Simulating models of polymer collapse

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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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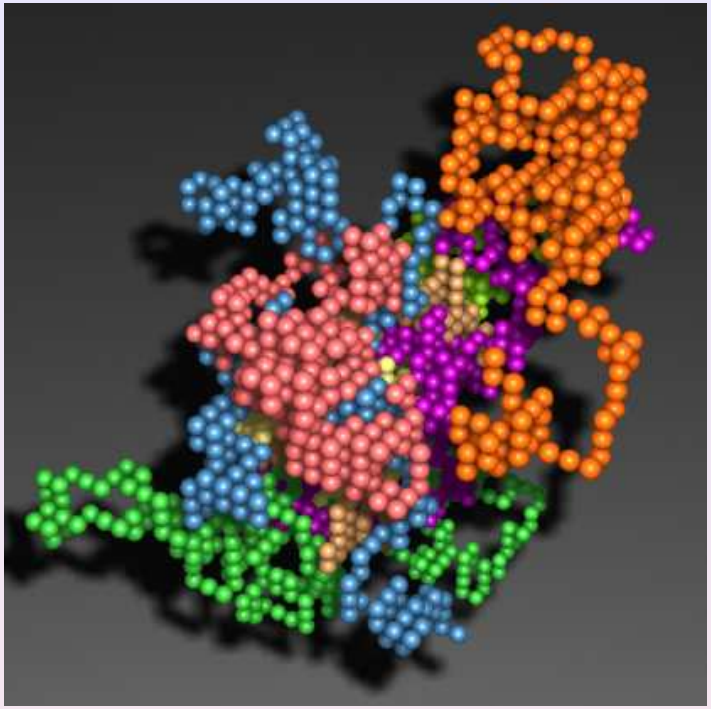
- Polymers in solution:
  - Equilibrium statistical mechanics, lattice model
- Algorithm:
  - Stochastic growth & flat histogram (PERM/flatPERM)
- Simulation of the canonical model:
  - Interacting self-avoiding walks (ISAW)
- Applications:
  - Protein groundstates (HP model)
  - Bulk vs surface phenomena:
    - confined polymers, force-induced desorption, interplay of collapse and adsorption
  - 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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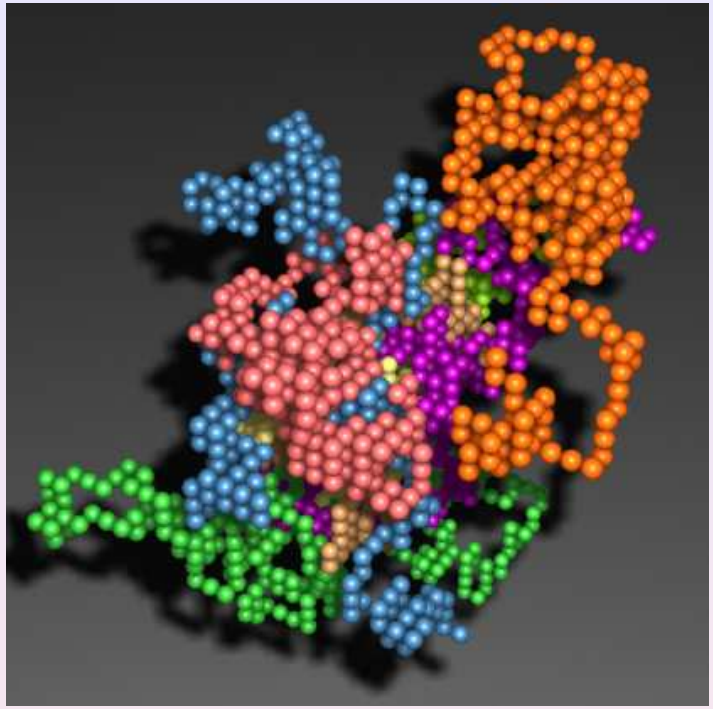
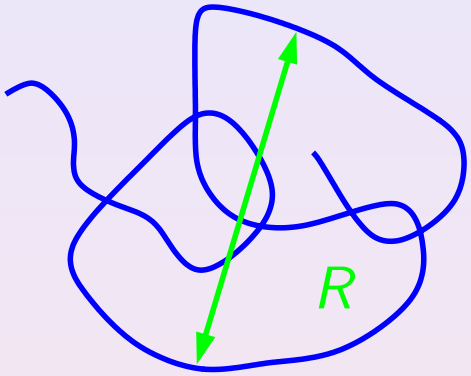


A Model of a Polymer in Solution

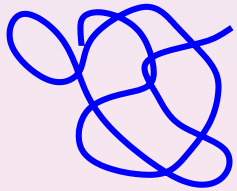
Random Walk + Excluded Volume + Short Range Attraction

Polymer Collapse, Coil-Globule Transition, Θ-Point

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



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



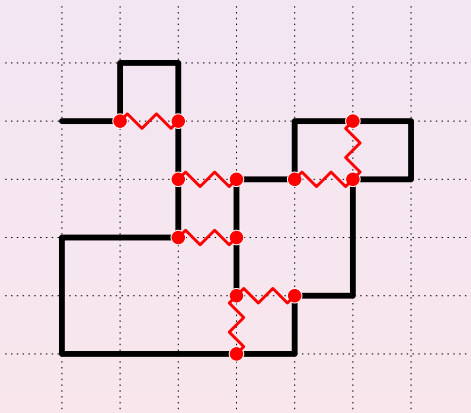
$T = T_c$:
Θ-polymer

$T < T_c$: 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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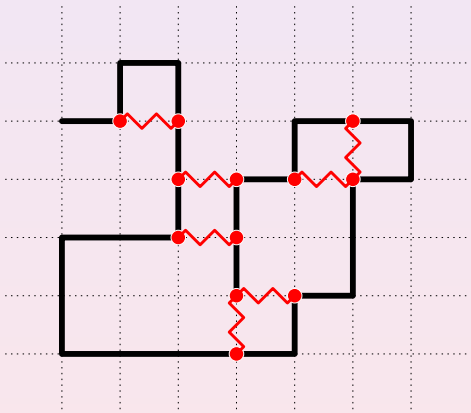
$$Z_N(\omega) = \sum_m C_{N,m}\omega^m$$

