Simulating models of polymer collapse

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Collaboration 2003-2008

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  - Clausthal University of Technology
  - University of Melbourne
  - University of Darmstadt
- Aleksander L Owczarek
  - University of Melbourne
- Andrew Rechnitzer
  - University of Melbourne
  - University British Columbia
- Thomas Prellberg
  - Clausthal University of Technology
  - Queen Mary, University of London

Outline

- Polymers in solution:
  - Equilibrium statistical mechanics, lattice model
- Algorithm:
  - Stochastic growth & flat histogram (PERM/flatPERM)
- Simulation of the canonical model:
  - Interacting self-avoiding walks (ISAW)

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- Applications:
  - Protein groundstates (HP model)
  - Bulk vs surface phenomena:
    - confined polymers, force-induced desorption, interplay of collapse and adsorption
  - Hydrogen-bond type interactions

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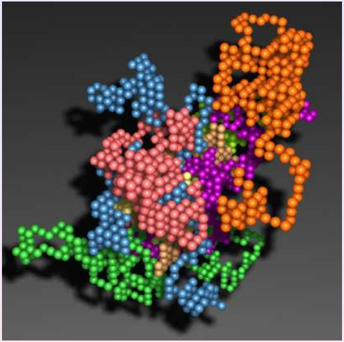
  - Hydrogen-bond type interactions
- Comparison with alternative lattice models

Polymers in Solution

Modelling of Polymers in Solution

- Polymers:
  long chains of monomers
- "Coarse-Graining":
  beads on a chain
- "Excluded Volume":
  minimal distance between beads
- Contact with solvent:
  effective short-range interaction
- Good/bad solvent:
  repelling/attracting interaction



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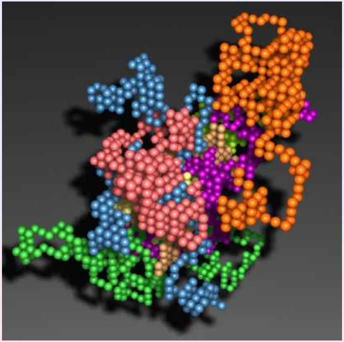
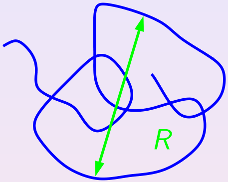


A Model of a Polymer in Solution

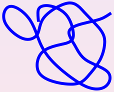
Random Walk + Excluded Volume + Short Range Attraction

Polymer Collapse, Coil-Globule Transition, Θ-Point

length N, spatial extension $R \sim N^{\nu}$



$T > T_c$: good solvent
swollen phase (coil)



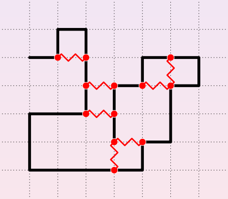
$T = T_c$:
Θ-polymer

$T < T_c$: bad solvent
collapsed phase (globule)

The Canonical Lattice Model

Interacting Self-Avoiding Walk (ISAW)

- Physical space $\longrightarrow$ simple cubic lattice $\mathbb{Z}^3$
- Polymer $\longrightarrow$ self-avoiding random walk (SAW)
- Quality of solvent $\longrightarrow$ short-range interaction ϵ



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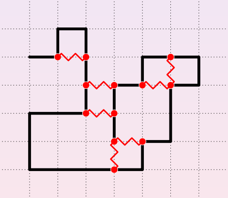
Partition function:

$$Z_N(\omega) = \sum_m C_{N,m}\omega^m$$



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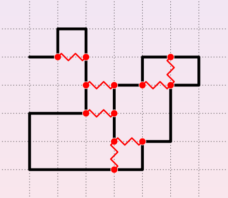

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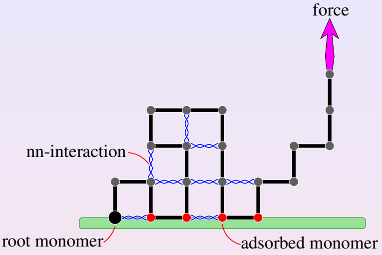
Thermodynamic Limit for a dilute solution:

$$V = \infty \quad \text{and} \quad N \to \infty$$

Extensions of the Model

- In addition to
  - solvent modelling (bulk interaction)
- add
  - adsorption (surface interaction)
  - micromechanical deformations
    e.g. force on chain end (optical tweezers)



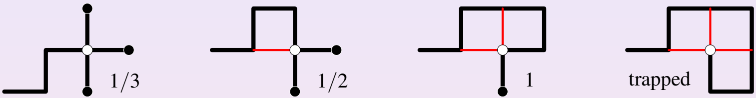
- Complete description through three-dimensional density of states:
  (a) bulk energy, (b) surface energy, (c) position of chain end

The Algorithm

PERM = Pruned and Enriched Rosenbluth Method

P Grassberger, Phys Rev E 56 (1997) 3682

- Rosenbluth Method: kinetic growth



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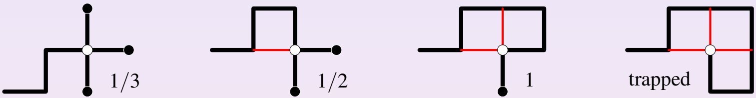

- Enrichment: weight too large → make copies of configuration
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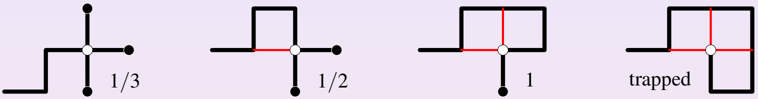

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Current work: flatPERM = flat histogram PERM

T Prellberg and J Krawczyk, PRL 92 (2004) 120602

- flatPERM samples a generalised multicanonical ensemble
- Determines the whole density of states in *one* simulation!

