Leipzig Spring School 2008

Monte Carlo Simulations of Domain Growth: Distortable Ising Nets

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- **Introduction and background**
- **Model and Method**
- **Results**
  - *Domain growth*
  - *Static critical behavior*
- **Summary and overview**

The Ising Model-Binary Alloy Equivalence

$$\mathcal{H} = -J \sum_{\langle i,j \rangle} \sigma_i \sigma_j$$

The **Ising Model** of magnetism

Draw the equivalence: $\sigma_i = 1$ for an A-type atom and $\sigma_i = -1$ for a B-type atom $\Rightarrow$ Binary Alloy model

Phase Transitions in the Ising Model

The Ising model is the "fruit fly" of statistical physics

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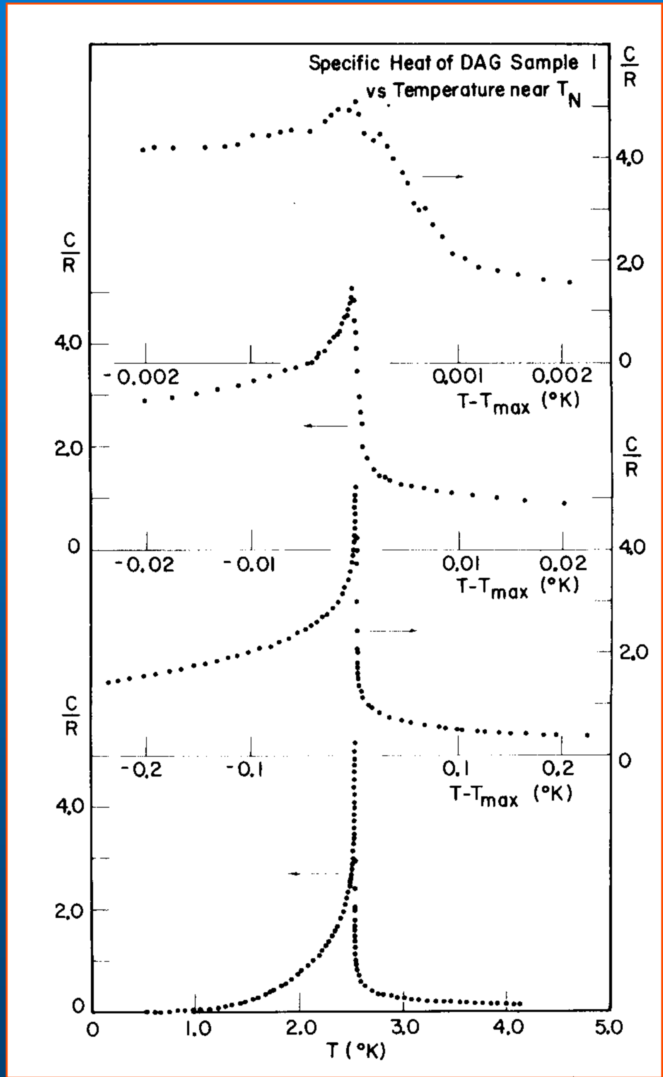
- Physical realizations of Ising models exist, e.g. DyAlG, $Dy(OH)_3$, $LiTbF_3$, binary alloys
- In real materials the lattice is not rigid. Does this matter?
- Theoretical studies began decades ago *(e.g. Mattis & Schulz, 1963; Larkin & Pikin, 1969; Bergmann & Halperin, 1976)*
  - *But different versions were studied*



(Keen, Landau, & Wolf, 1967)

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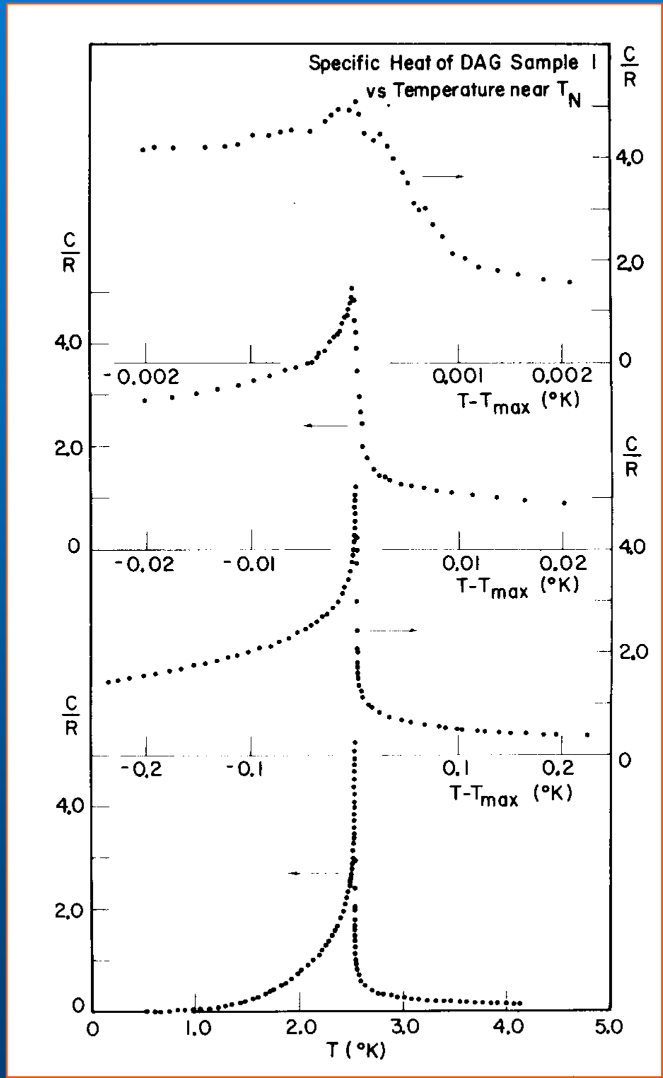

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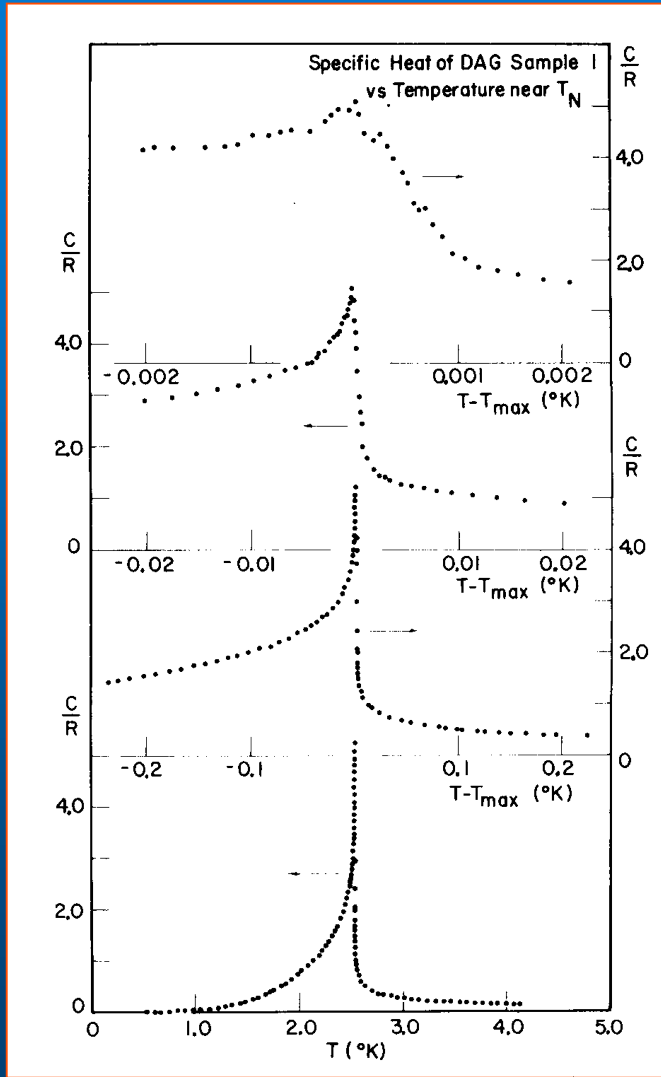

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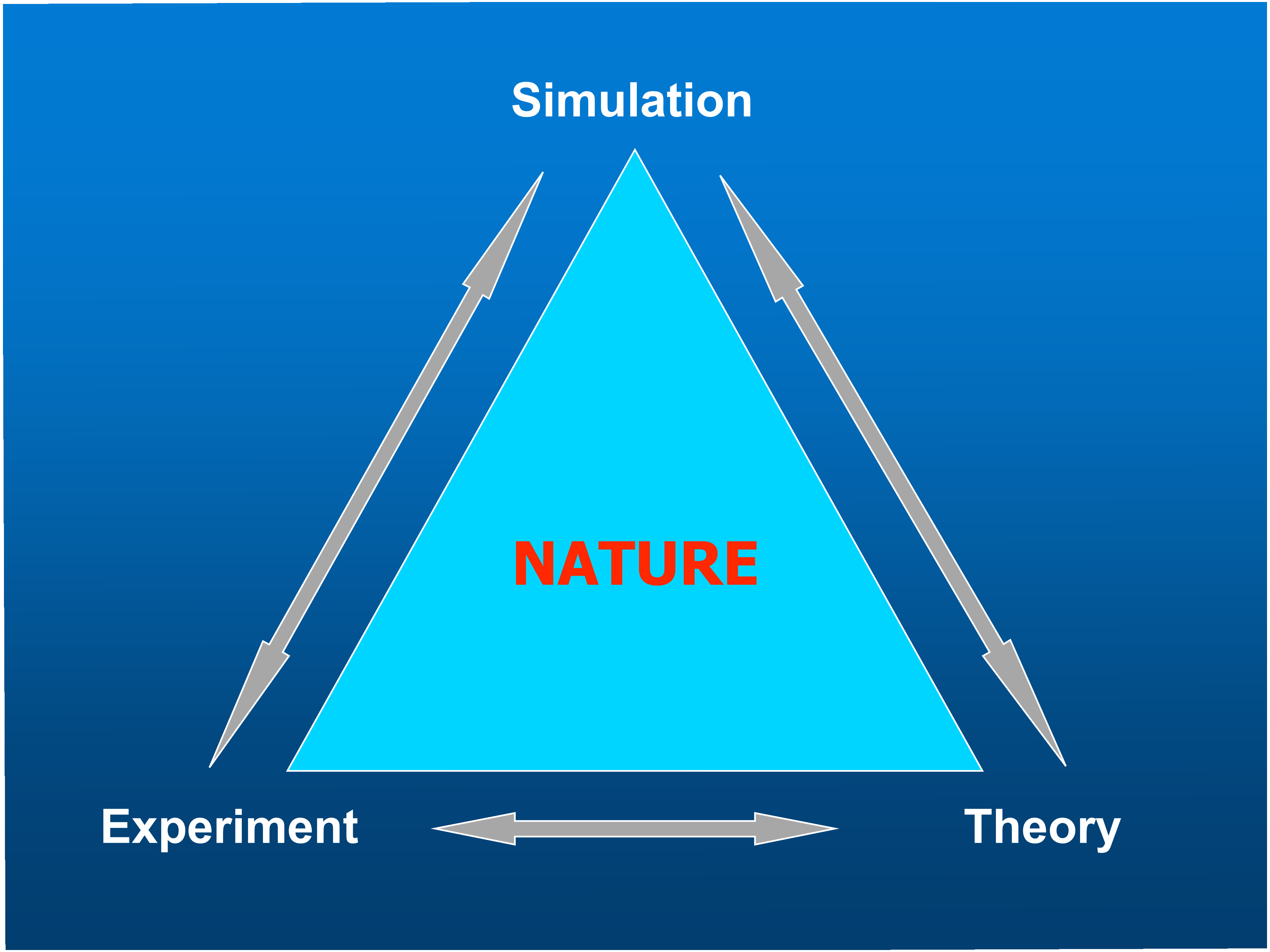
Simulation
NATURE
Experiment
Theory

