Lectures on Quantum Monte Carlo Methods

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Progression of Lectures

1. *Stochastic Integration*
2. *Random Numbers*
3. ***Classical Statistical Mechanical Simulations***
4. *Cluster algorithms for classical models*
5. *Quantum Monte Carlo*
6. *The continuum limit*
7. *Observables and Estimators*
8. *Finite-size scaling*
9. *More about the correlation length*
10. *Survey of other applications*

3. Classical Statistical Mechanical Simulations

Or, shortcomings of the Metropolis method...

Partition function generates statistical mechanical observables

- probability of state μ: $p_\mu \propto \exp\left(-\beta E_\mu\right),\ \beta = 1/T$
- sum over states $Z \equiv \sum_\mu \exp\left(-\beta E_\mu\right)$ ("partition function")
- $\exp\left(-\beta F\right) = \sum_\mu \exp\left(-\beta E_\mu\right) \Rightarrow F = -T \ln Z$ ("free energy")
- expectation $\langle Q \rangle = \sum_\mu Q_\mu p_\mu = \frac{1}{Z} \sum_\mu Q_\mu \exp\left(-\beta E_\mu\right)$
- $U = \langle E \rangle = \frac{1}{Z} \sum_\mu E_\mu \exp\left(-\beta E_\mu\right) = -\frac{1}{Z}\frac{\partial Z}{\partial \beta} = -\frac{\partial \ln Z}{\partial \beta}$

Couplings to conjugate fields enable measurements

- H contains $-XY \Rightarrow \langle X \rangle = \frac{1}{\beta Z}\frac{\partial Z}{\partial Y} = -\frac{\partial F}{\partial Y}$

  ⇨e.g. X=magnetization M and Y= field B

- $-\frac{1}{\beta}\frac{\partial^2 F}{\partial Y^2} = \frac{1}{\beta}\frac{\partial \langle X \rangle}{\partial Y} = \langle X^2 \rangle - \langle X \rangle^2$

  $\Leftrightarrow$ fluctuations from 2nd derivative

- $\chi \equiv \frac{\partial \langle X \rangle}{\partial Y}$ ("susceptibility") “Linear response theorem”

  $\Leftrightarrow$ fluctuations $\propto$ susceptibility

Correlation functions from local fields

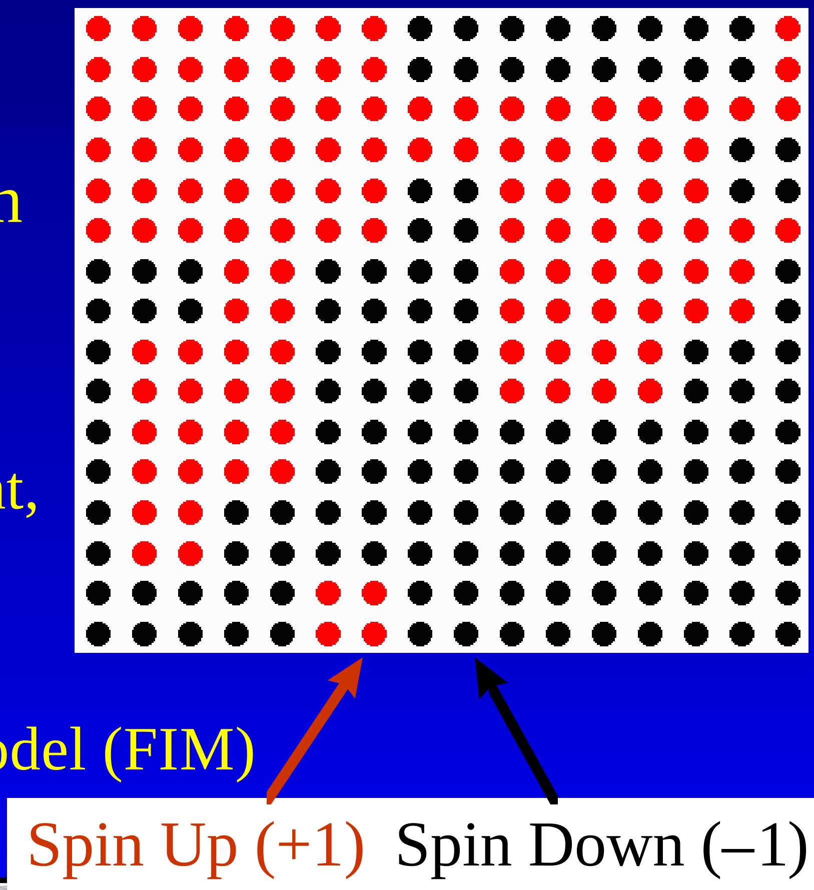
- Promote Y to local field Y_{i}
- Promote X to (intensive) local observable x_{i}
- Let H contain $-\Sigma\, x_i Y_i$