$C_{N,m}$ is the number of SAWs
with N steps and m interactions



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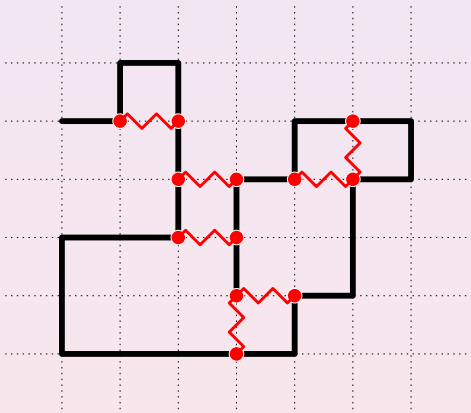

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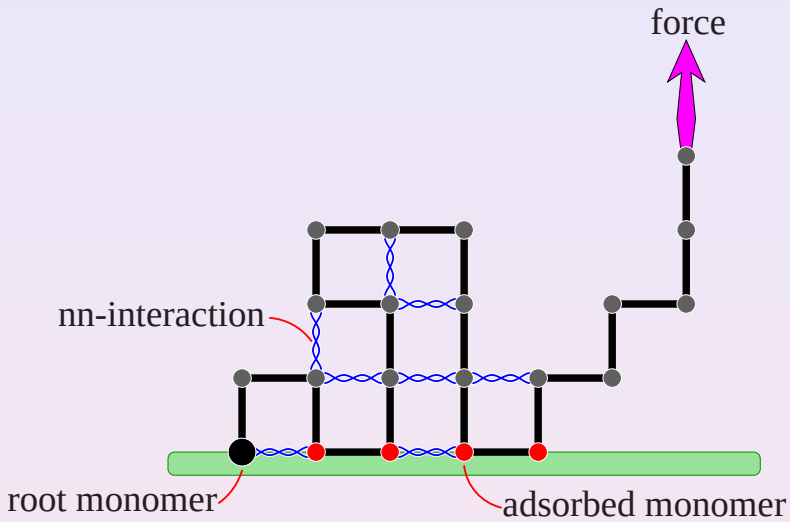
Thermodynamic Limit for a dilute solution:

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

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

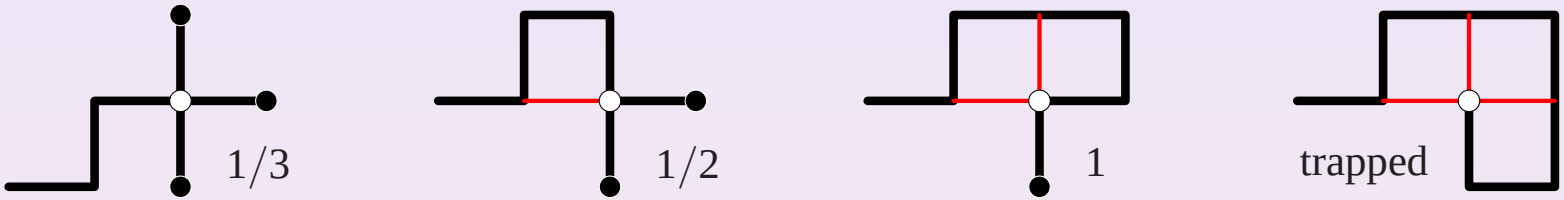
The Algorithm

PERM: "Go With The Winners"

PERM = Pruned and Enriched Rosenbluth Method

P Grassberger, Phys Rev E 56 (1997) 3682

- Rosenbluth Method: kinetic growth



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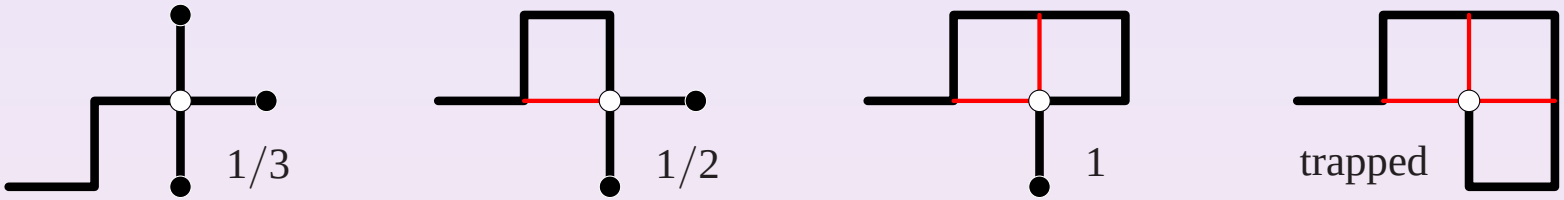

