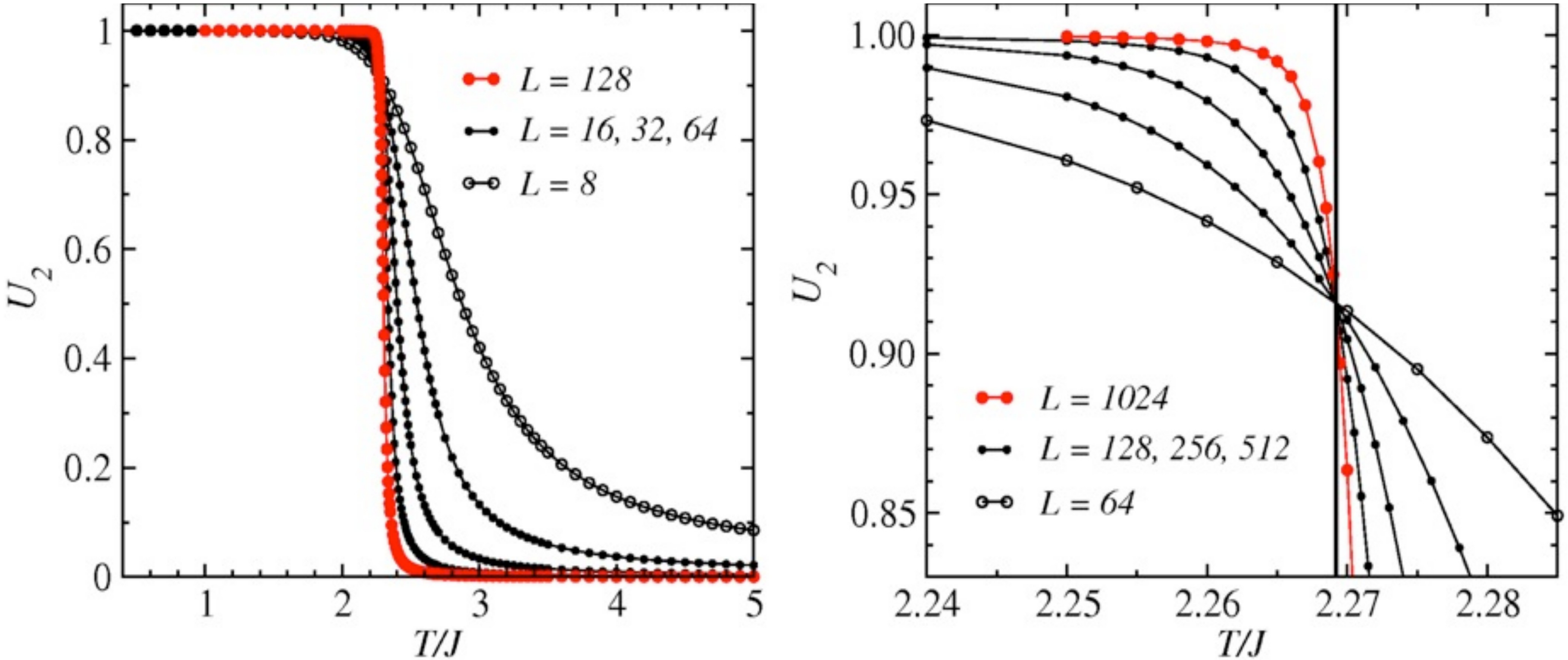
First order phase transition



Finite size effects



Binder Cumulant: Determination of Tc



$$U = \frac{1}{2}\left(3 - \frac{\langle m^4 \rangle}{\langle m^2 \rangle^2}\right)$$

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