$$G_c^{(2)}(i,j) \equiv \left\langle \left(x_i - \langle x_i \rangle \right)\left(x_j - \langle x_j \rangle \right) \right\rangle = \langle x_i x_j \rangle - \langle x_i \rangle \langle x_j \rangle$$

$$= \frac{1}{\beta^2} \frac{\partial^2 \ln Z}{\partial Y_i \partial Y_j} = \frac{1}{\beta^2 Z} \frac{\partial^2 Z}{\partial Y_i \partial Y_j} - \left(\frac{1}{\beta Z} \frac{\partial Z}{\partial Y_i} \right)\left(\frac{1}{\beta Z} \frac{\partial Z}{\partial Y_j} \right)$$

Ising model:
The mother of all lattice models

- $H = \sum_{\langle ij \rangle} J_{ij} s_i s_j - B \sum_{s_i} s_i$
- $s_i = \pm 1, \; J_{ij} =$ coupling strength
- $\langle ij \rangle =$ nearest-neighbor i, j
- Often we take $J_{ij} = -J =$ constant,
- $H = -J \sum_{\langle ij \rangle} s_i s_j - B \sum_{i} s_i$
- $J > 0 \Rightarrow$ ferromagnetic Ising model (FIM)



2d FIM exhibits phase transition

- Spins aligned ⇔ low energy
- Anti-aligned ⇔ high energy
- Low T: ordered
- High T: disordered
- Critical : $T_c = 2J/\ln\left(1+\sqrt{2}\right)$
  $= 2.269\,J$

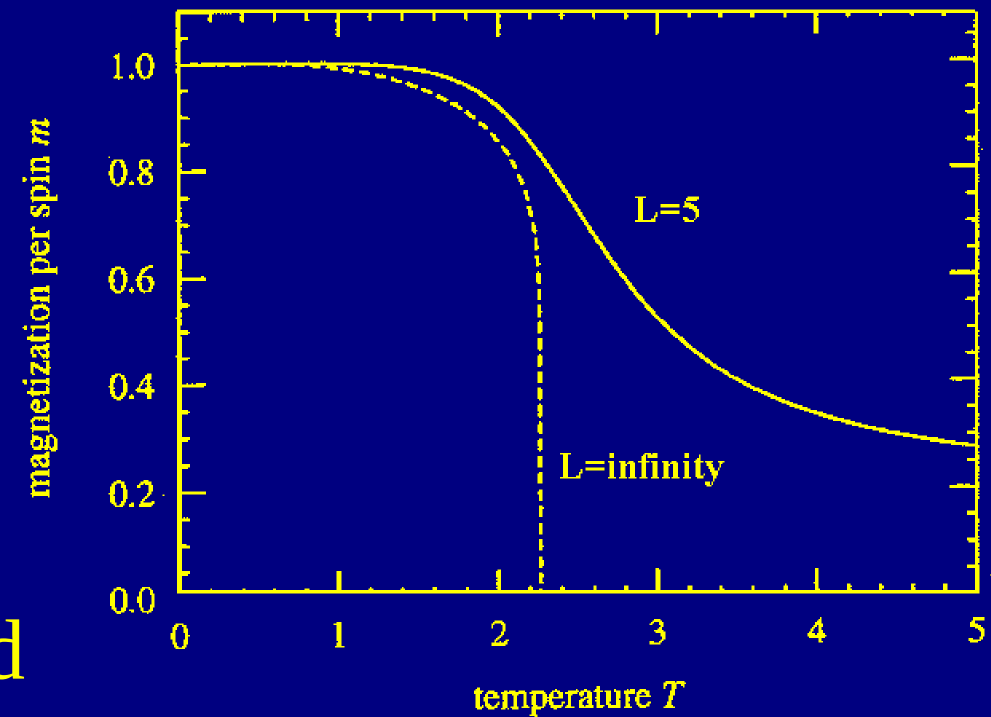


Fig 1.1 from
Newman & Barkema

2dFIM explicit calculation only feasible for small L

- $Z = \sum_{\mu} \exp\left(-\beta \left(J \sum_{\langle ij \rangle} s_i s_j - B \sum_i s_i \right) \right)$ has 2^{L^2} terms
- $2^{25} = 33{,}554{,}432$ but $2^{36} = 68{,}719{,}476{,}736$
- **Sounds like a job for Monte Carlo**
- Note: Onsager solved 2dFIM exactly for L→∞ (“thermodynamic limit”)