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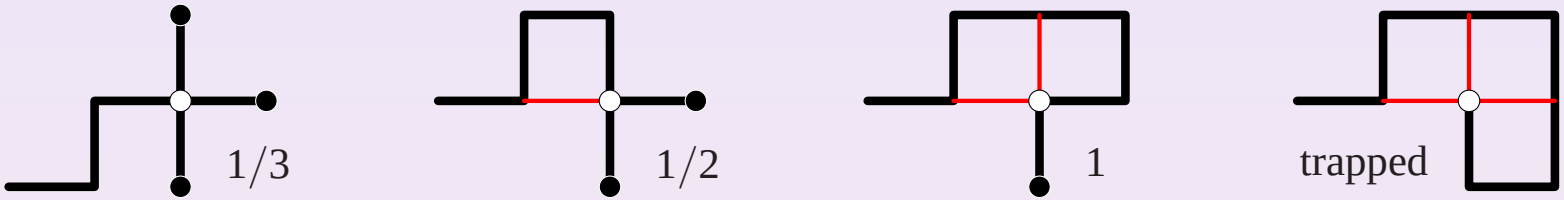

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Current work: flatPERM = flat histogram PERM

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

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  - Number of samples generated for each N is roughly constant
  - We have a 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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  - thermal PERM: estimate partition function $Z_N(\beta)$
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    - $Z_N^{est}(\beta) = \langle W \exp(-\beta E) \rangle_N$
    - $r = W_N^{(i)} \exp(-\beta E^{(i)}) / Z_N^{est}(\beta)$
- 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?

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There is little theory and this is notoriously difficult to simulate