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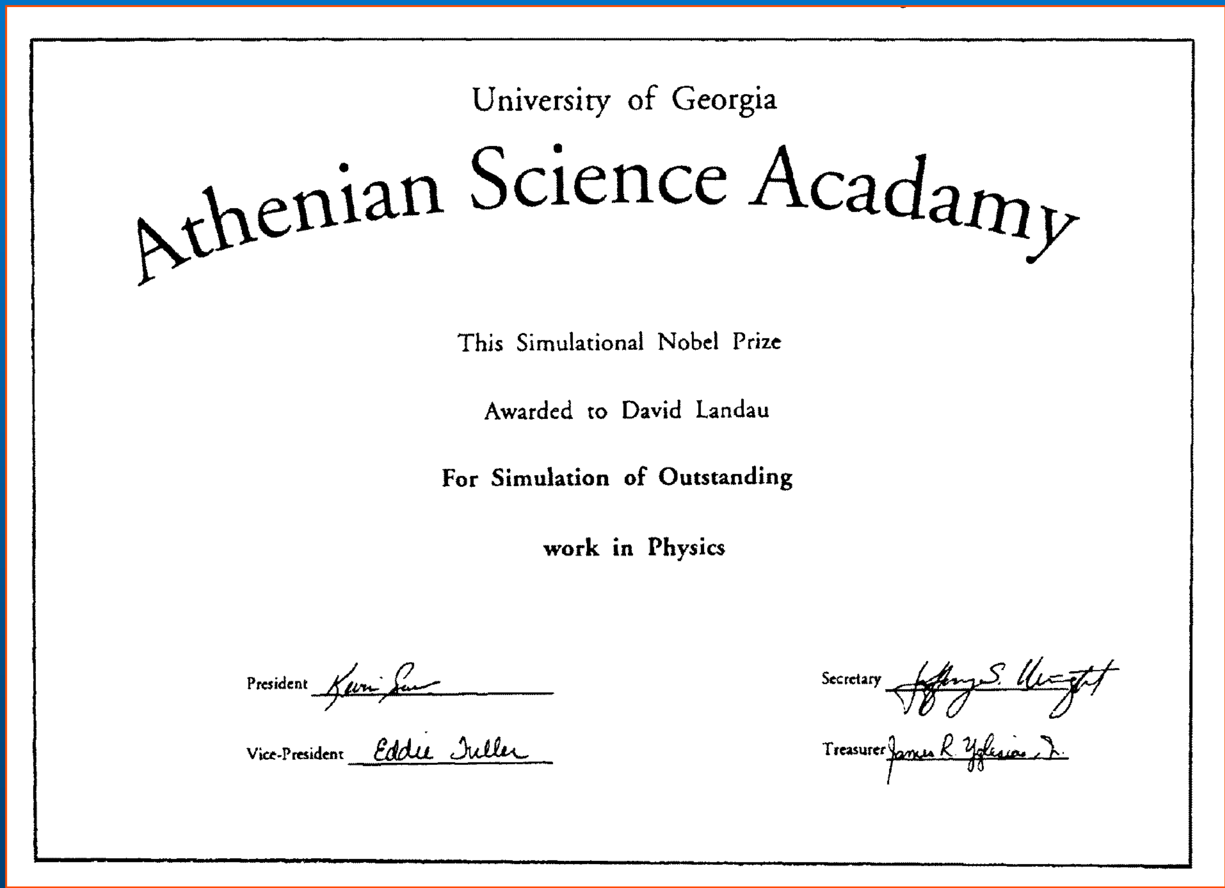
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Athenian Science Acadamy

This Simulational Nobel Prize

Awarded to David Landau

For Simulation of Outstanding

work in Physics

President

Vice-President Eddie Fuller

Secretary

Treasurer

Time Dependence in Monte Carlo Simulations

- **Approach to equilibrium**

  (non-linear relaxation)

- **Fluctuations within equilibrium**

  (linear relaxation)

Spin-flip algorithms

Time Dependence in Monte Carlo Simulations

- **Approach to equilibrium**

  (non-linear relaxation)

- **Fluctuations within equilibrium**

  (linear relaxation)

Spin-flip algorithms

- **Non-equilibrium behavior – domain growth**

  (Note that the magnetization is conserved!)

Spin-exchange algorithms

Single spin-flip sampling for the Ising model

$$\mathcal{H} = -J \sum_{\langle i,j \rangle} \sigma_i \sigma_j \qquad \sigma_i = \pm 1$$

Produce the n^{th} state from the m^{th} state, *e.g.* flip a spin … relative probability is $P_n / P_m \rightarrow$ need only the *energy difference, i.e.* $\Delta E = (E_n - E_m)$ between the states

Any transition rate that satisfies ***detailed balance*** is acceptable, usually the Metropolis form:

$$\begin{aligned} W(m \rightarrow n) &= \tau_o^{-1} \exp(-\Delta E / k_B T), \quad \Delta E > 0 \\ &= \tau_o^{-1} \qquad\qquad\qquad\qquad\quad , \quad \Delta E < 0 \end{aligned}$$

where τ_o is the time required to attempt a spin-flip.

Spin-exchange sampling for the Ising model

$$\mathcal{H} = -J \sum_{\langle i,j \rangle} \sigma_i \sigma_j \qquad \sigma_i = \pm 1$$

Produce the n^{th} state from the m^{th} state, exchange a pair of spins … relative probability is P_n / P_m → need only the *energy difference, i.e.* $\Delta E = (E_n - E_m)$ between the states

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$$= \tau_o^{-1} \quad , \quad \Delta E < 0$$

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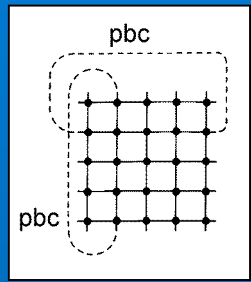
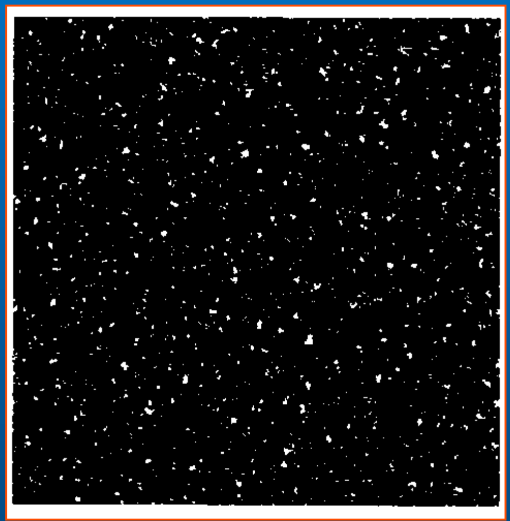
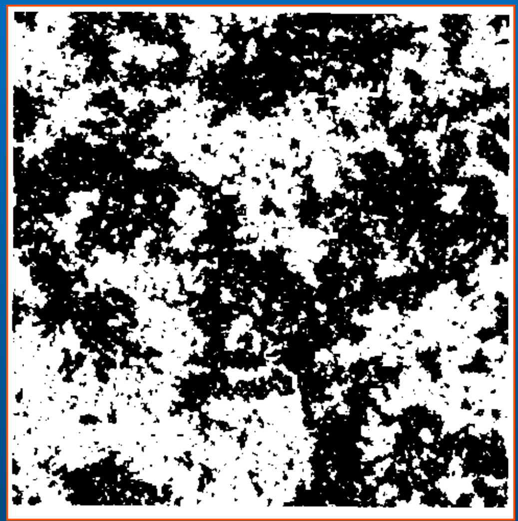
Single Spin-Flip Monte Carlo Simulations

Typical ***equilibrium*** spin configurations
for the **rigid** Ising square lattice with pbc

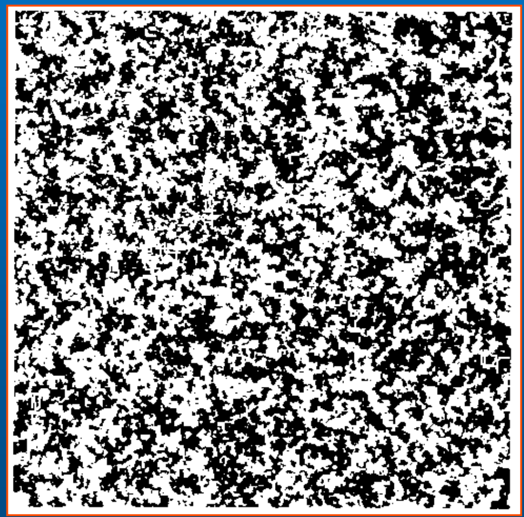




$T << T_c$



$T \sim T_c$

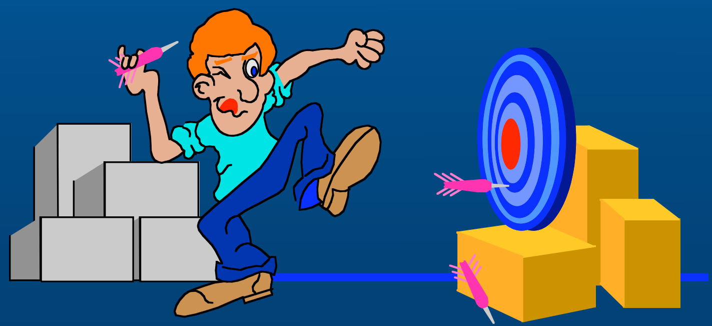


$T >> T_c$

Types of Computer Simulations

Deterministic methods . . . (Molecular dynamics)

Stochastic methods . . . (*Monte Carlo*)



Historical Background *(from The Mathematical Intelligencer)*

Montmorency Royce Sebastian Carlow (1878-1927). The son of a Buckinghamshire peat-digger, he was born in the sedate village of Gossoon two years after Alexander Graham Bell's invention of the telephone, and died the year Lindberg flew the Atlantic.

Montmorency Carlow's contribution to science is no less striking. He displayed no noticeable mathematical talent - indeed no talent at all worth speaking of - until the age of forty-eight, when he succeeded in destroying the entire village of Gossoon, and much of the surrounding countryside, in a singlehanded air-raid mounted from a Handley Page 0/0400 Night Bomber. At his subsequent trial he offered the defence that he was attempting to estimate the area of Gossoon's village pond by calculating the proportion of hits from a random bombing pattern; adding that since the total area of Gossoon was 946.32 acres and he had hit the pond exactly once using 143 bombs, the area of the pond was approximately 6.6176224 and a bit acres.

Lord Justice Milnesshawe-Ffeebes, failing to appreciate the revolutionary nature of the method, commented that since the bomb crater had obliterated all trace of the pond, the calculation left something to be desired. Before the conclusion of the trial, Carlow attempted to estimate the probability of surviving a fall by repeatedly jumping from a high window, fell on his head at the first attempt, and broke his neck. His name lingers on, however: the techniques of estimation that he pioneered are known throughout the world as Monty Carlow Methods.

The Compressible Ising Model: Statics

$$\mathcal{H} = -\sum_{nn} J(r_{ij}, \theta_{ijk}) \sigma_i \sigma_j - \sum_i H(r_i) \sigma_i \, , \quad \sigma_i = \pm 1$$

Couple the order parameter to the elastic degrees of freedom:

Theoretical predictions: *(Dünweg, Habilitationschrift)*

	Linear coupling (F)	**Quadratic coupling (AF)**
Constant pressure	*Mean-field-like*	*1st order*
Constant volume	*Two transition lines, mean-field-like*	*Fisher renormalized*

The Compressible Ising Model ⇔ Si/Ge Alloy

What if the model is on an elastic net instead of a rigid lattice?

$$\mathcal{H} = -\sum_{nn} J\,(r_{ij}, \theta_{ijk})\sigma_i\sigma_j - \sum_i H(r_i)\sigma_i\ , \qquad \sigma_i = \pm 1$$

$$\Leftrightarrow \mathcal{H}_{Si\text{-}Ge} = \mathcal{H}_1 + \mathcal{H}_2 + \mathcal{H}_3 \qquad \sigma_i = 1(Si);\ \sigma_i = -1(Ge)$$

$$= -\tfrac{1}{2}\Delta\mu \sum_i \sigma_i + \sum_{nn} \varepsilon(\sigma_i, \sigma_j)\mathcal{F}_2(r_{ij})$$

$$+ \sum_{nn} \sqrt{\varepsilon(\sigma_i, \sigma_j) * \varepsilon(\sigma_i, \sigma_k)}\ \mathcal{F}_3(r_{ij}, r_{ik}, \theta_{ijk})$$

Now, Monte Carlo moves must include:

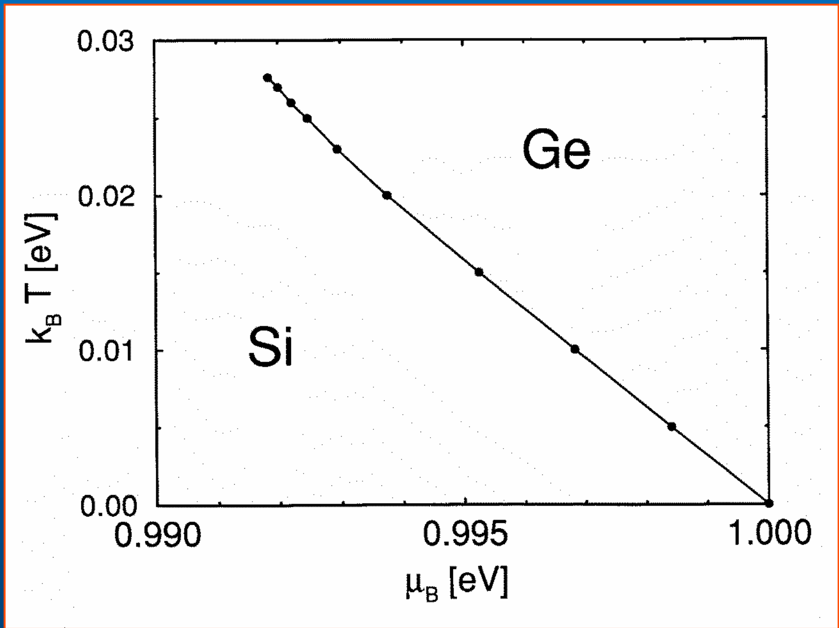
- Spin flips
- Spin moves
- Volume changes