First try: Metropolis sampling with Boltzmann weights

- Example: measure magnetization
- $\langle |m| \rangle = \frac{1}{Z} \sum_{\mu} |m| \exp(-\beta H)$
- Use Boltzmann weight as sampling function
  - ⇨Pick a spin site at random
  - ⇨Test flip + ⇔ –
  - ⇨If energy decreases, accept flip
  - ⇨If energy increases, accept with $p = \exp(-\beta \Delta H)$

Example program: 2dSpin.exe

- 100x100 spins, $0 < T < 2T_c$, staggered start
- 1 Monte Carlo "sweep"$=100^2$ flips
- Current configuration magnetization per spin *m* shown on meter

Ctrl-Shift-S

Noteworthy

- Low T: ordered, large domains
- High T: disordered, small domains
- Simulation may start far from an equilibrium configuration
  - ⇨"thermalization period" may be needed
- Metropolis produces highly correlated series of measurements
  - ⇨Long "autocorrelation time"

Thermalization of Metropolis algorithm for 2dFIM

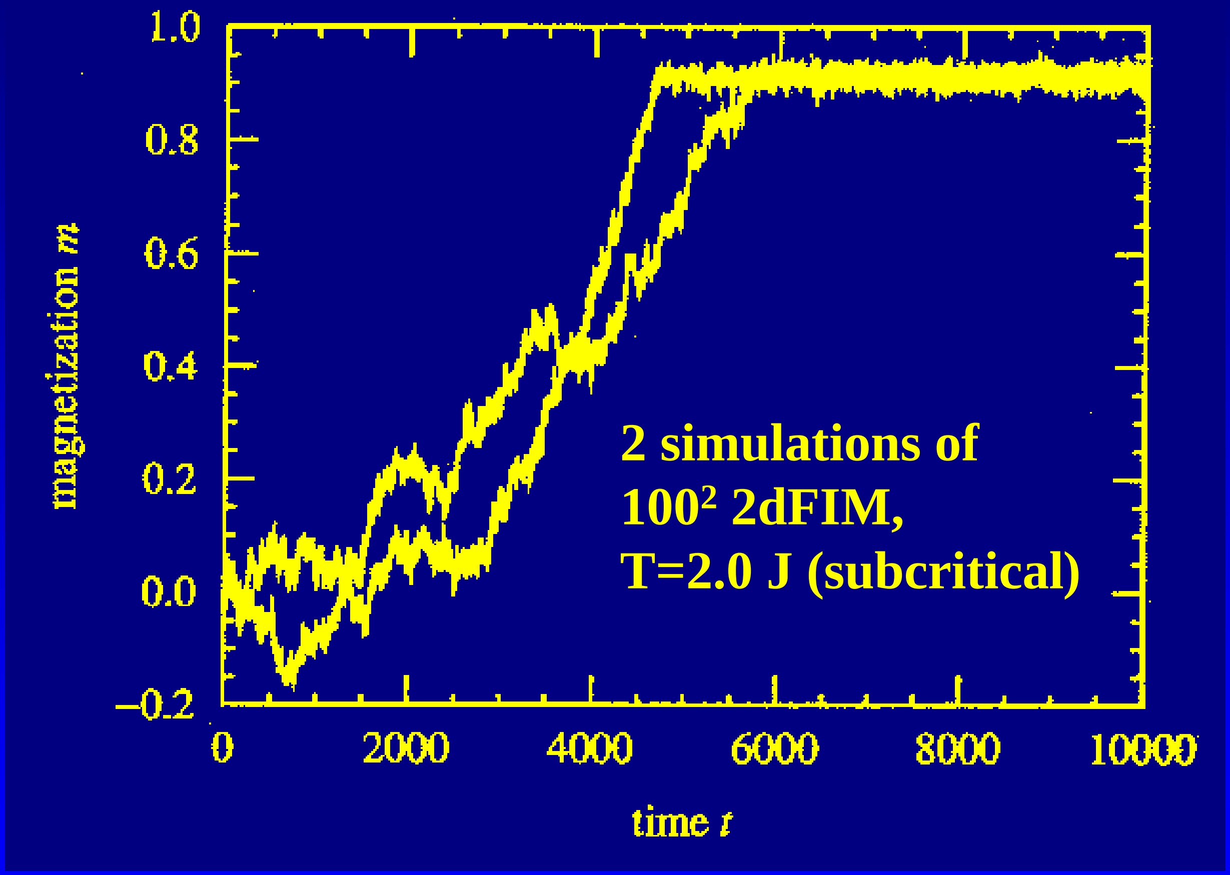
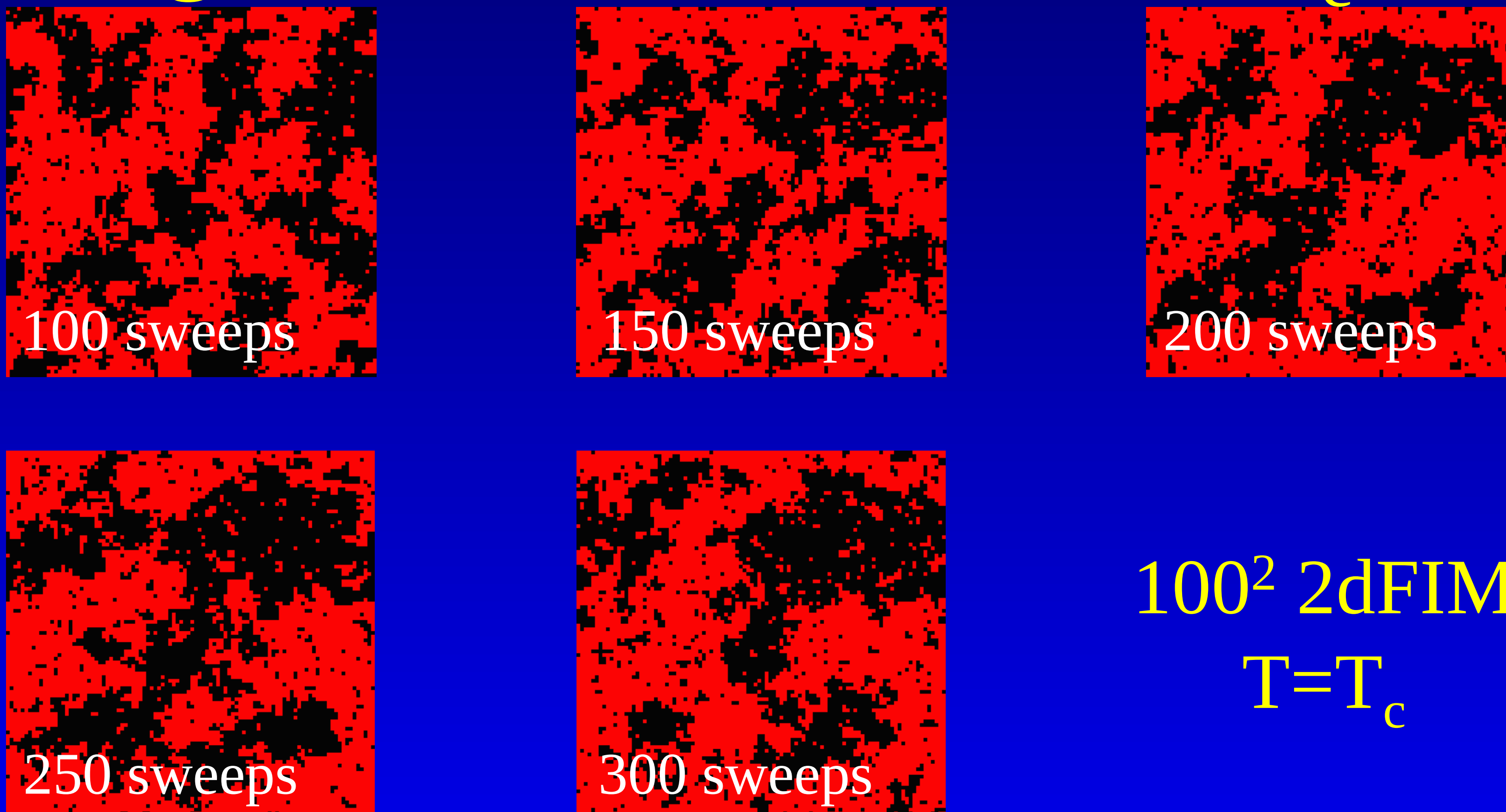