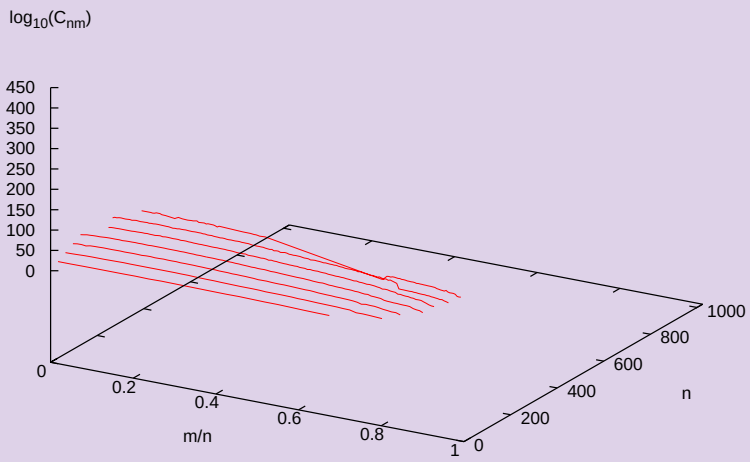
Simulations and Results

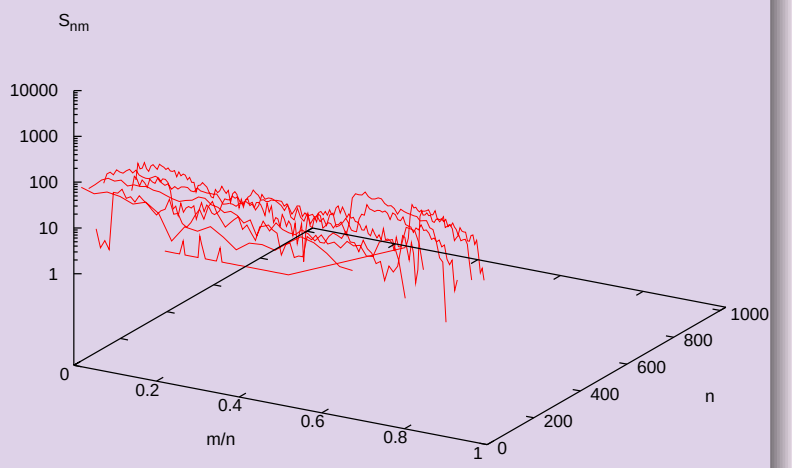
2d ISAW simulation up to $N = 1024$

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 $N = 1024$

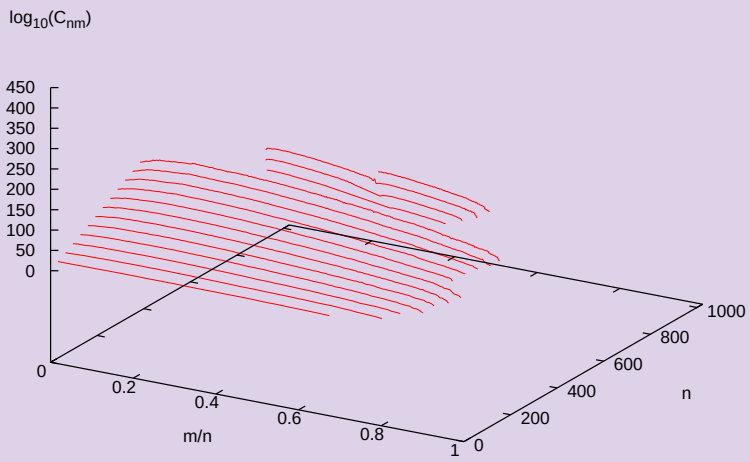
Total sample size: $1,000,000$

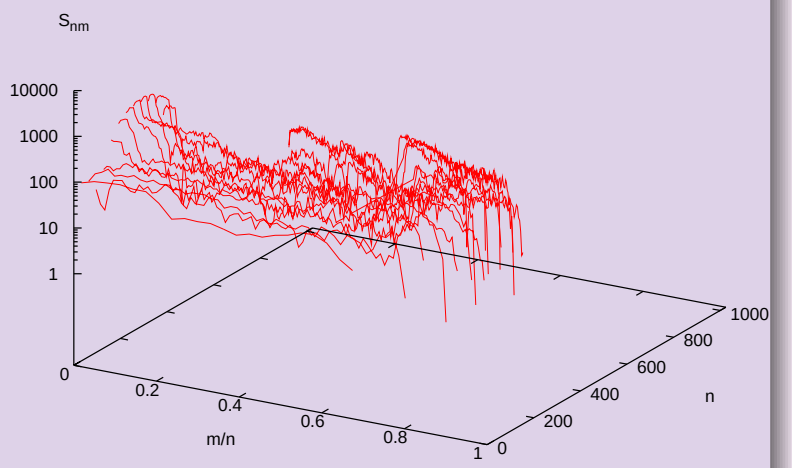




2d ISAW simulation up to $N = 1024$

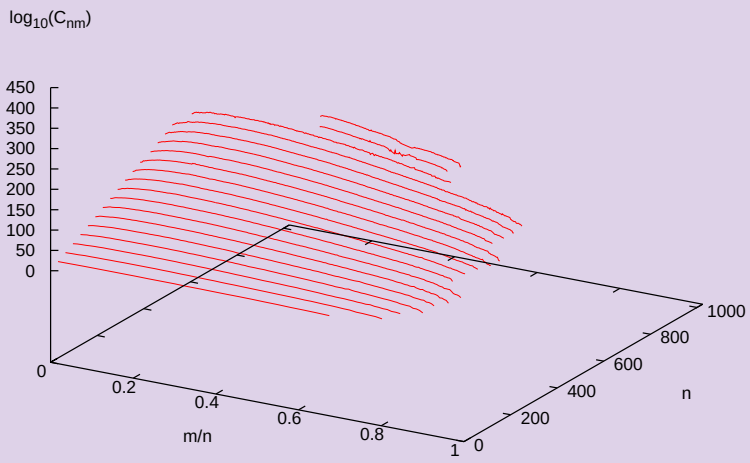