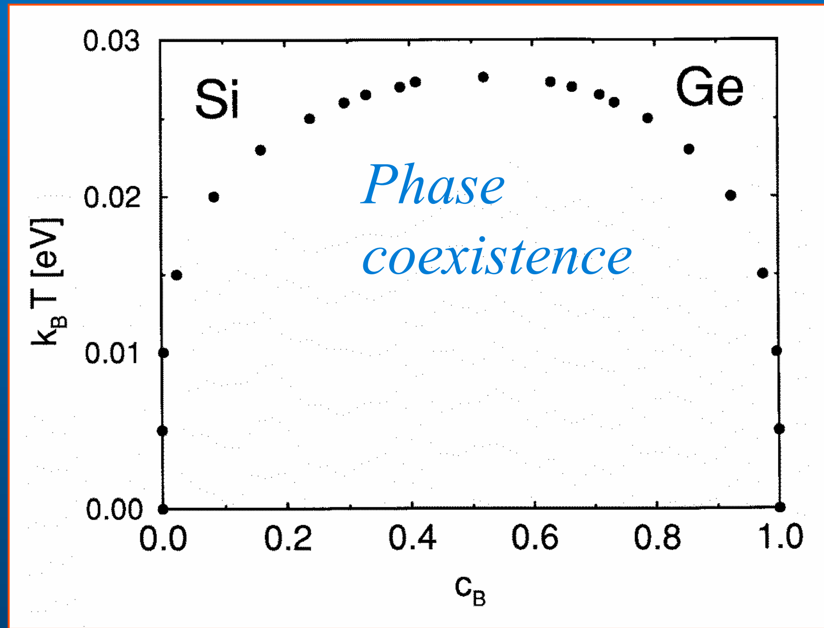
(Duenweg and Landau, 1993)

The Ising Ferromagnet on a Distortable Diamond Net at Constant Pressure

$$\mathcal{H} = -\sum_{nn} J\,(r_{ij}, \theta_{ijk})\sigma_i\sigma_j - \sum_i H(r_i)\sigma_i, \qquad \sigma_i = \pm 1$$

Phase diagram *Note:* $c \Leftrightarrow M\,; \quad \mu \Leftrightarrow H$





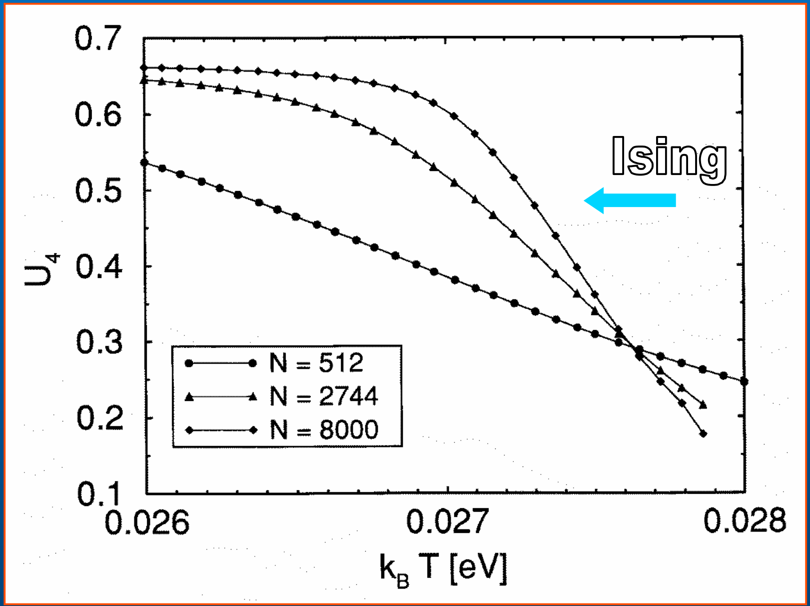
(Dünweg & Landau, 1993)

The Ising Ferromagnet on a Distortable Diamond Net at Constant Pressure

Critical behavior is mean-field-like!

Finite size scaling:

4th order cumulant



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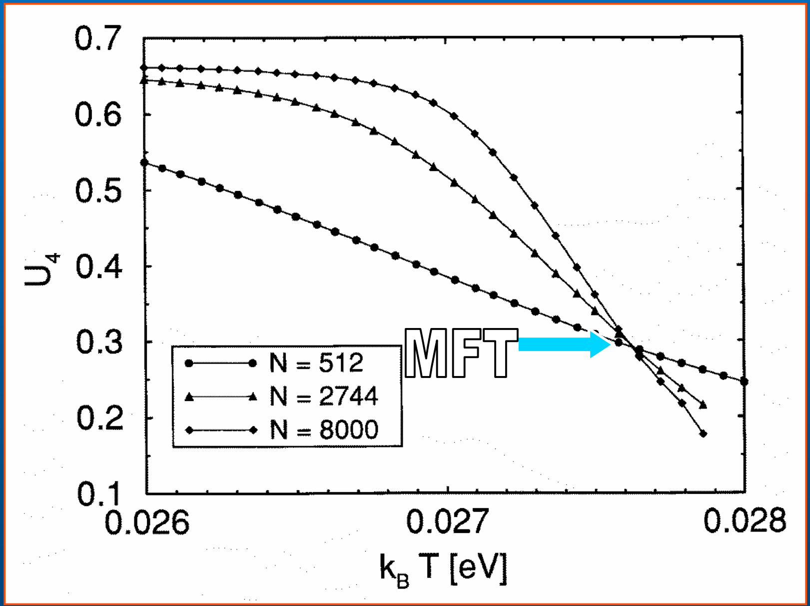

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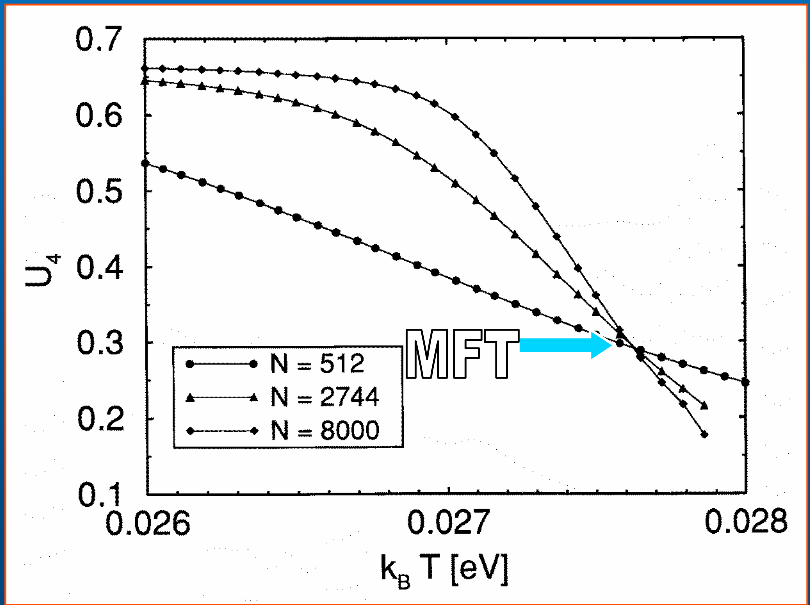
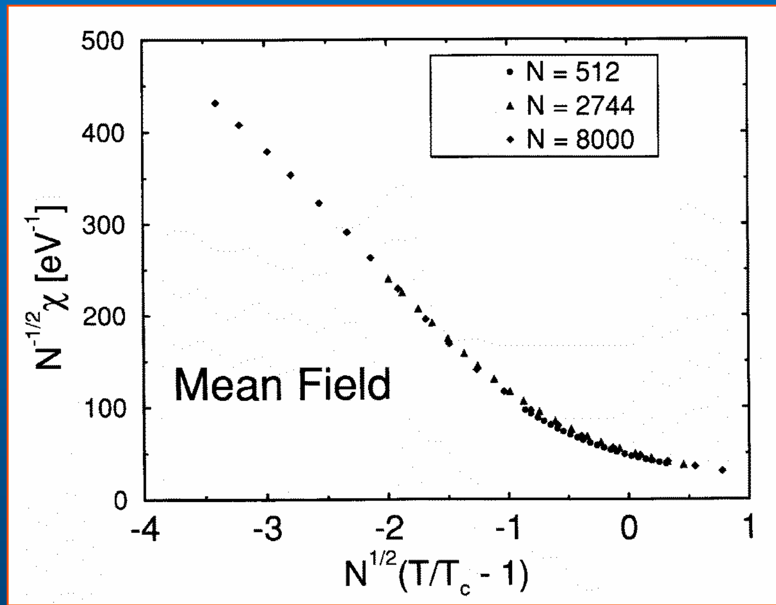


susceptibility



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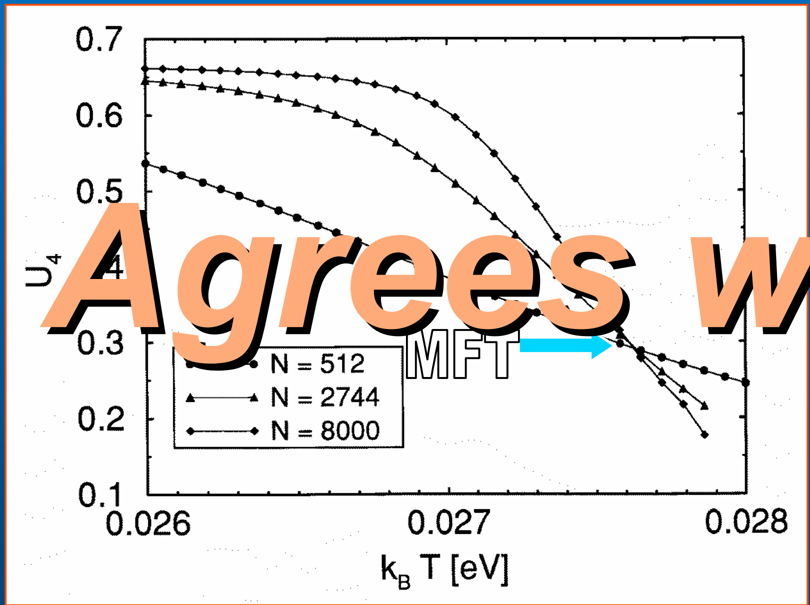