Algorithm details

View kinetic growth as *approximate enumeration*

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- Add pruning/enrichment with respect to ratio $r = W_N^{(S+1)}/C_N^{est}$
  - Number of samples generated for each N is roughly constant
  - We have a $\boxed{\text{flat histogram algorithm}}$ in system size

From PERM to flatPERM

- Consider athermal case
  - PERM: estimate number of configurations C_N
    - $C_N^{est} = \langle W \rangle_N$
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- Consider energy E, temperature $\beta = 1/k_B T$
  - thermal PERM: estimate partition function $Z_N(\beta)$
    - $Z_N^{est}(\beta) = \langle W \exp(-\beta E) \rangle_N$
    - $r = W_N^{(i)} \exp(-\beta E^{(i)}) / Z_N^{est}(\beta)$

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    - $r = W_N^{(i)} \exp(-\beta E^{(i)}) / Z_N^{est}(\beta)$
- Consider parametrisation $\vec{m}$ of configuration space
  - flatPERM: estimate density of states $C_{N,\vec{m}}$
    - $C_{N,\vec{m}}^{est} = \langle W \rangle_{N,\vec{m}}$
    - $r = W_{N,\vec{m}}^{(i)} / C_{N,\vec{m}}^{est}$

Why Simulations?

- Most interesting open questions for dense and geometrically restricted configurations

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There is little theory and this is notoriously difficult to simulate

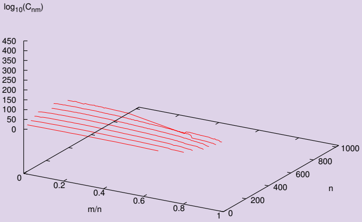
Simulations and Results

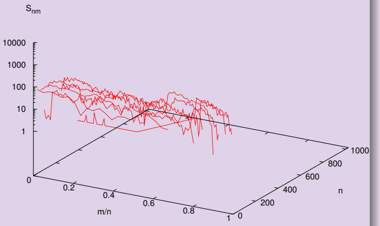
2d ISAW simulation up to $N = 1024$

To stabilise algorithm (avoid initial overflow/underflow):
Delay growth of large configurations
Here: after t tours growth up to length $10t$