Fig 3.4 from
Newman & Barkema

Metropolis algorithm exhibits long autocorrelation time at T_c



100^2 2dFIM

$T=T_c$

Autocorrelation time τ measures evolution of MC series

- Autocorrelation function for observable A

$$C_{AA}(t) \equiv \langle A_s A_{s+t} \rangle - \langle A \rangle^2$$

- Decays with "exponential autocorrelation time"

$$C_{AA}(t) \propto \exp\left(-t/\tau_{\exp,A}\right)$$

- Related to "integrated autocorrelation time"

$$\tau_{\mathrm{int},A} \equiv \frac{1}{2} \sum_{t=-\infty}^{+\infty} C_{AA}(t)/C_{AA}(0)$$

Example autocorrelation function

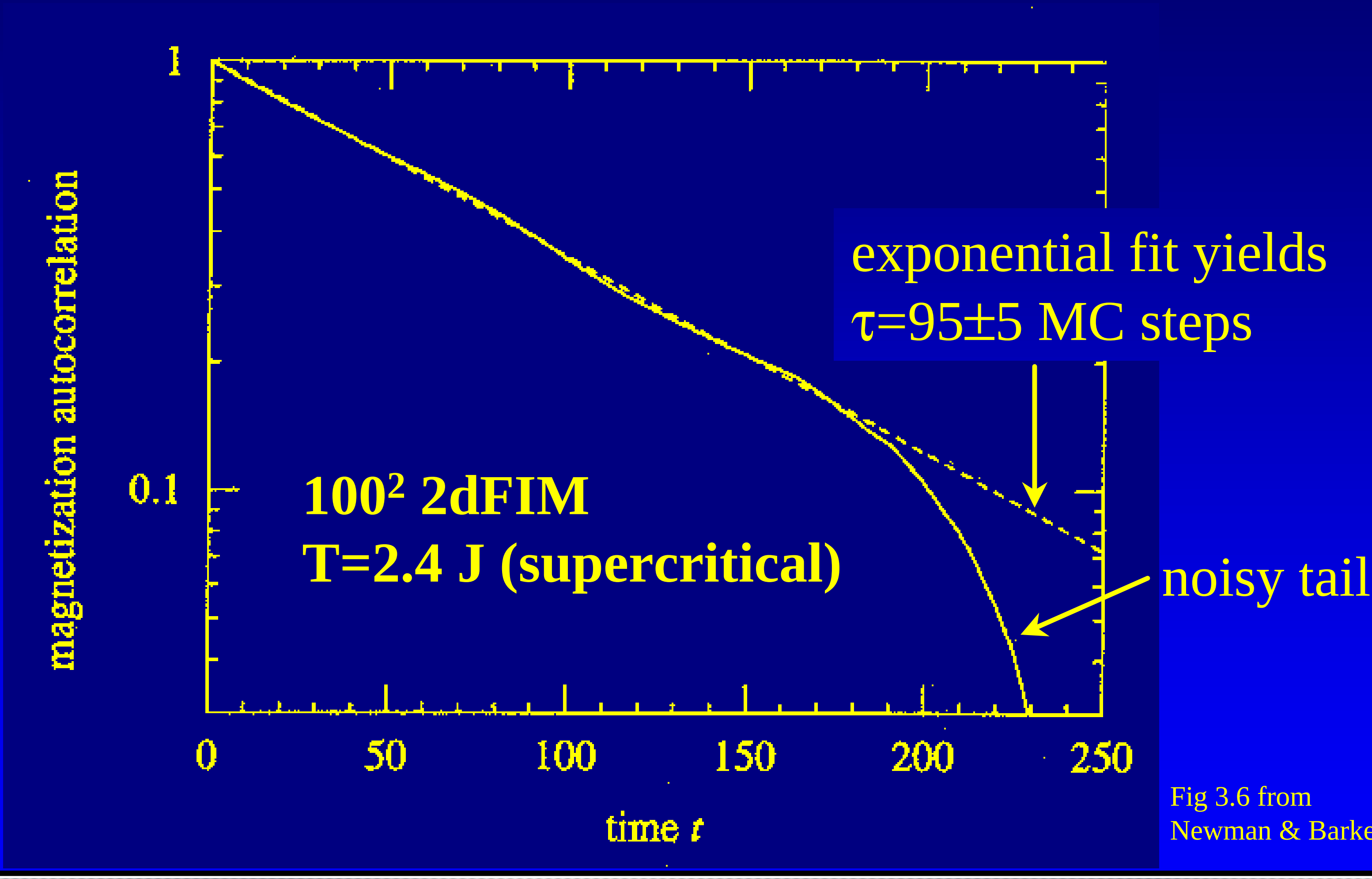


Fig 3.6 from Newman & Barkema

CPU time ∝ autocorrelation time

- Finite samples are used to estimate <A>

$$\overline{A} = \frac{1}{n}\sum_{t=1}^{n} A_t$$

- Naïve variance of estimate for <A>

$$\left(\delta \overline{A}_{naive}\right)^2 = \frac{1}{n} C_{AA}(0)$$

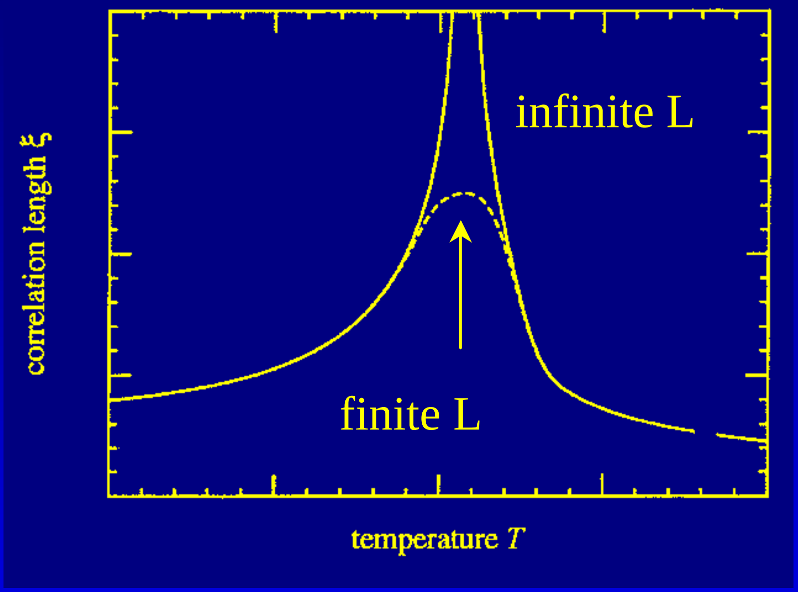
- $\tau_{\text{int},A}$ governs actual uncertainty

$$\left(\delta \overline{A}\right)^2 = 2\tau_{\text{int},A}\left(\delta \overline{A}_{naive}\right)^2 = 2\frac{\tau_{\text{int},A}}{n} C_{AA}(0)$$