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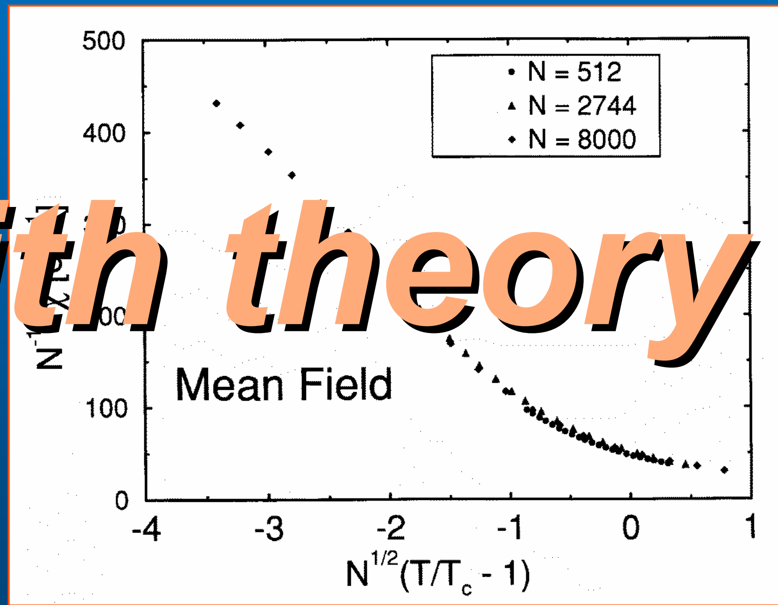
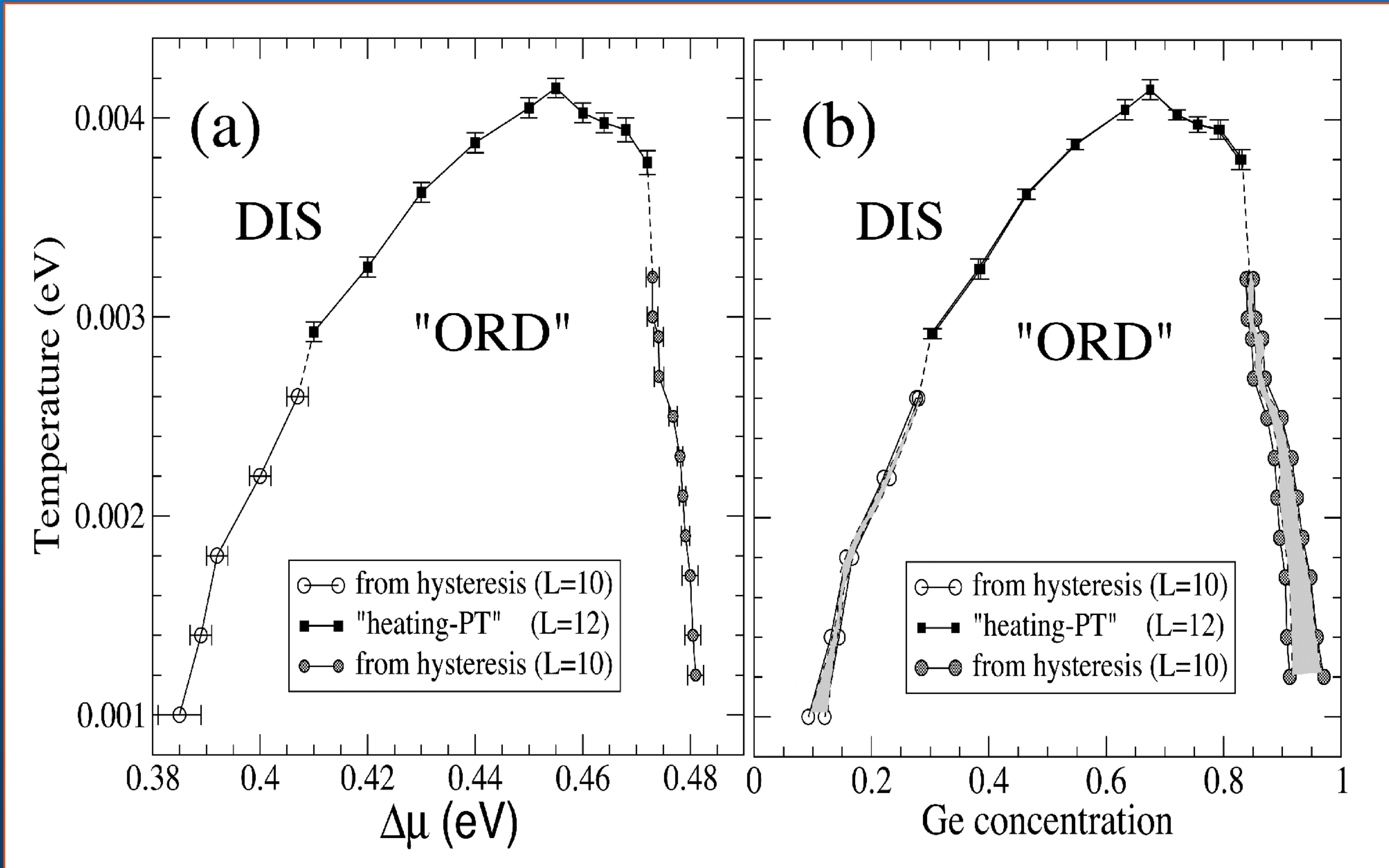


Agrees with theory

(Dünweg & Landau, 1993)

The Ising Ferromagnet on a Distortable Diamond Net at Constant Volume

Phase diagrams - 1st order transitions everywhere!



(Tavazza et al., 2004)

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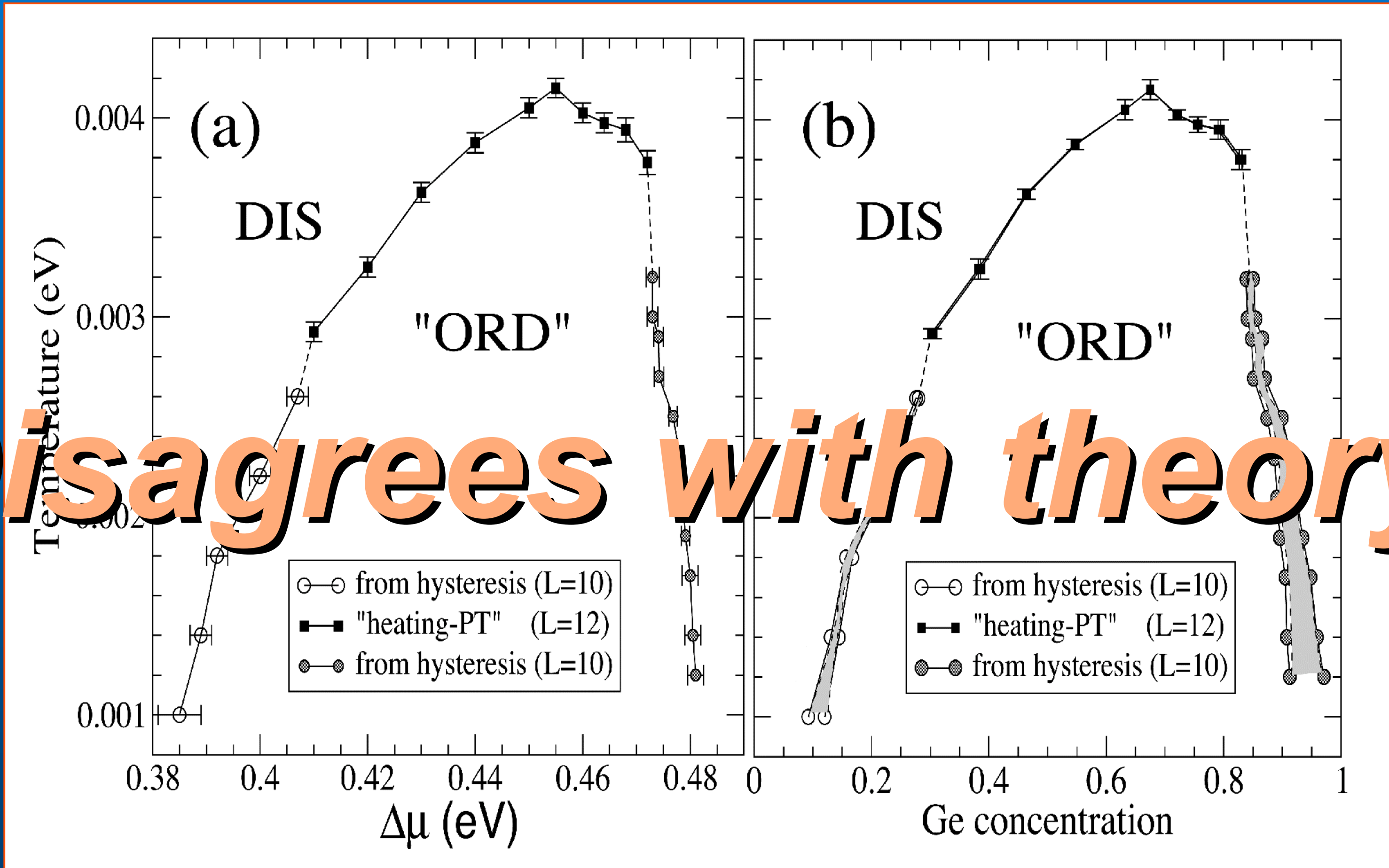


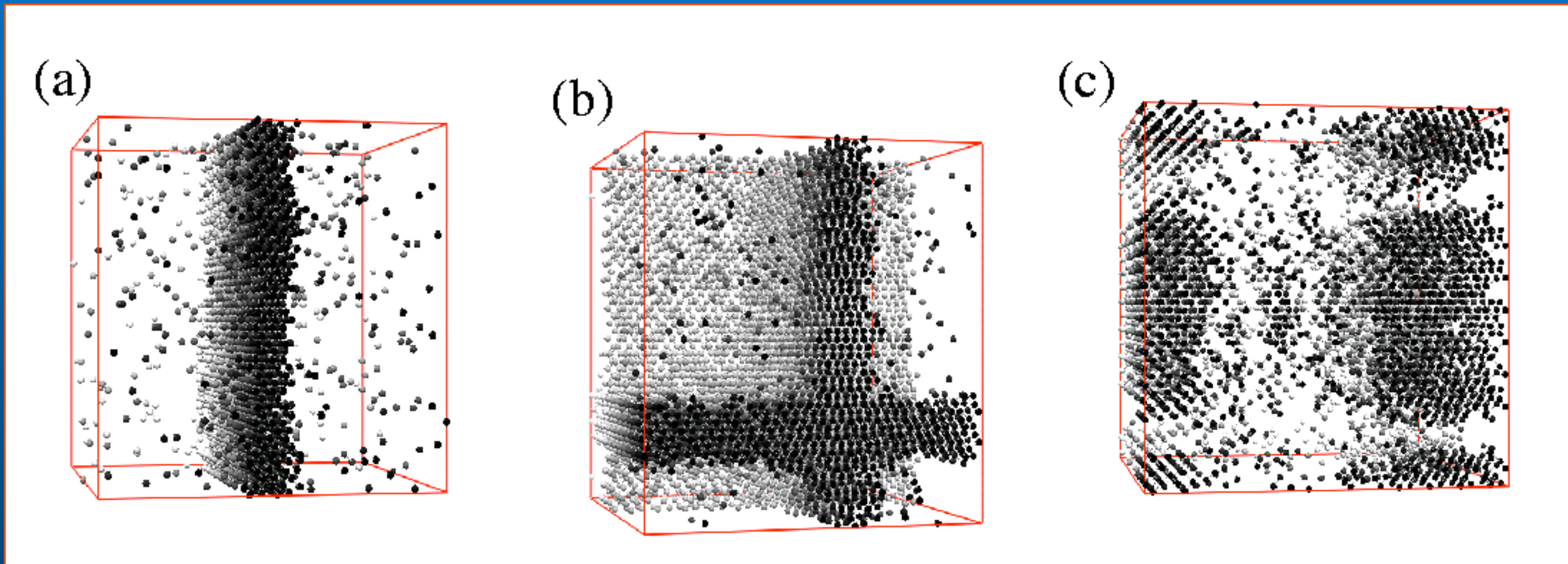
Disagrees with theory

(Tavazza et al., 2004)

The Ising Ferromagnet on a Distortable Diamond Net at Constant Volume

What structures form near the phase transition?

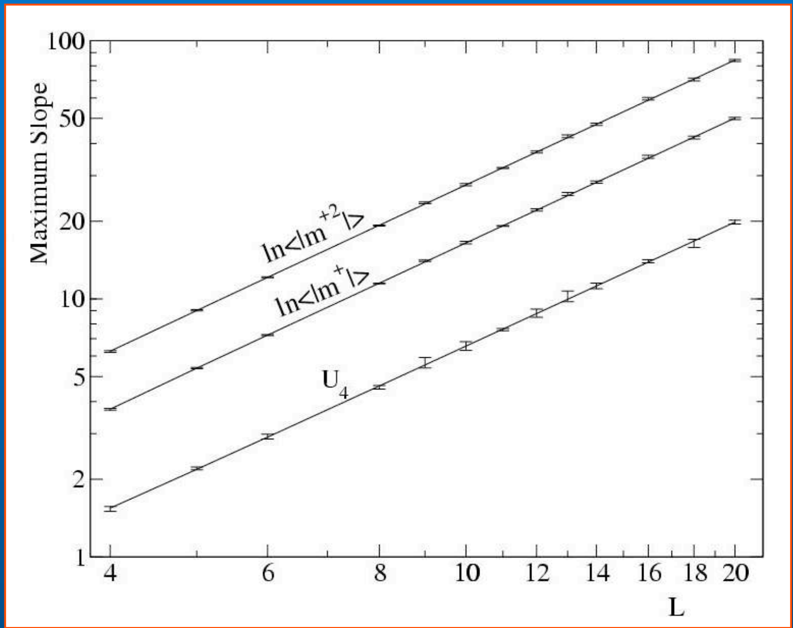
T=0.0029eV

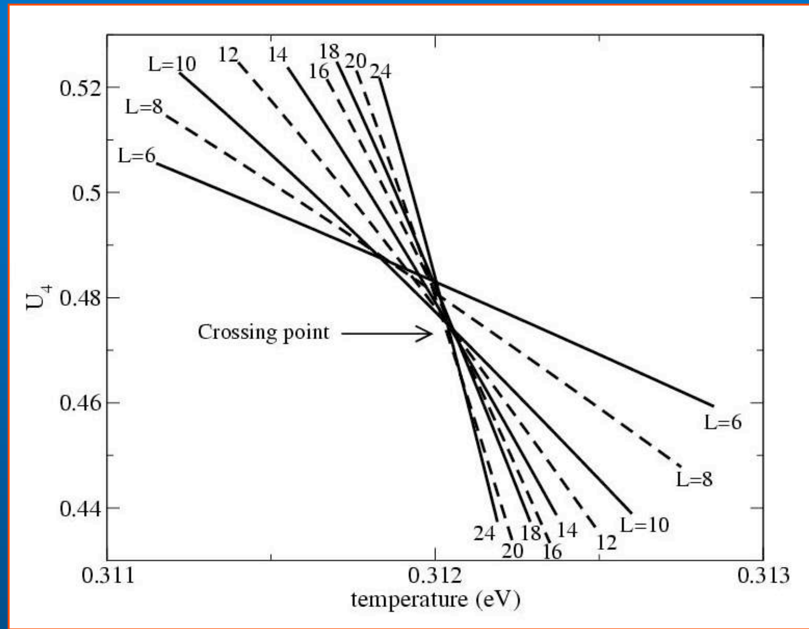


$\Delta\mu$=0.472 (Si only) c(Ge)~0.83 $\Delta\mu$=0.440 (Si only) ~0.55 $\Delta\mu$=0.410 (Ge only) ~0.30