2d ISAW simulation up to $N = 1024$

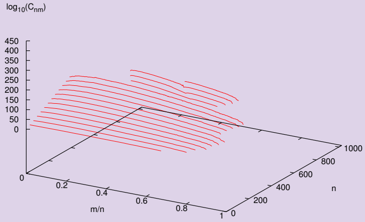
Total sample size: $1,000,000$

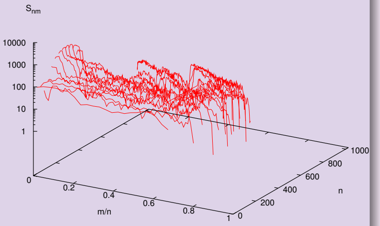




2d ISAW simulation up to $N = 1024$

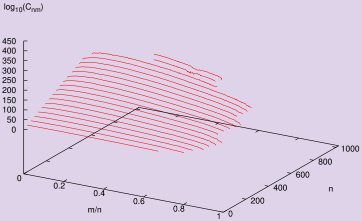
Total sample size: $10,000,000$

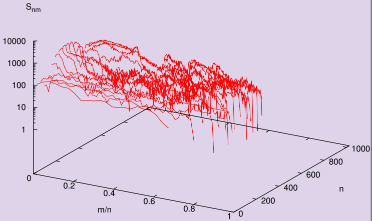




2d ISAW simulation up to $N = 1024$

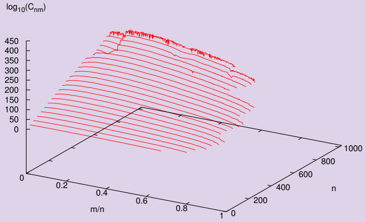
Total sample size: $20,000,000$

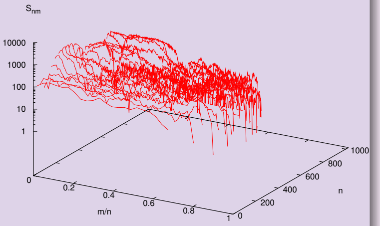




2d ISAW simulation up to $N = 1024$

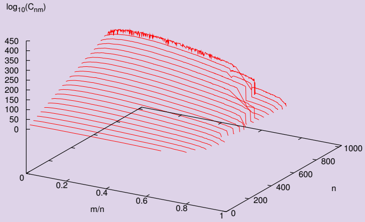
Total sample size: $30,000,000$

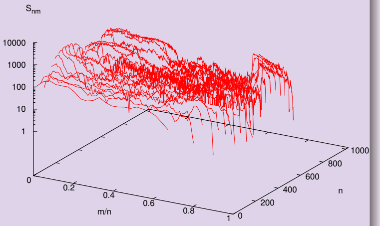




2d ISAW simulation up to $N = 1024$

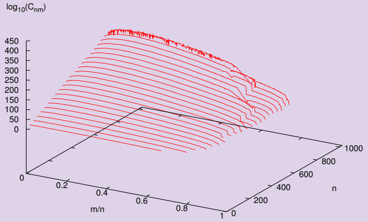
Total sample size: $40,000,000$

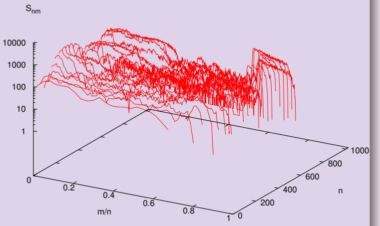




2d ISAW simulation up to $N = 1024$

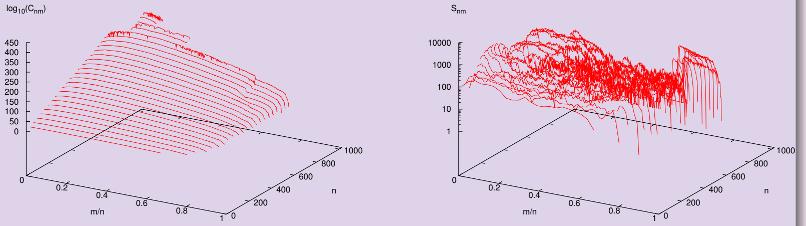
Total sample size: $50,000,000$





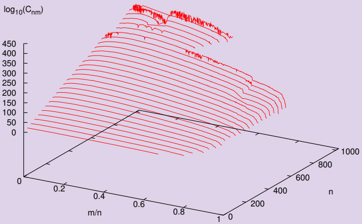
2d ISAW simulation up to $N = 1024$

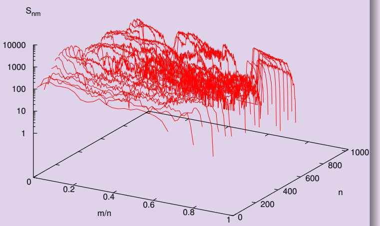
Total sample size: $60,000,000$



2d ISAW simulation up to $N = 1024$

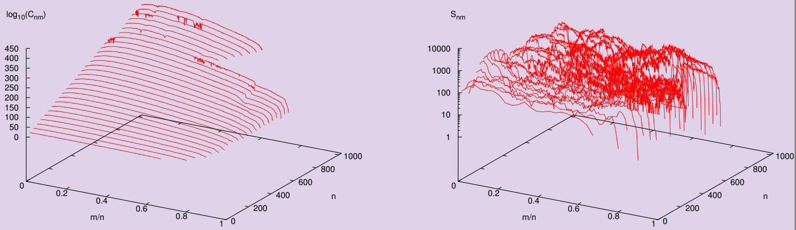
Total sample size: $70,000,000$





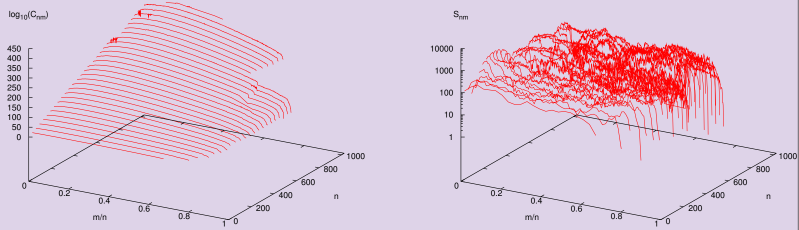
2d ISAW simulation up to $N = 1024$

Total sample size: $80,000,000$



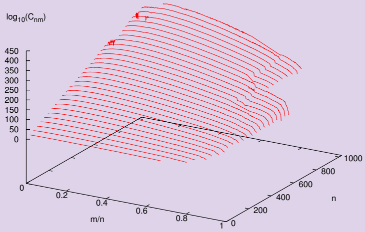
2d ISAW simulation up to $N = 1024$

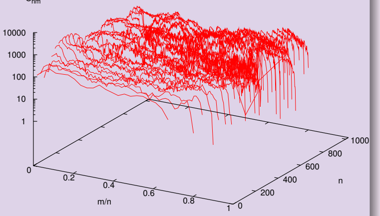
Total sample size: $90,000,000$



2d ISAW simulation up to $N = 1024$

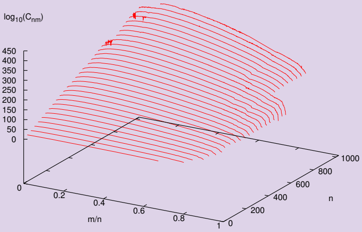
Total sample size: $100,000,000$

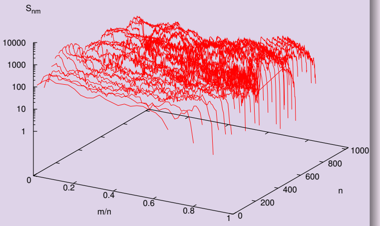




2d ISAW simulation up to $N = 1024$