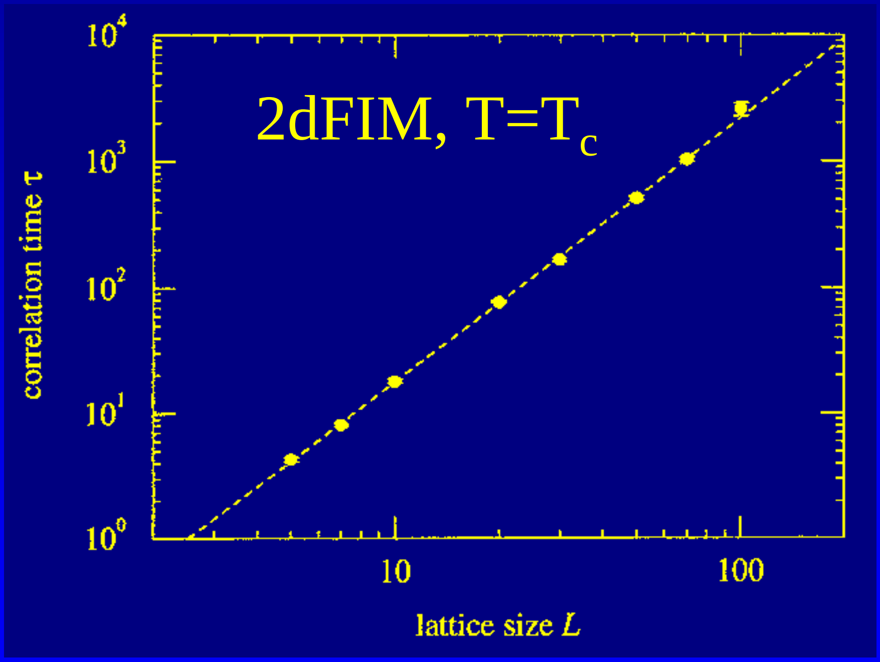
↖ µ **CPU time**

Finite-size effects keep τ, ξ finite

Correlation length ξ vs T



Autocorrelation time τ vs T



Figs 4.1-2 from
Newman & Barkema

Autocorrelation τ for 2dFIM exhibits jump near $T=T_c$

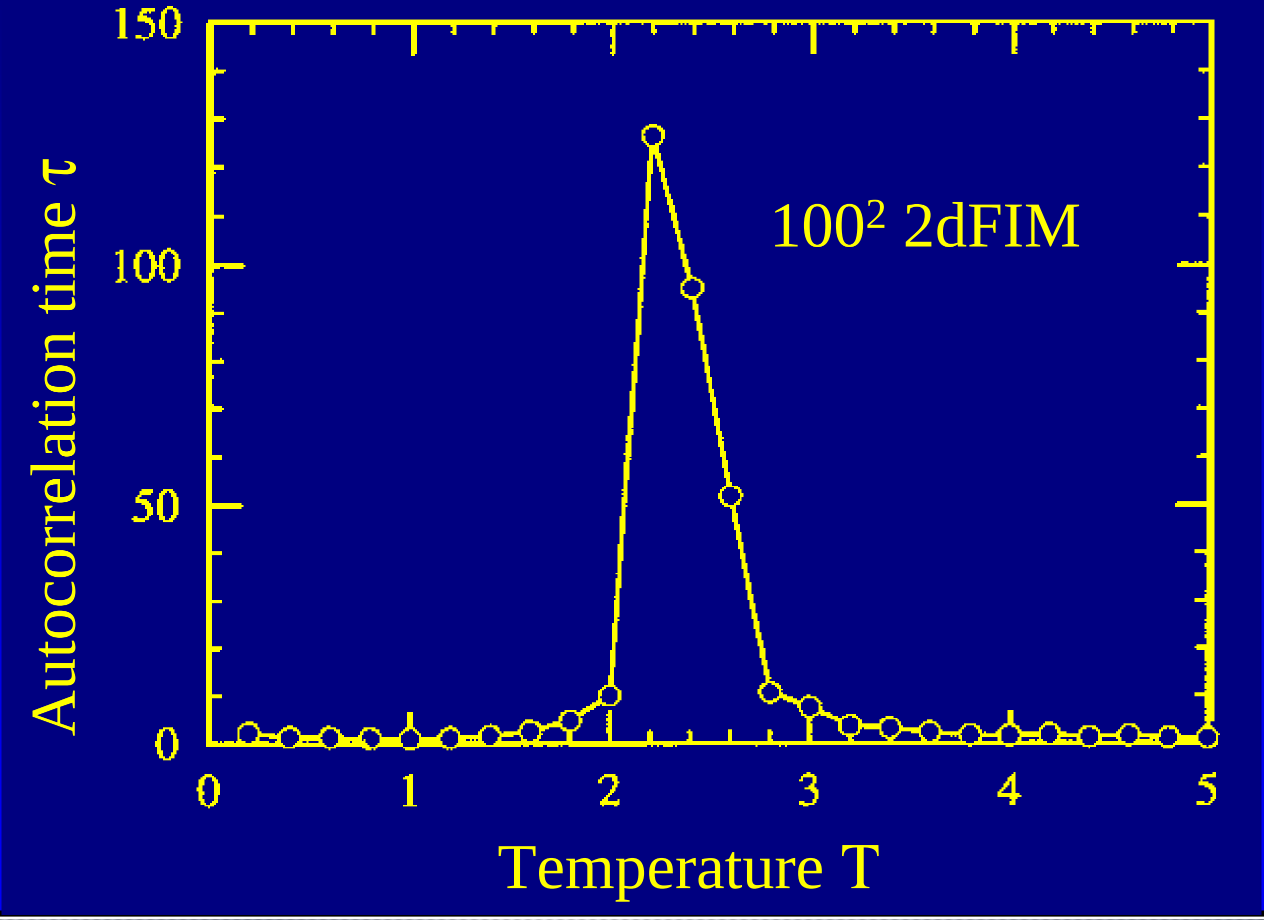


Fig 3.8 from
Newman & Barkema

Bad news: Metropolis τ blows up near critical point

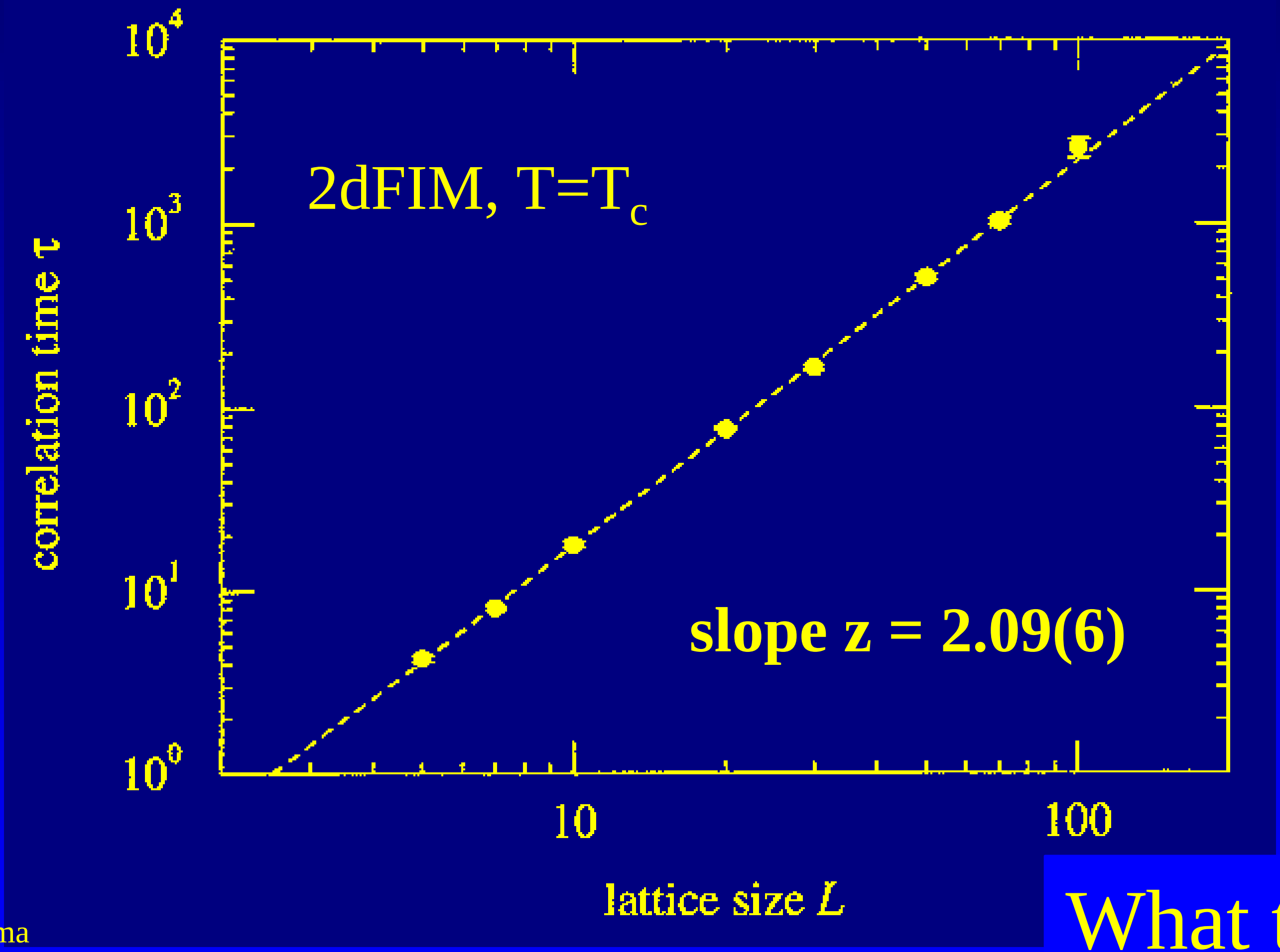
- Near a critical point, autocorrelation time goes as power of correlation length

$$\tau_{\text{int},A} \approx c\xi^{z}$$

- z = “dynamic critical exponent”
- For Metropolis applied to 2dFIM, *z » 2*

  ⇨**“Critical slowing down”**
- But note: z depends on our algorithm

Metropolis $\tau \propto \xi^2$



Figs 4.2 from
Newman & Barkema

What to do???

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1 Stochastic Integration

2 Random Numbers

3 Classical Statistical Mechanical Simulations

4 Cluster algorithms for classical models

5 Quantum Monte Carlo

6 The continuum limit

7 Observables and Estimators

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9 More about the correlation length

10 Survey of other applications