Compressible Ising antiferromagnet

Critical behavior



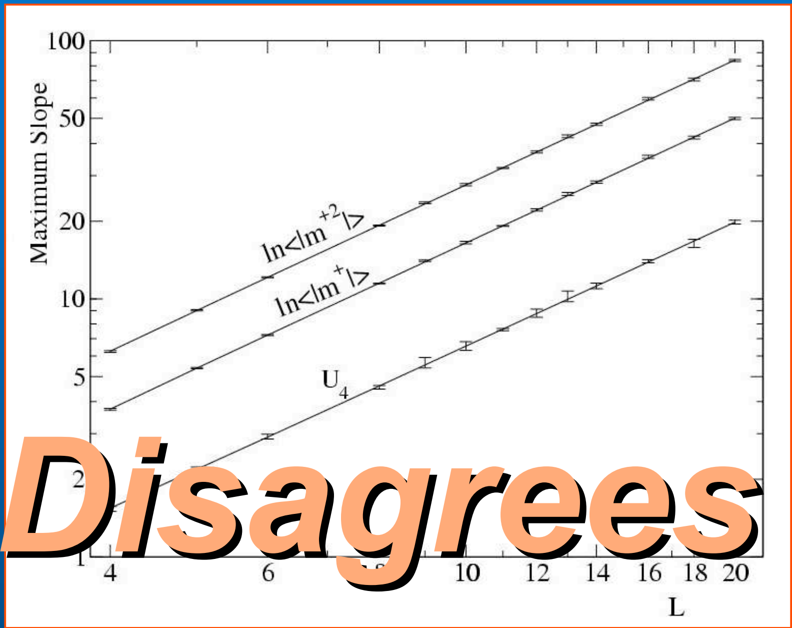


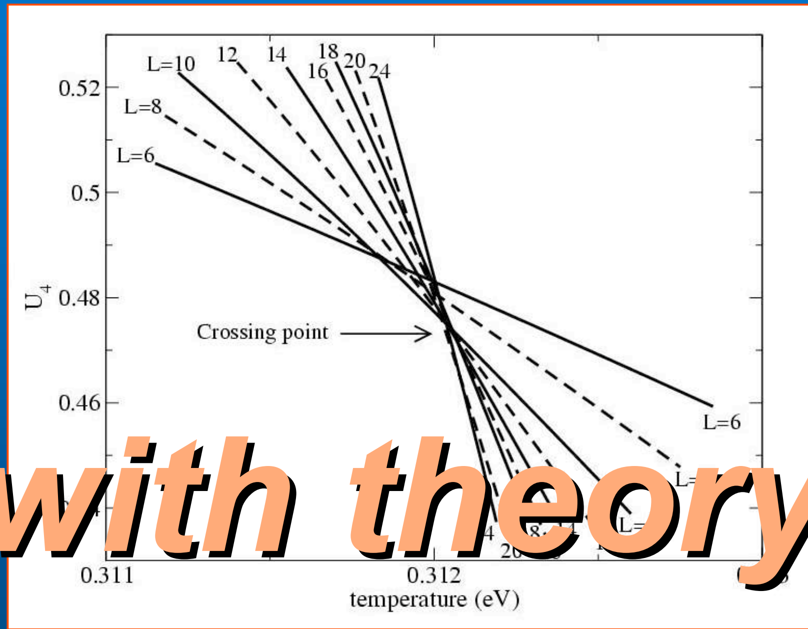
- *Critical exponents and U_4^* are Ising-like !*

(Zhu et al, 2005)

Compressible Ising antiferromagnet

Critical behavior





Disagrees with theory

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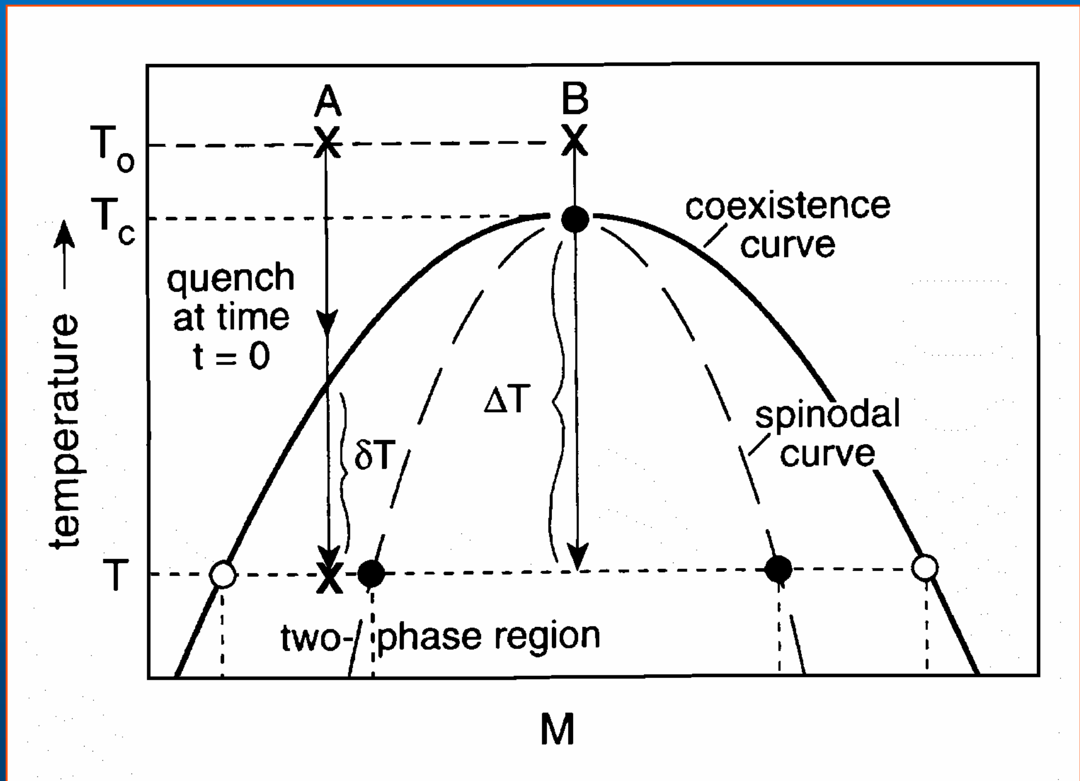
What happens if we quench an Ising model from high T to below T_c?

⇒ domains form and grow with time



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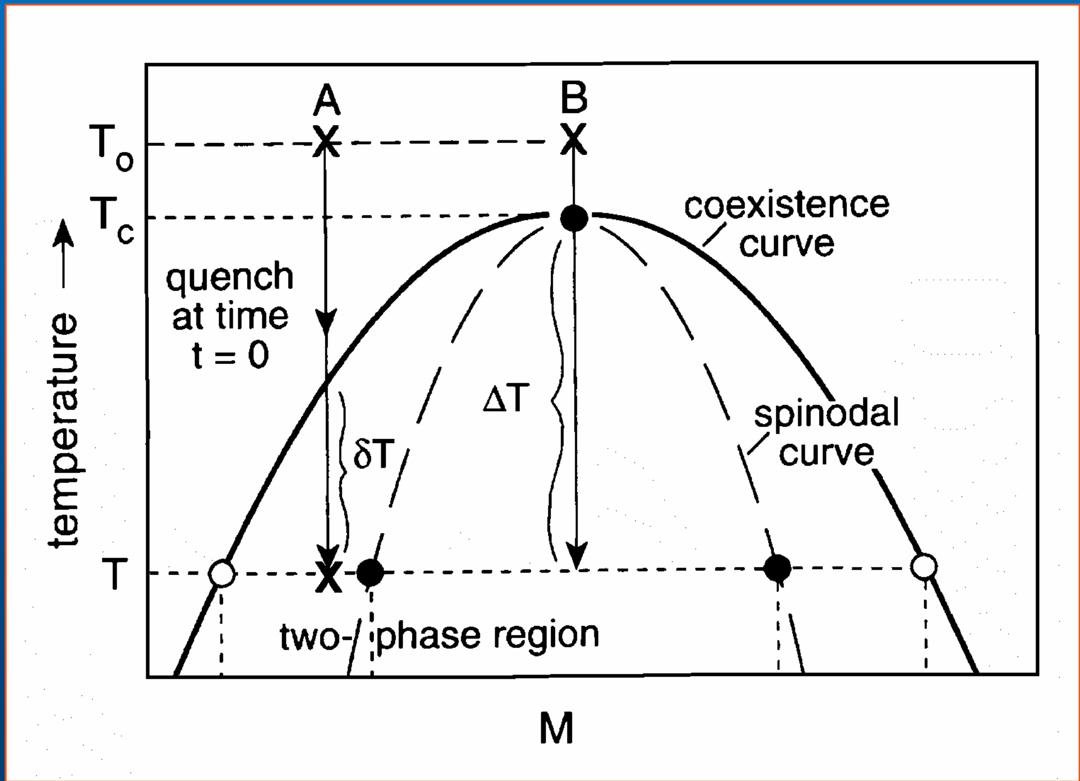
What happens in a compressible system?



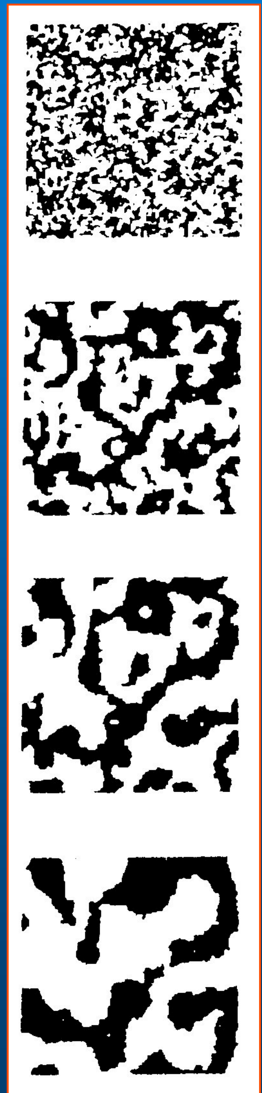
Domain growth (quench from high T)

Monte Carlo simulation – rigid Ising model

Quench to

$T=0.6\ T_c$

Spin flip



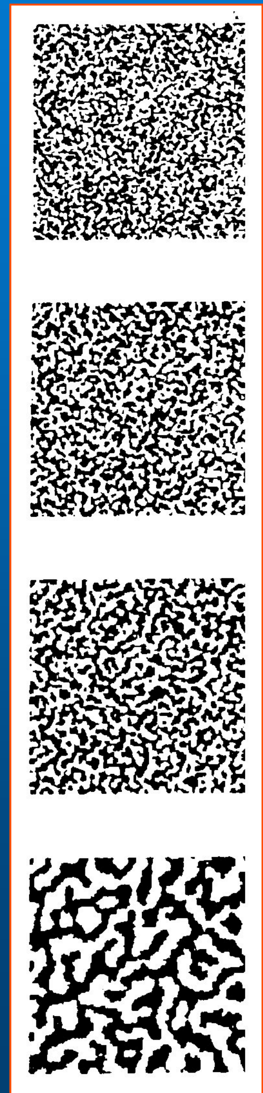
t=2 MCS

15 MCS

15 MCS

120 MCS

Spin exchange



t=10 MCS

60 MCS

200 MCS

10,000 MCS

(Gunton et al., 1988)

Domain growth (quench from high T)

Late stage of domain growth

$$R(t) \propto t^n$$

Domain growth exponent

Domain size

Lifshitz-Slyozov theory

n=1/3, independent of dimension

Huse (1986) predicted: $R(t) \propto a + bt^n$

Domain growth (quench from high T)

Looking at the late stage of domain growth requires large system sizes $\Rightarrow$ simulate a 2-dim system (512×512 with p.b.c., $T_{quench} \sim 0.6\, T_c$)

- Analyze the correlation function
- Visualization!