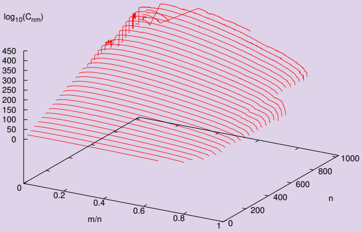
Total sample size: $110,000,000$

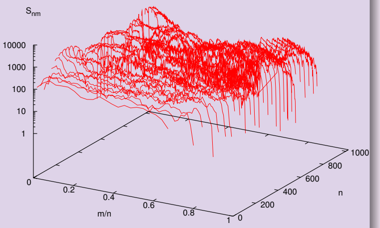




2d ISAW simulation up to $N = 1024$

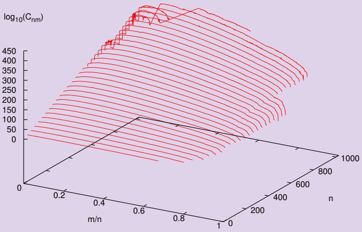
Total sample size: $120,000,000$





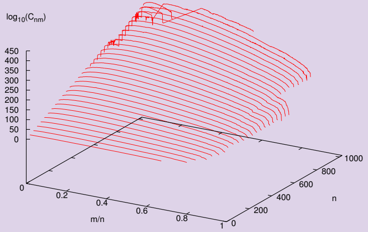
2d ISAW simulation up to $N = 1024$

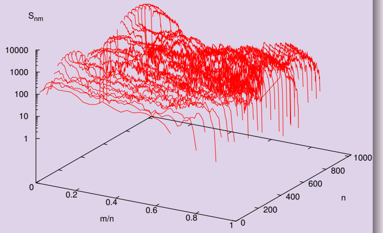
Total sample size: $130,000,000$



2d ISAW simulation up to $N = 1024$

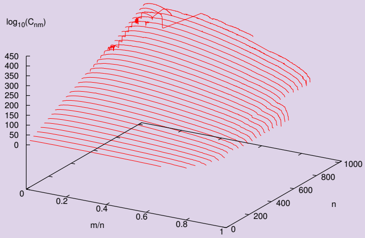
Total sample size: $140,000,000$





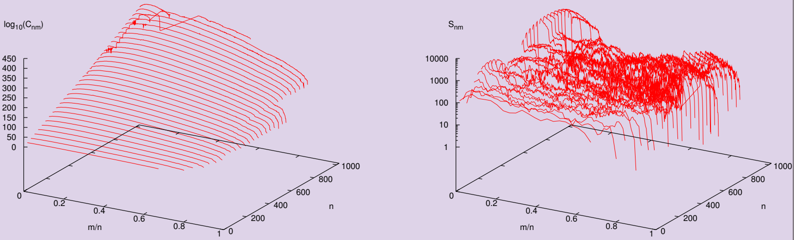
2d ISAW simulation up to $N = 1024$

Total sample size: $150,000,000$



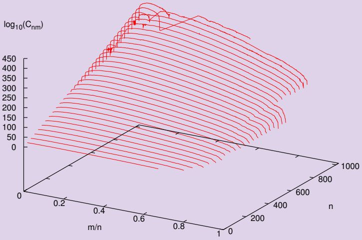
2d ISAW simulation up to $N = 1024$

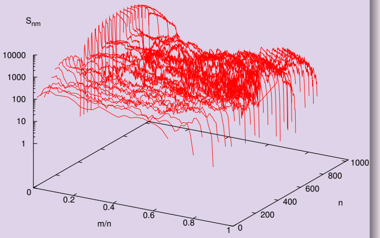
Total sample size: $160,000,000$



2d ISAW simulation up to $N = 1024$

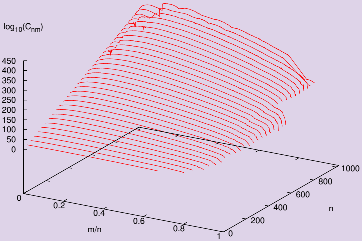
Total sample size: $170,000,000$

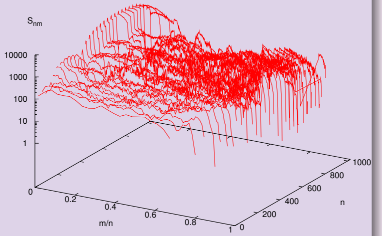




2d ISAW simulation up to $N = 1024$

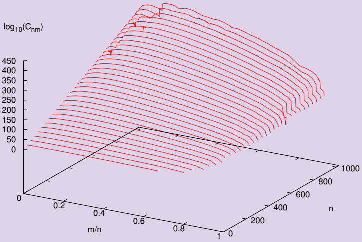
Total sample size: $180,000,000$

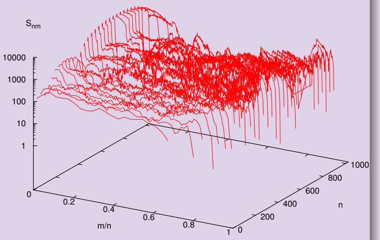




2d ISAW simulation up to $N = 1024$

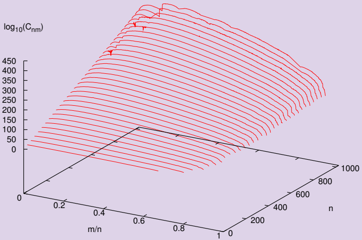
Total sample size: $190,000,000$

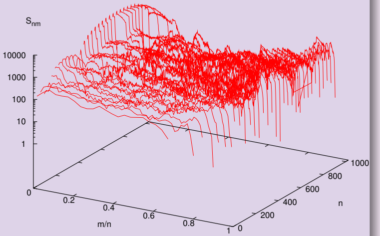




2d ISAW simulation up to $N = 1024$

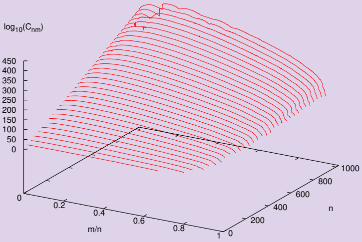
Total sample size: $200,000,000$

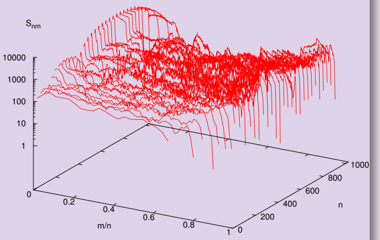




2d ISAW simulation up to $N = 1024$

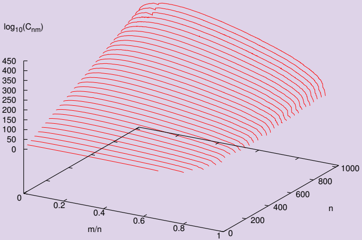
Total sample size: $210,000,000$

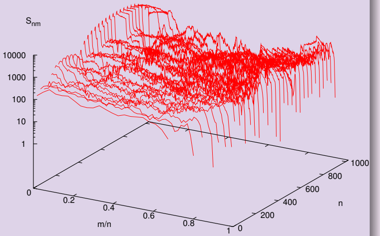




2d ISAW simulation up to $N = 1024$

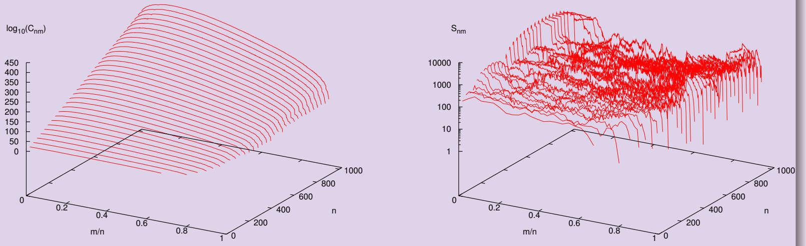