Total sample size: $10,000,000$

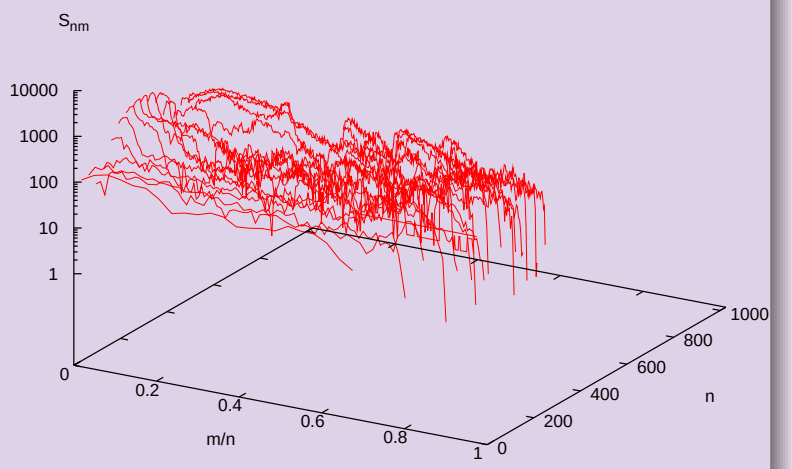




2d ISAW simulation up to $N = 1024$

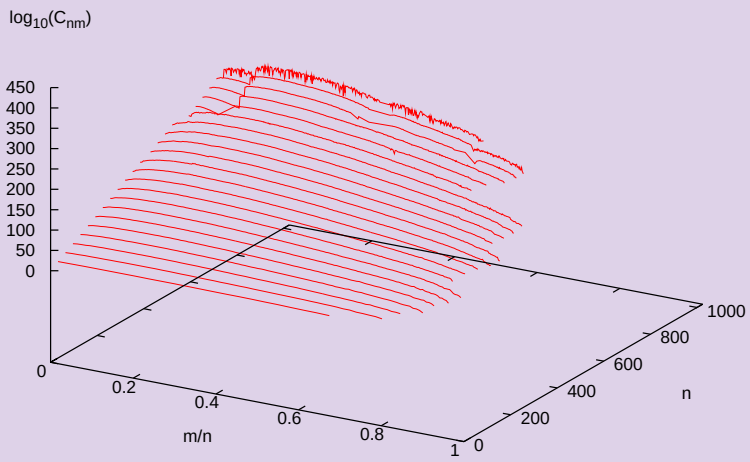
Total sample size: $20,000,000$

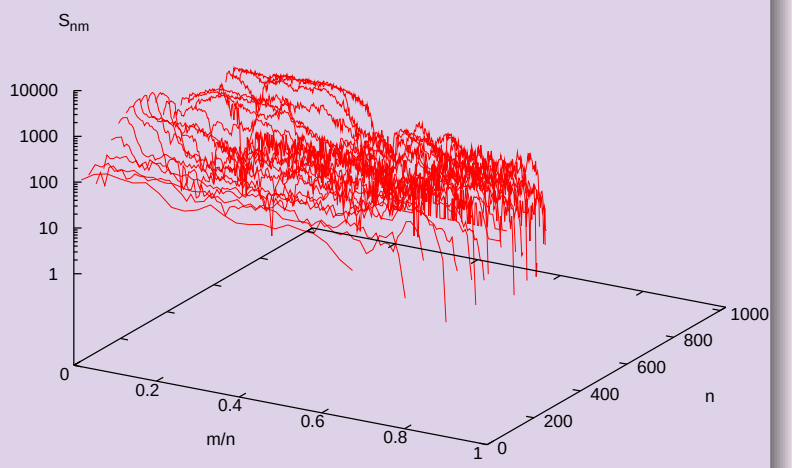




2d ISAW simulation up to $N = 1024$

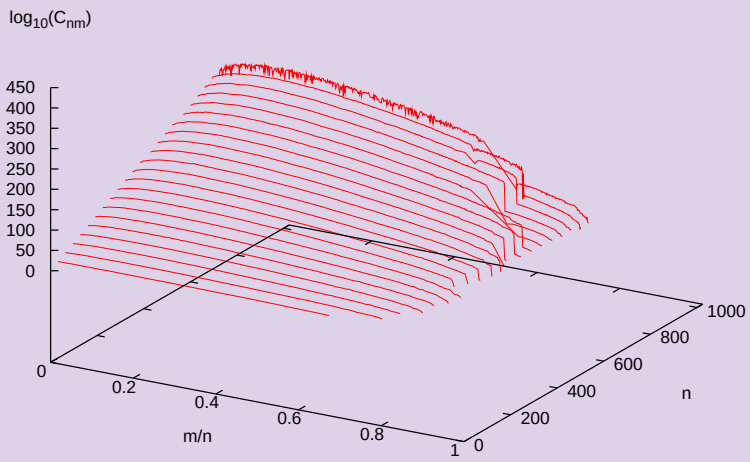
Total sample size: $30,000,000$

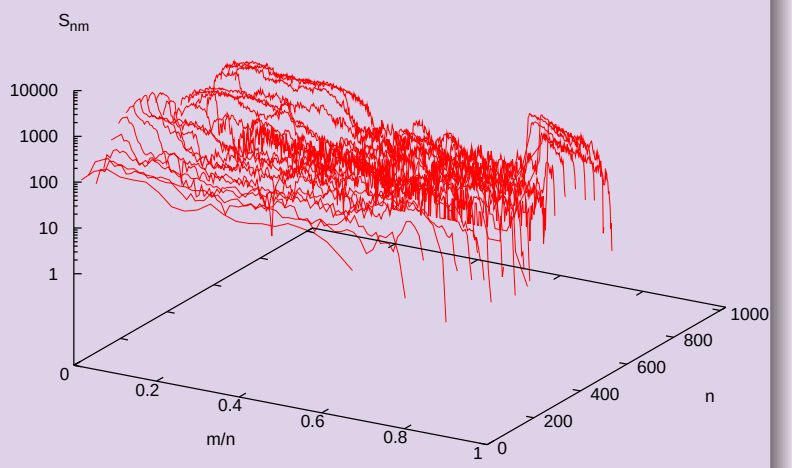




2d ISAW simulation up to $N = 1024$