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- Visualization!

Total computational effort

~ 5 cpu years

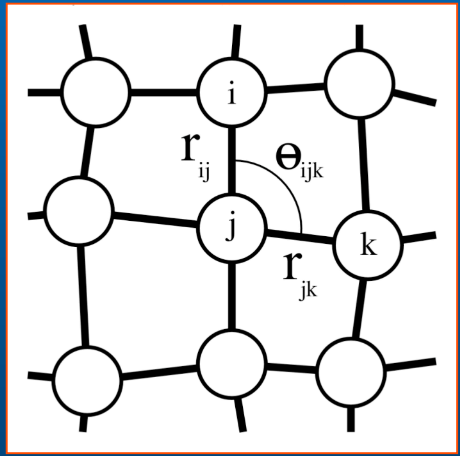
~ 1 Terabyte storage

The Ising Ferromagnet on a Distortable Square Net at Constant Pressure

$$\mathcal{H} = -\sum_{nn} f(r_{ij}, \sigma_i, \sigma_j) + J_\theta \sum_i \cos^2(\theta_{ijk}) \;, \quad \sigma_i = \pm 1$$

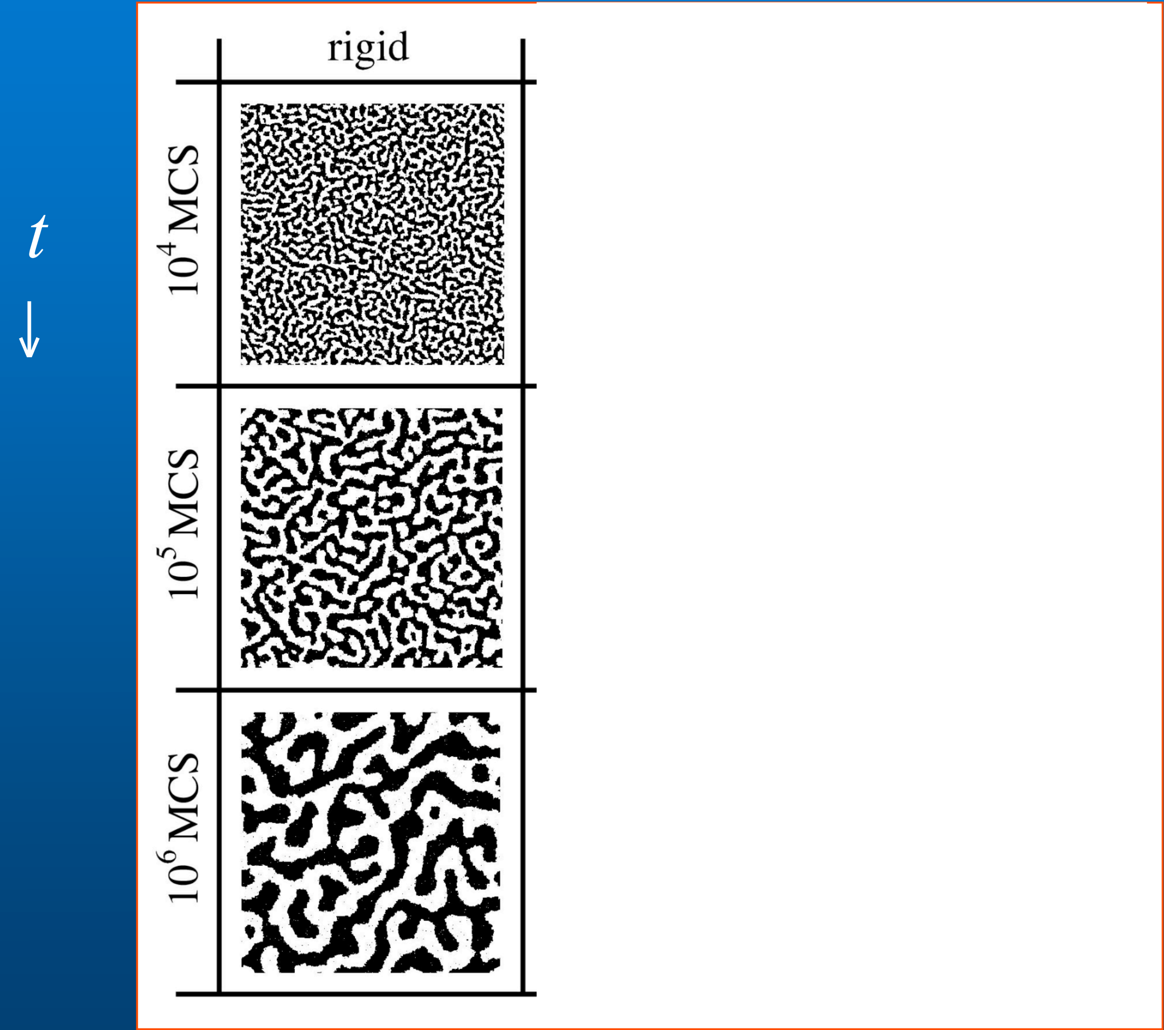
Lennard-Jones potential

Distortable net…apply p.b.c.



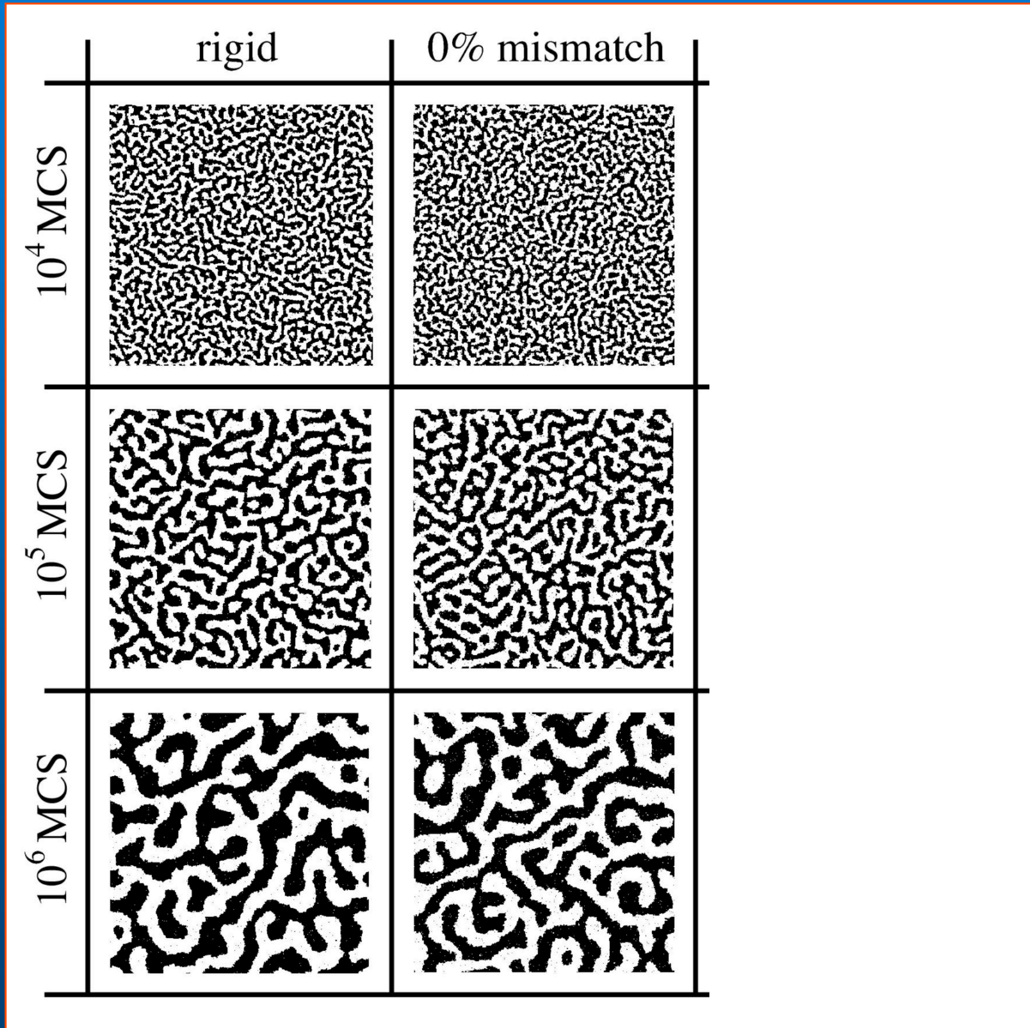
The ***mismatch*** *is the difference between bond lengths at minimum energy for ++ and -- neighbors*

The Ising Ferromagnet on a Distortable Square Net at Constant Pressure



The Ising Ferromagnet on a Distortable Square Net at Constant Pressure

t
↓



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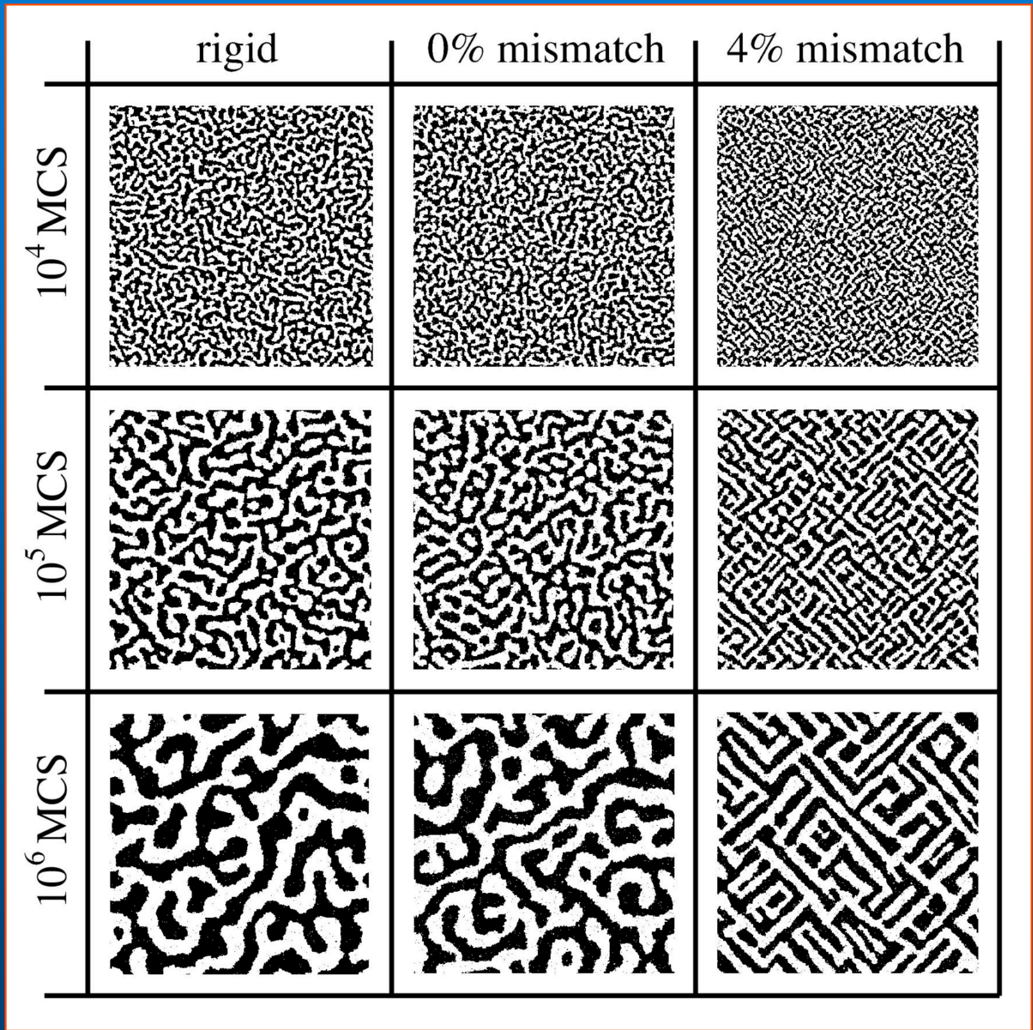
t
↓