Total sample size: $220,000,000$





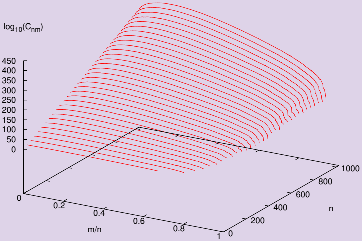
2d ISAW simulation up to $N = 1024$

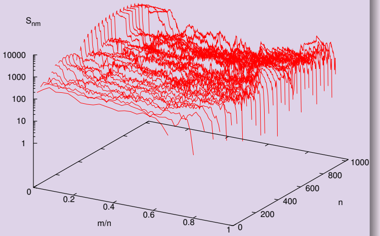
Total sample size: $230,000,000$



2d ISAW simulation up to $N = 1024$

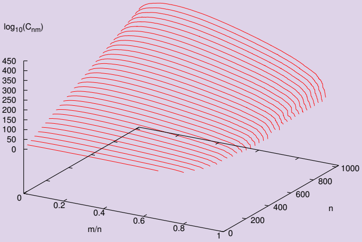
Total sample size: $240,000,000$

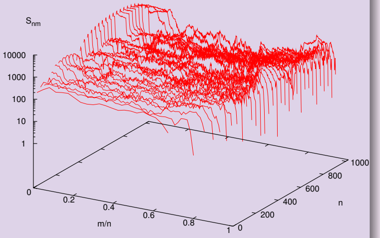




2d ISAW simulation up to $N = 1024$

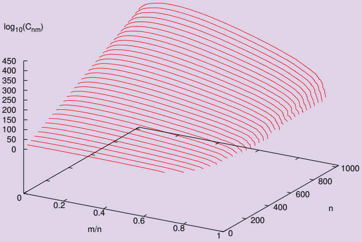
Total sample size: $250,000,000$

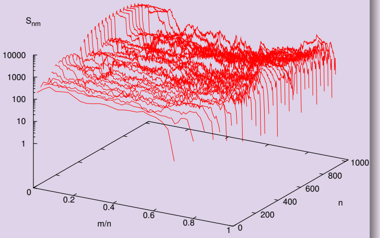




2d ISAW simulation up to $N = 1024$

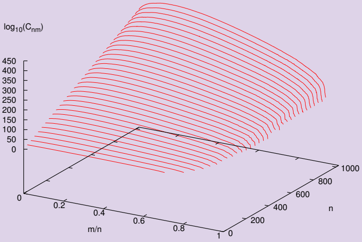
Total sample size: $260,000,000$

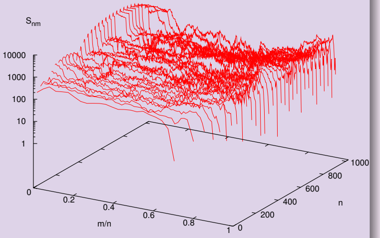




2d ISAW simulation up to $N = 1024$

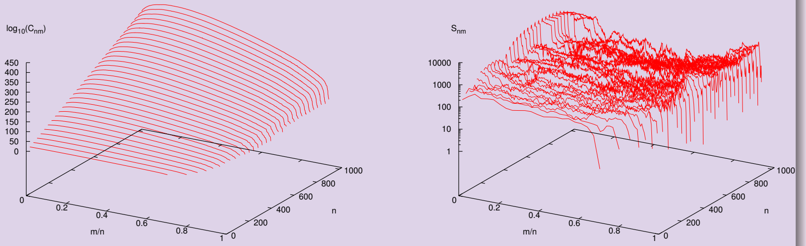
Total sample size: $270,000,000$





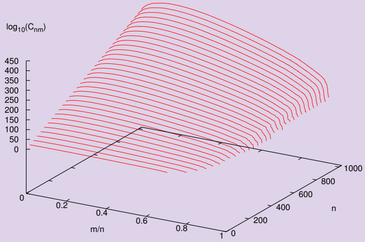
2d ISAW simulation up to $N = 1024$

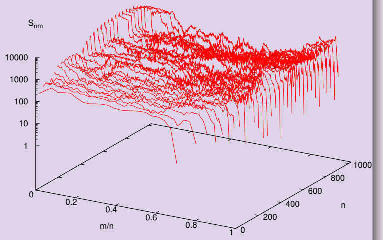
Total sample size: $280,000,000$



2d ISAW simulation up to $N = 1024$

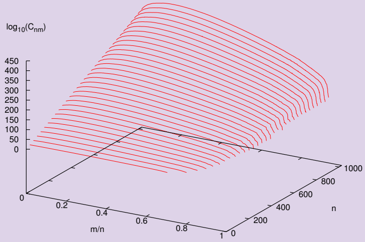
Total sample size: $290,000,000$





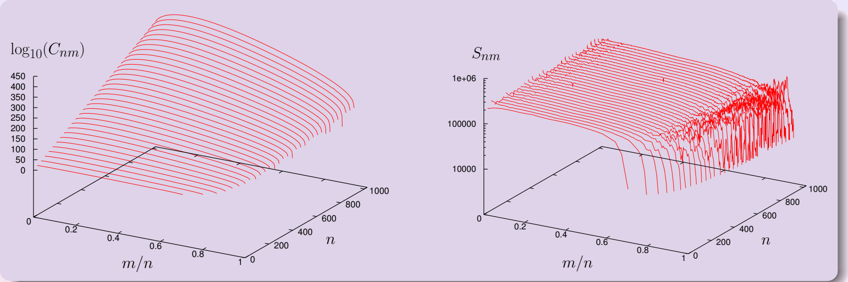
2d ISAW simulation up to $N = 1024$

Total sample size: $300,000,000$



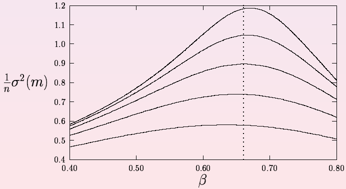
ISAW simulations

T Prellberg and J Krawczyk, PRL 92 (2004) 120602



- 2d ISAW up to $n = 1024$
- One simulation suffices
- 400 orders of magnitude

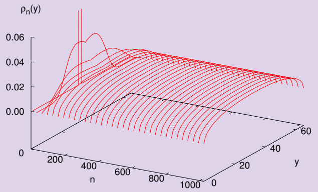
(only 2d shown, 3d similar)

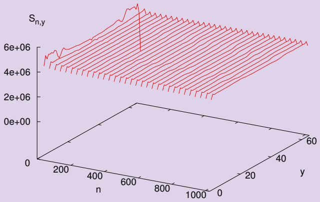


Simulation results: SAW in a strip

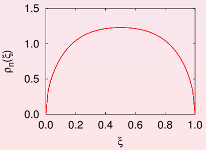
T Prellberg et al, in: Computer Simulation Studies in Condensed Matter Physics XVII, Springer Verlag, 2006