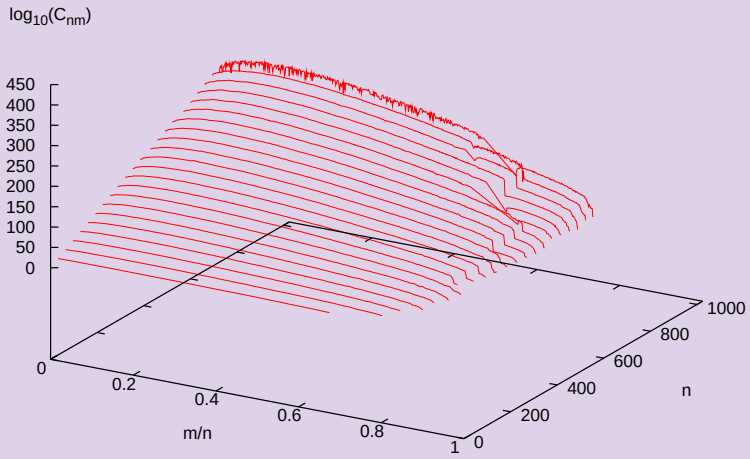
Total sample size: $40,000,000$

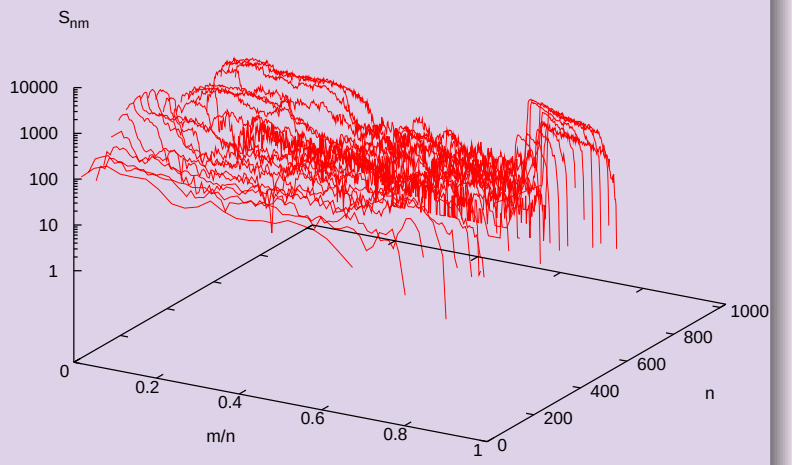




2d ISAW simulation up to $N = 1024$

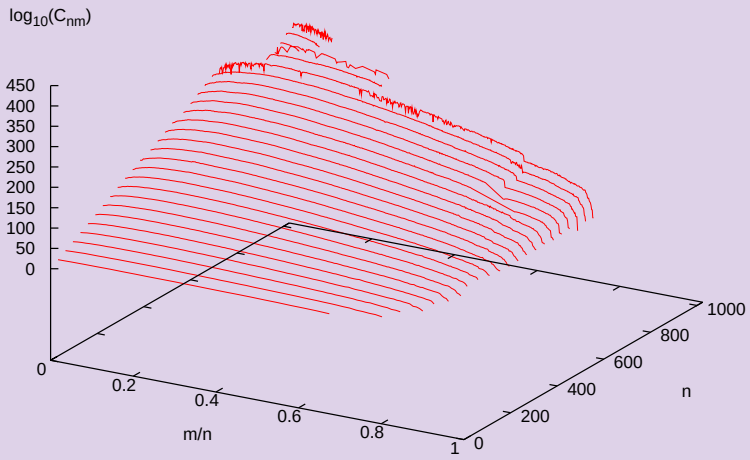
Total sample size: $50,000,000$

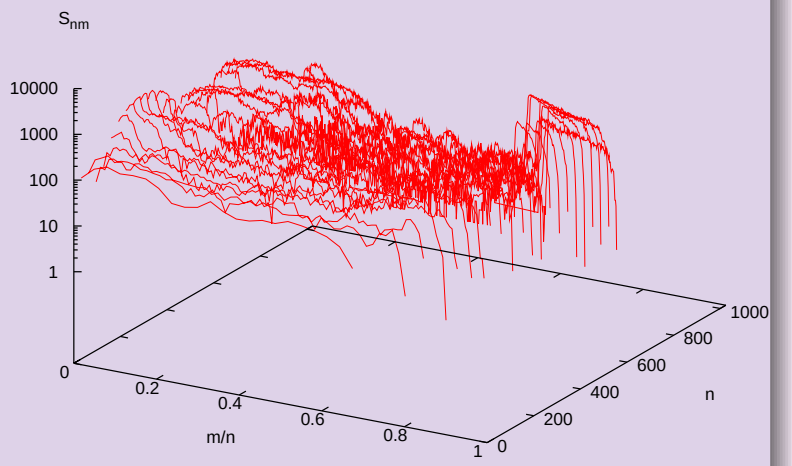




2d ISAW simulation up to $N = 1024$

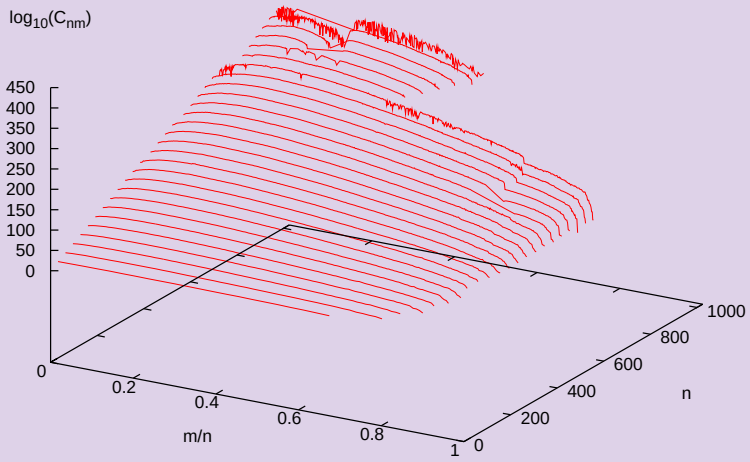
Total sample size: $60,000,000$

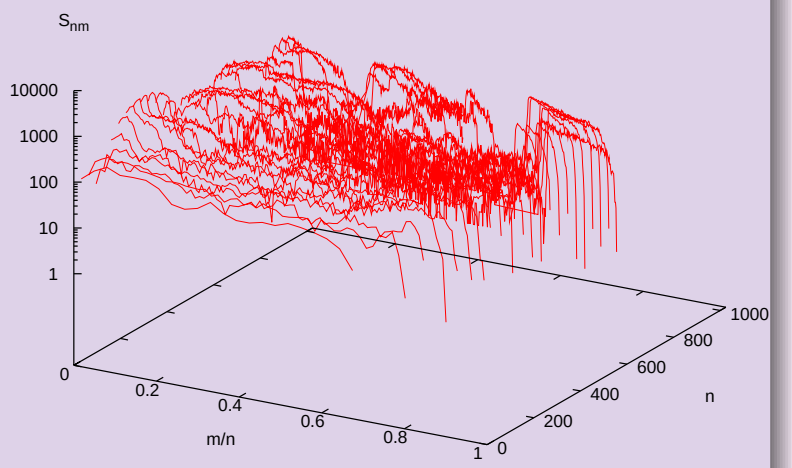