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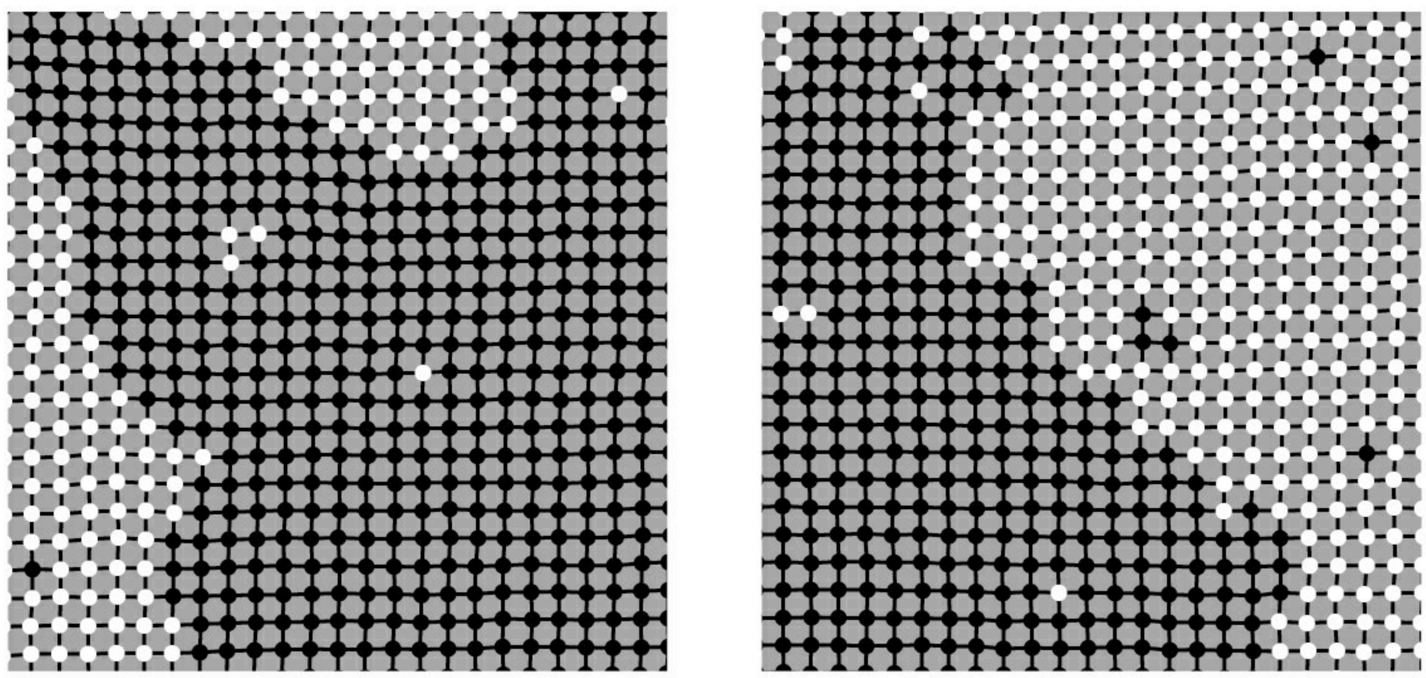


(a) (b)

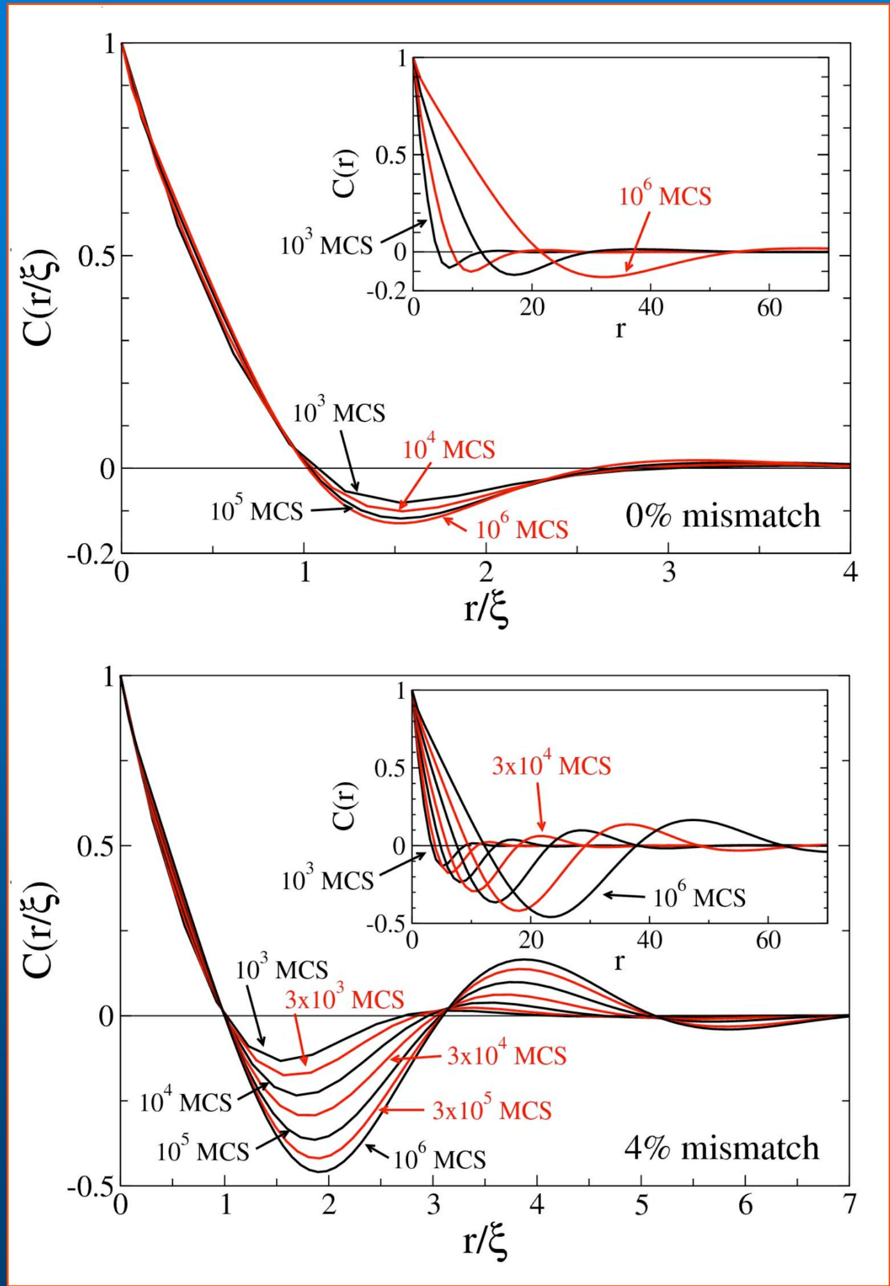
Domain growth: The Ising Ferromagnet on a Distortable Square Net at Constant Pressure

Spin-spin correlation function $C(r) = <\sigma_i\sigma_j> - <\sigma_i>^2$

Define the 1^{st} zero of $C(r)$ as the correlation length ξ

Correlation function:

The Ising Ferromagnet on a distortable square net at constant pressure



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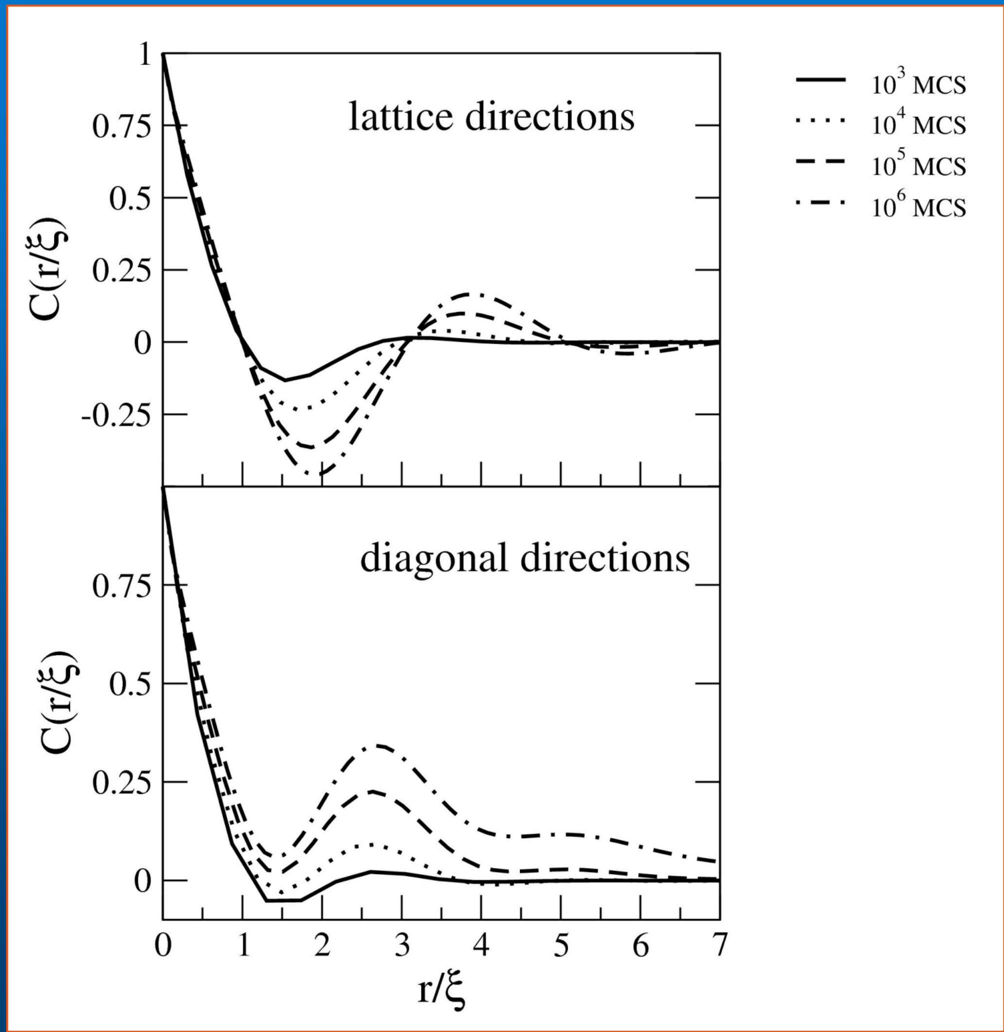
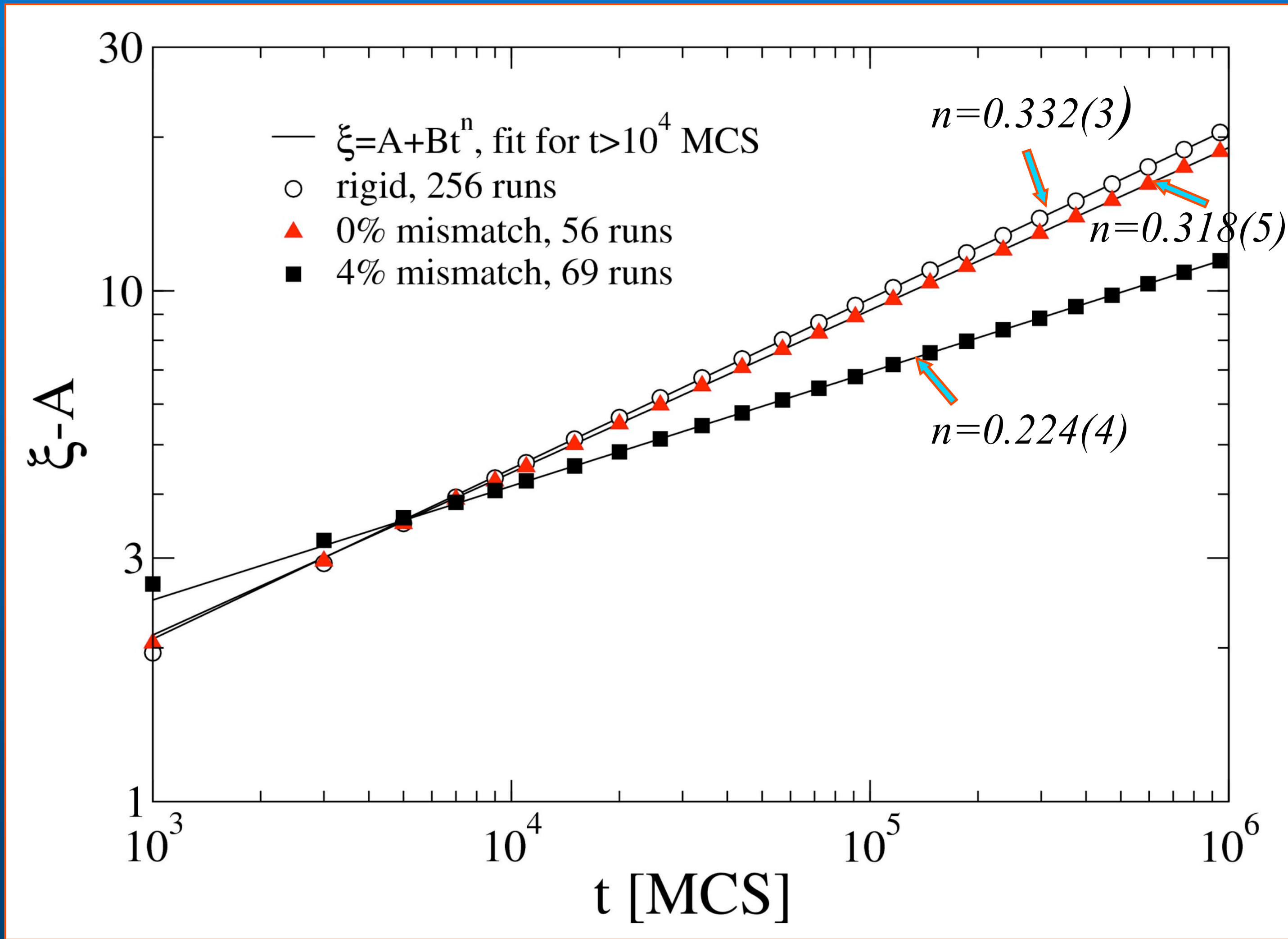
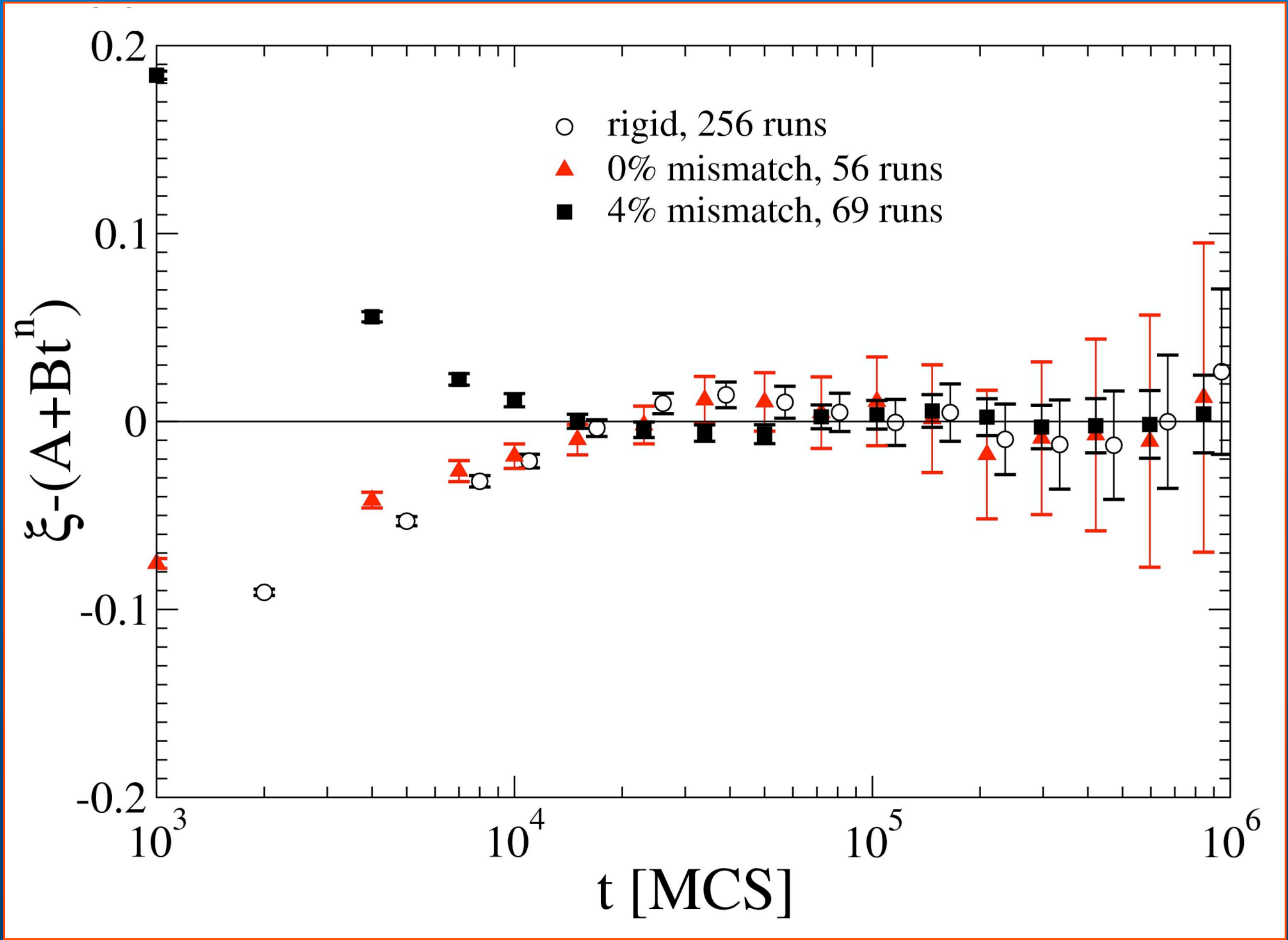