- 2d SAW in a strip: strip width 64, up to $n = 1024$





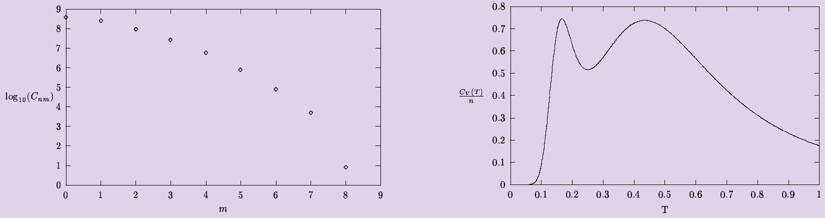
- Scaled endpoint density



HP model simulations

T Prellberg et al, in: Computer Simulation Studies in Condensed Matter Physics XVII, Springer Verlag, 2006

- Engineered sequence HPHPHHPHPHHPPH in $d = 3$:

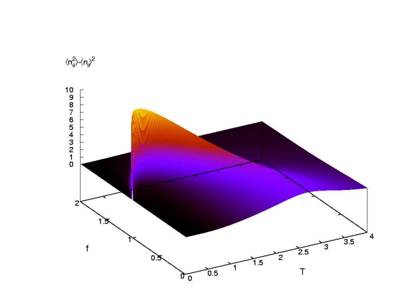


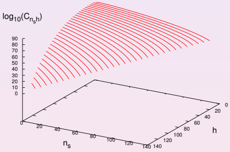
- Investigated other sequences up to $N \approx 100$ in $d = 2$ and $d = 3$
- Collapsed regime accessible
- Reproduced known ground state energies
- Obtained density of states $C_{n,m}$ over large range ($\approx 10^{30}$)

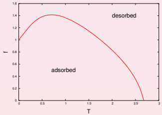
2-Dimensional Density of States

J Krawczyk et al, JSTAT (2004) P10004

- Force-induced desorption of adsorbed polymers
  - Relevance: optical tweezers, AFM; related to DNA unzipping
- 3-dim polymer in a half space, one simulation, up to $n = 256$
  - Fluctuations of surface coverage





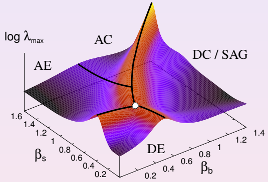


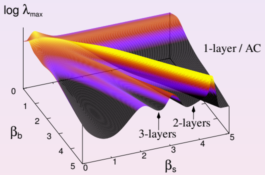
2-Dimensional Density of States

J Krawczyk et al, Europhys Lett 70 (2005) 726-732

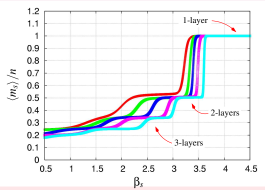
AL Owczarek et al, J Phys A 40 (2007) 13257-13267

- Layering transitions of adsorbed polymers in poor solvents





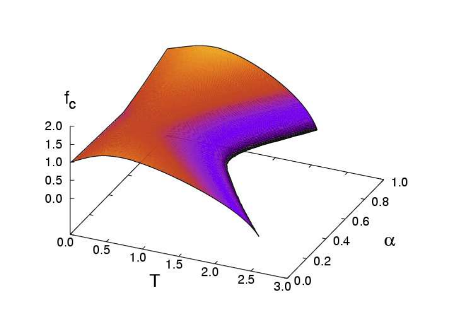
- whole phase diagram at once
- low temperatures accessible
- hierarchy of layering transitions
- resolved controversy over "surface attached globule"

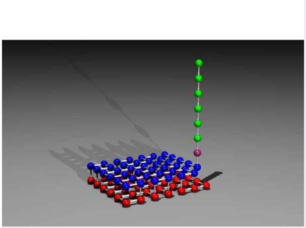


3-Dimensional Density of States

J Krawczyk et al, JSTAT (2005) P05008

- Pulling adsorbing and collapsing polymers off a surface





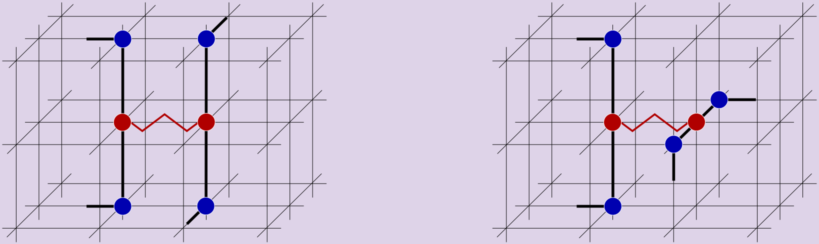
$\epsilon_s = \alpha$, $\epsilon_b = 1 - \alpha$

- simulations up to $n = 91$ (4-dimensional histogram)
- interplay of (both force-induced and thermal) desorption ($\alpha = 1$) and stretching ($\alpha = 0$)

Hydrogen-bond type interactions

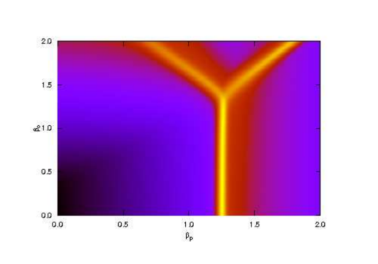
J Krawczyk et al, Phys. Rev. E 76 (2007) 051904

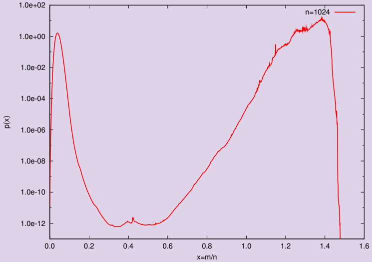
Hydrogen-like interactions between *straight* segments of the walk



Distinguish parallel and orthogonal interactions: layering of β-sheets

Hydrogen-bond type interactions (ctd.)