2d ISAW simulation up to $N = 1024$

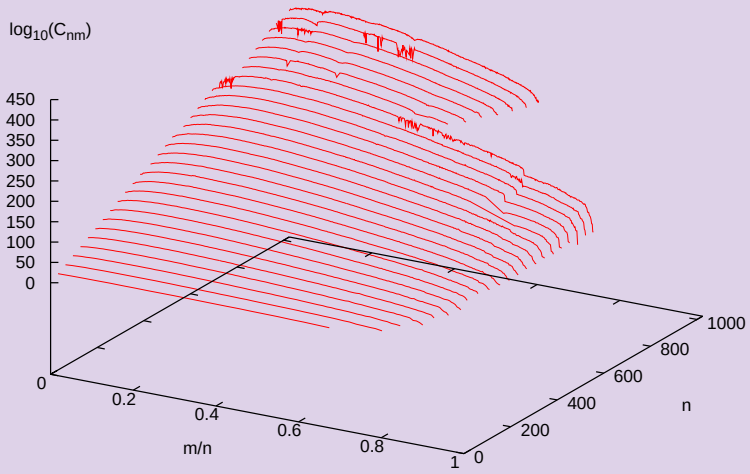
Total sample size: $70,000,000$

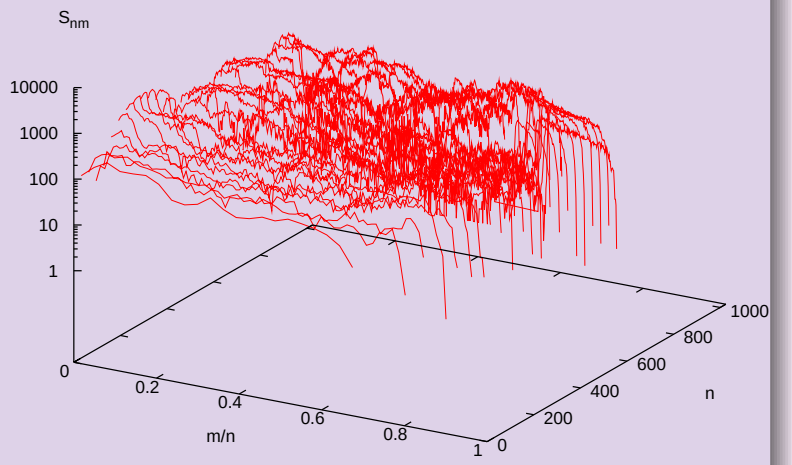




2d ISAW simulation up to $N = 1024$

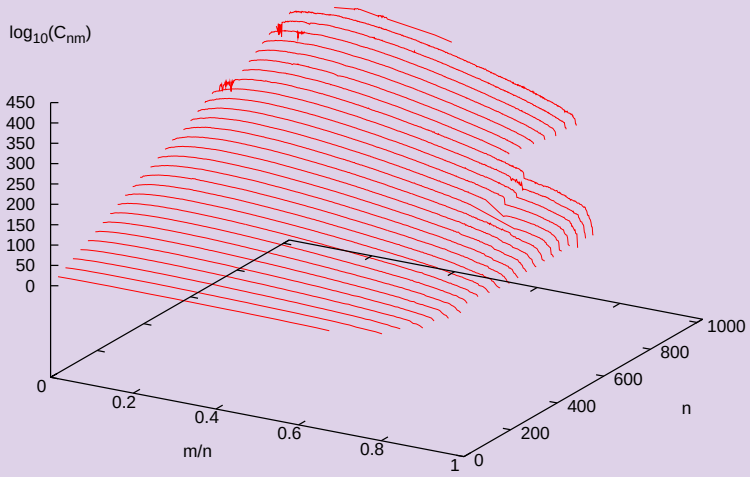
Total sample size: $80,000,000$

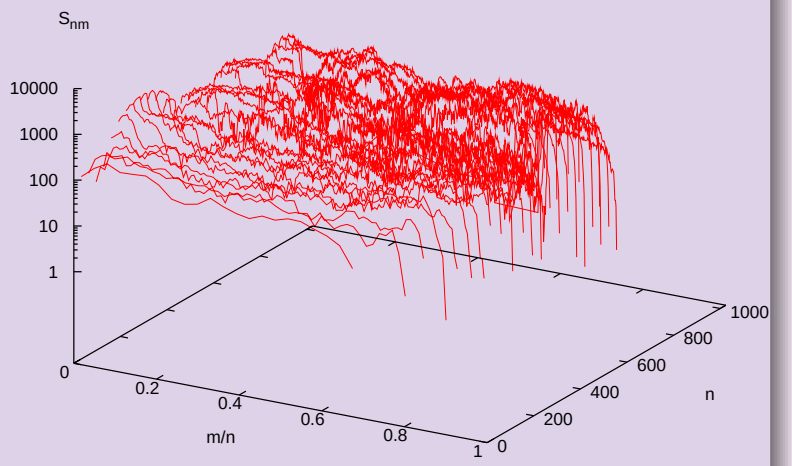




2d ISAW simulation up to $N = 1024$

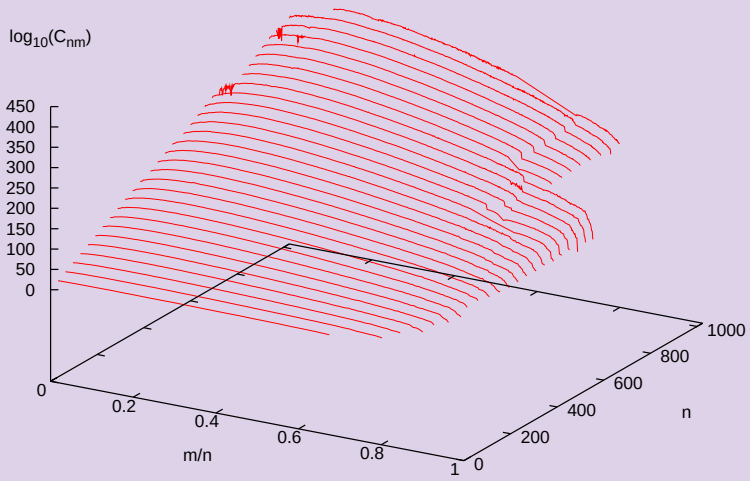