Correlation length: The Ising Ferromagnet on a Distortable Square Net at Constant Pressure



Ising Ferromagnet on a Distortable Square Net at Constant Pressure

fitting to long time behavior



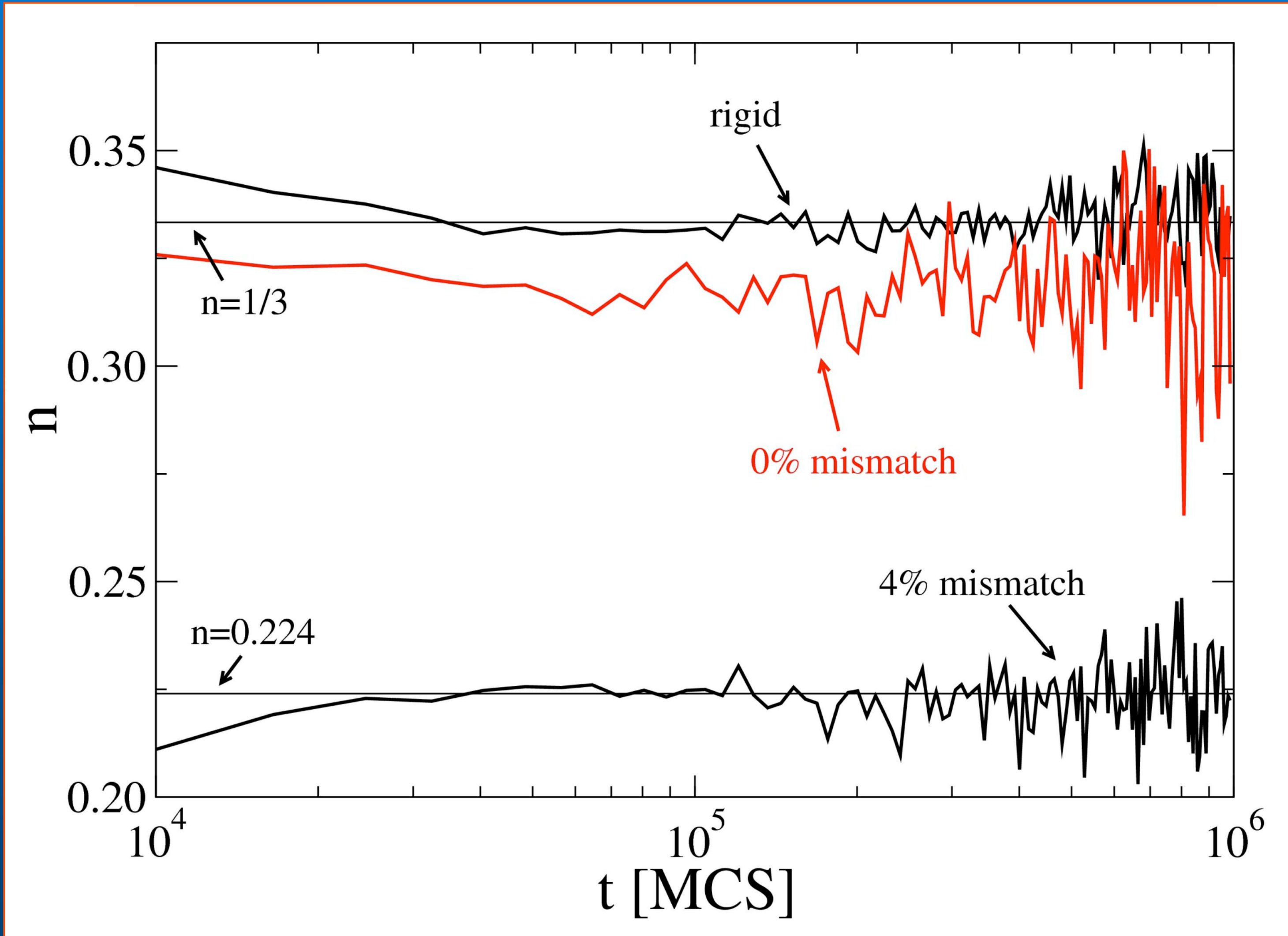
Domain growth exponent: The Ising Ferromagnet on a distortable square net at constant Pressure

Determine the **"local" exponent** and extrapolate to $t \to \infty$

$$n(t) = \frac{\log\left[\dfrac{\xi'(t+\Delta)}{\xi'(t-\Delta)}\right]}{\log\left[\dfrac{t+\Delta}{t-\Delta}\right]}$$

use $10^3 < \Delta < 10^4$ *MCS*

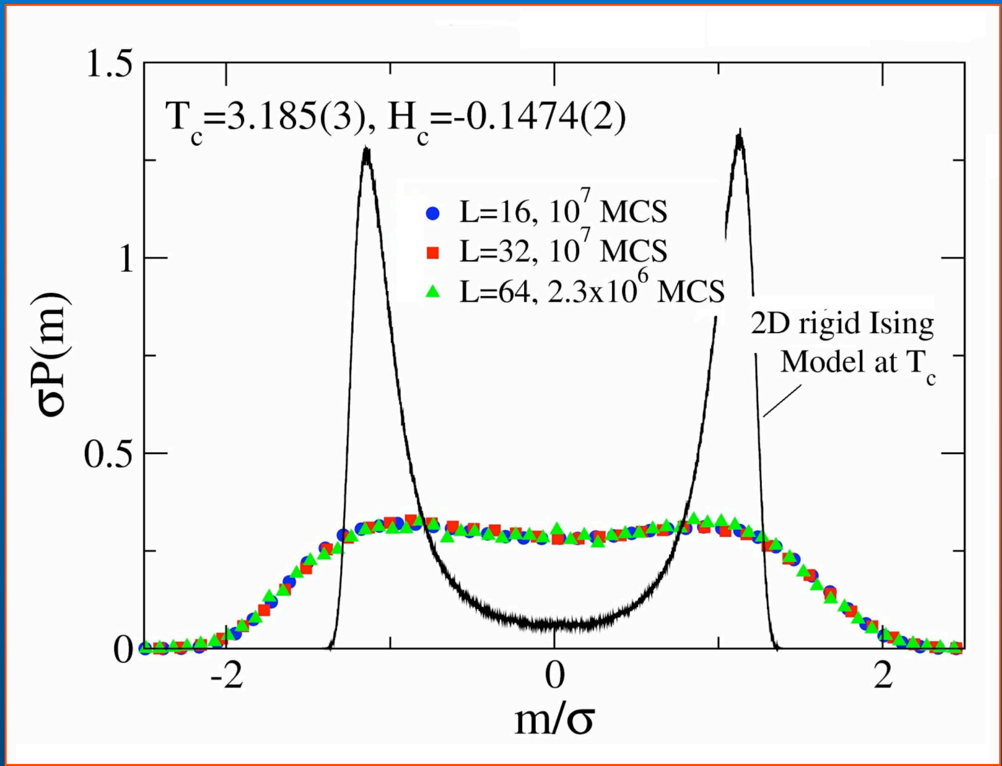
The "local" exponent: Ising Ferromagnet on a Distortable Square Net at Constant Pressure



Last minute update…

Preliminary results:

Probability distributions for the magnetization scaled by the 2nd moment σ should be **Universal**.



Overview and Conclusion

Effects of compressibility in the Ising model are important, but subtle:

- Static behavior in compressible systems is only partially understood
- Domain growth after a quench in the 2-dim compressible ferromagnet at constant pressure differs from that in the rigid model and depends upon “details”

Acknowledgements

Collaborators:

B. Dünweg
M. Laradji
F. Tavazza
L. Cannavacciuolo
X. Zhu
J. Adler

$$$

National Science Foundation

cpu cycles, bits, and bytes

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