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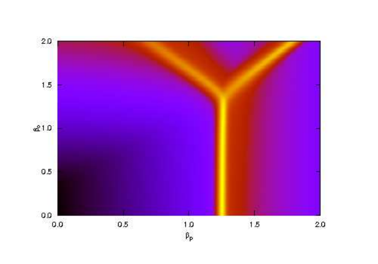
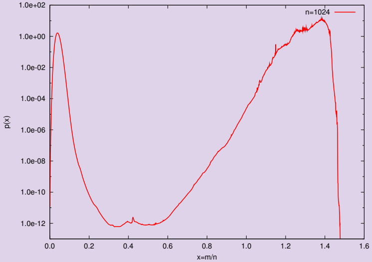
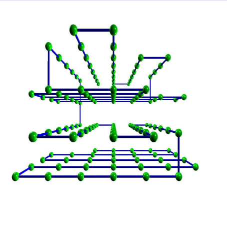
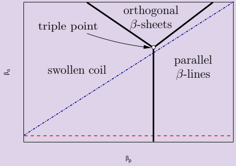
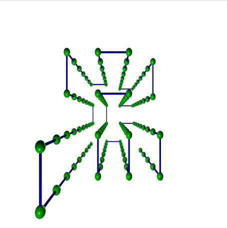






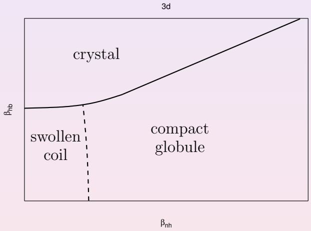


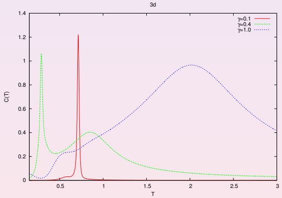


Hydrogen-bond vs. isotropic interactions

J Krawczyk et al, JSTAT (2007) P09016

Interplay of hydrogen-bond interactions (equal strength parallel and orthogonal) with isotropic interactions





First-order globule-crystal transition

Alternative Lattice Models

Alternative lattice models

General "universality" assumption:

A Model of a Polymer in Solution

Random Walk + Excluded Volume + Short Range Attraction

Alternative lattice models

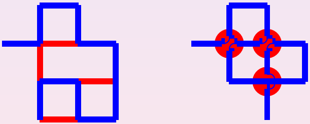
General "universality" assumption:

A Model of a Polymer in Solution

Random Walk + Excluded Volume + Short Range Attraction

- Canonical model: interacting self-avoiding walks (ISAW)
- Alternative model: interacting self-avoiding trails (ISAT)

vertex avoidance (walks) $\Leftrightarrow$ edge avoidance (trails)



nearest-neighbour interaction $\Leftrightarrow$ contact interaction

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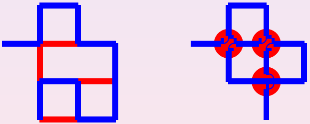

nearest-neighbour interaction $\Leftrightarrow$ contact interaction

- simulations of ISAW confirm predictions from theory

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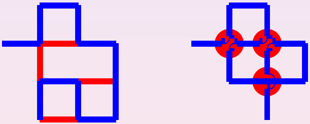


nearest-neighbour interaction $\Leftrightarrow$ contact interaction

- simulations of ISAW confirm predictions from theory
- simulations of ISAT confound predictions from theory: SAW = SAT, but ISAW $\neq$ ISAT (different collapse exponents)

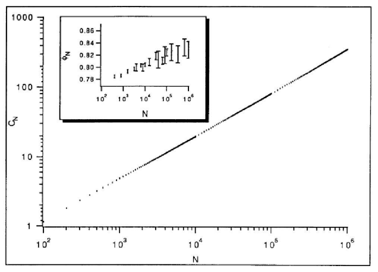
Simulations of ISAT

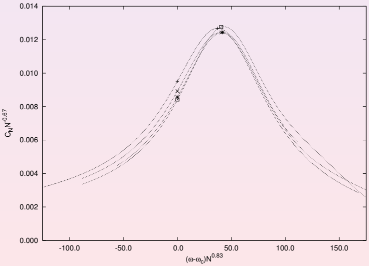
- At critical T_c, ISAT can be modelled as kinetic growth; simulations up to $N = 10^6$

AL Owczarek and T Prellberg, J. Stat. Phys. 79 (1995) 951-967

- Pruned Enriched Rosenbluth Method enables simulations for $T \neq T_c$; new simulations up to $N = 2 \cdot 10^6$

AL Owczarek and T Prellberg, Physica A **373** (2007) 433-438





A Proposal of a New Model

J Krawczyk et al, Phys Rev Lett 96 (2006) 240603

- ISAW/ISAT contain on-site and nearest-neighbour interactions
- The field-theory is formulated with purely local interactions
- Field theory is equivalent to Edwards model:
  - Brownian motion + suppression of self-intersections + attractive interactions
  - field theory is $\phi^4 - \phi^6$ $O(n)$-model for $n \to 0$

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Formulate a lattice model with purely local interactions

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Formulate a lattice model with purely local interactions

- Site-weighted random walk:
  - lattice random walk weighted by multiple visits of sites
  - few visits to same site are favoured (attractive interaction)
  - too many visits are disfavoured (excluded volume)

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(technically, this is an extension of a Domb-Joyce model)

Site-Weighted Random Walk

- An N-step random walk $\xi = (\vec{\xi}_0, \vec{\xi}_1, \ldots, \vec{\xi}_N)$ induces a density-field ϕ_ξ on the lattice sites $\vec{x}$ via

$$\phi_\xi(\vec{x}) = \sum_{i=0}^{N} \delta_{\vec{\xi}_i, \vec{x}}$$

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- Define the energy as a functional of the field $\phi = \phi_\xi$

$$E(\xi) = \sum_{\vec{x}} f\left(\phi(\vec{x})\right)$$

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- Define the energy as a functional of the field $\phi = \phi_\xi$

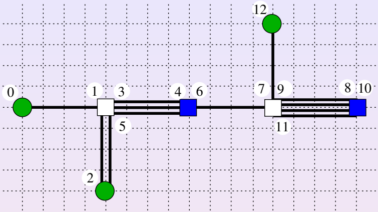
$$E(\xi) = \sum_{\vec{x}} f\left(\phi(\vec{x})\right)$$

- Incorporate self-avoidance and attraction via choice of $f(t)$. For example, $f(0) = f(1) = 0$,

$$f(2) = \varepsilon_1 \ , \quad f(3) = \varepsilon_2 \ ,$$

and $f(t \geq 4) = \infty$.

Site-Weighted Random Walk (ctd)



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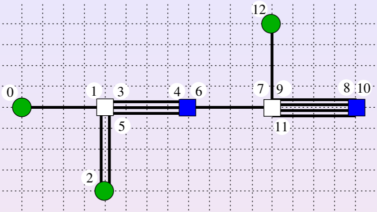
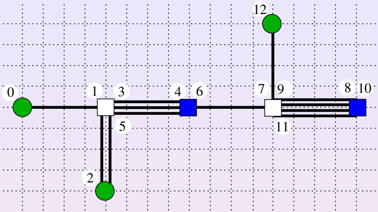


- Partition function

$$Z_N(\beta) = \sum_{m_1,m_2} C_{N,m_1,m_2} e^{-\beta(m_1\varepsilon_1+m_2\varepsilon_2)}$$

with density of states C_{N,m_1,m_2}

Site-Weighted Random Walk (ctd)



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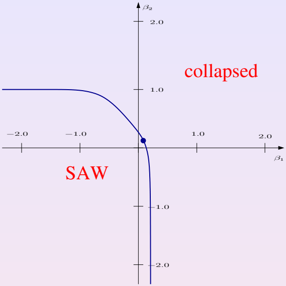
  with density of states C_{N,m_1,m_2}

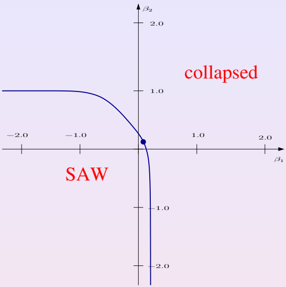
- Simulate two variants of the model on the square and simple cubic lattice
  - random walks with immediate reversal allowed (RA2, RA3)
  - random walks with immediate reversal forbidden (RF2, RF3)

SWRW in 3d, reversal forbidden (RF3)



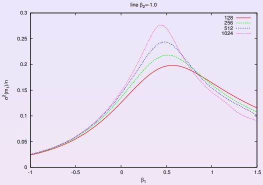
Phase diagram

SWRW in 3d, reversal forbidden (RF3)



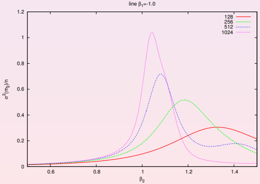
Phase diagram

$\beta_2 = -1.0$:



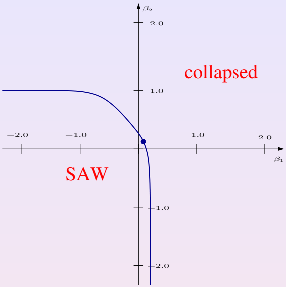
2nd order transition

$\beta_1 = -1.0$:

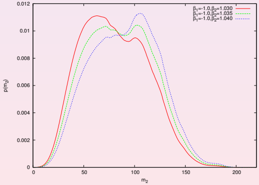


1st order transition

SWRW in 3d, reversal forbidden (RF3)

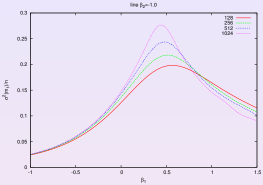


Phase diagram



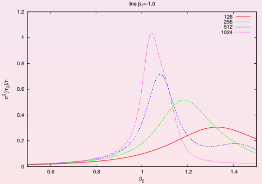
bimodal distribution

$\beta_2 = -1.0$:



2nd order transition

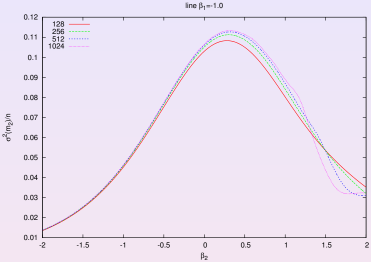
$\beta_1 = -1.0$:

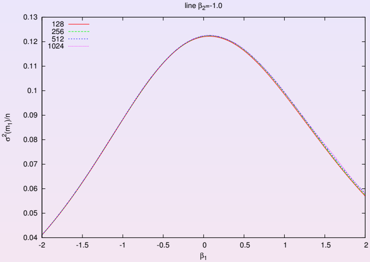


1st order transition

SWRW in 2d, reversal allowed (RA2)

We find a smooth crossover:

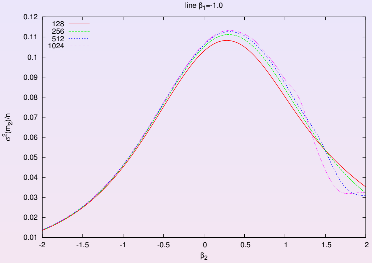


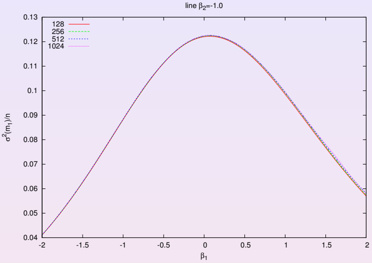


Both 1st order and 2nd order transitions have disappeared!

SWRW in 2d, reversal allowed (RA2)

We find a smooth crossover:





Both 1st order and 2nd order transitions have disappeared!

RA3 and RF2

2nd order transition disappears as in RA2

1st order transition weakens

SWRW summarised

Model	2d	3d
RA	no transitions	one transition
RF	one transition	two transitions

SWRW summarised

Model	2d	3d
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Unexpected and intriguing behaviour

Changing the dimension and/or allowing reversals removes the phase transition

SWRW summarised

Model	2d	3d
RA	no transitions	one transition
RF	one transition	two transitions

Unexpected and intriguing behaviour

Changing the dimension and/or allowing reversals removes the phase transition

Many open questions remain . . .

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