Total sample size: $90,000,000$

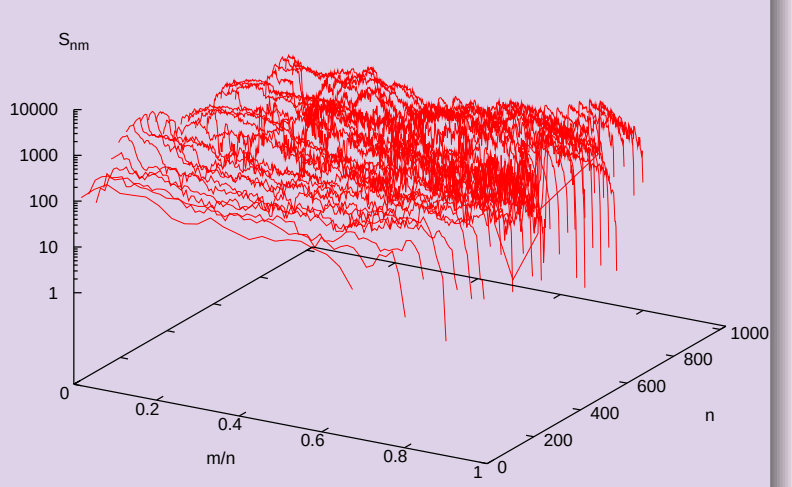




2d ISAW simulation up to $N = 1024$

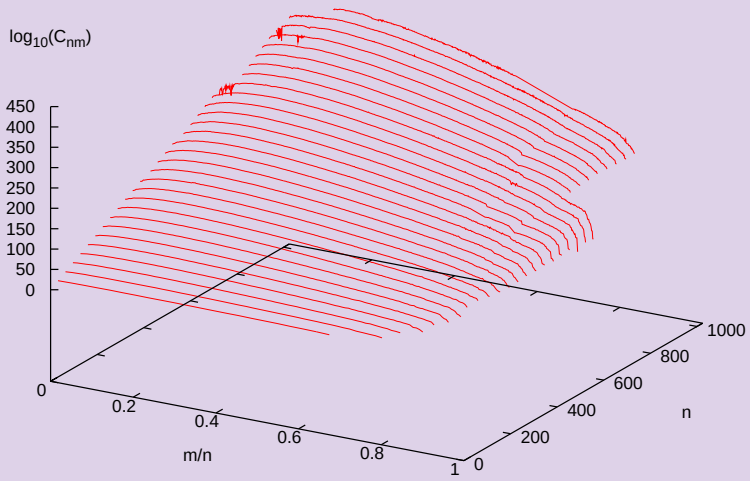
Total sample size: $100,000,000$

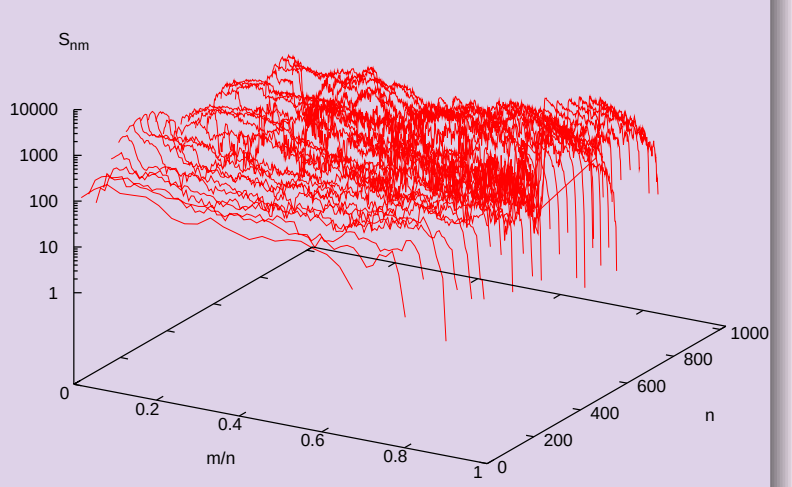




2d ISAW simulation up to $N = 1024$

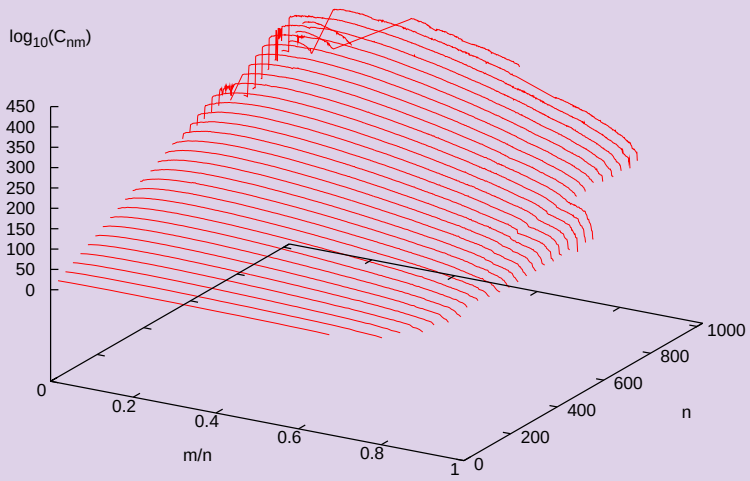
Total sample size: $110,000,000$

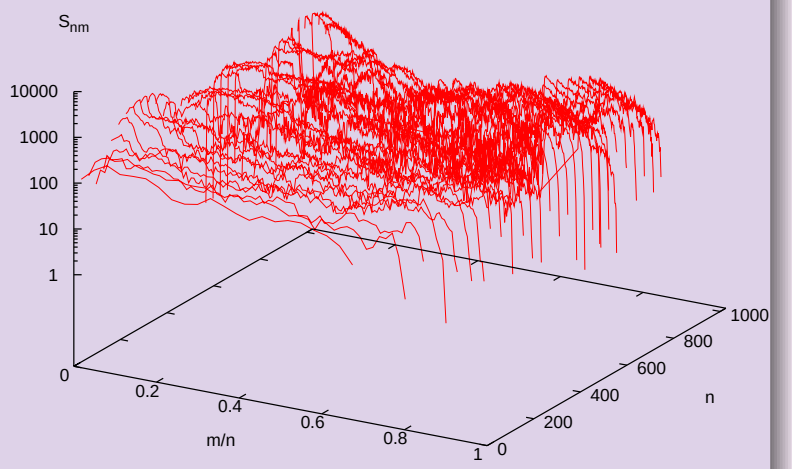




2d ISAW simulation up to $N = 1024$

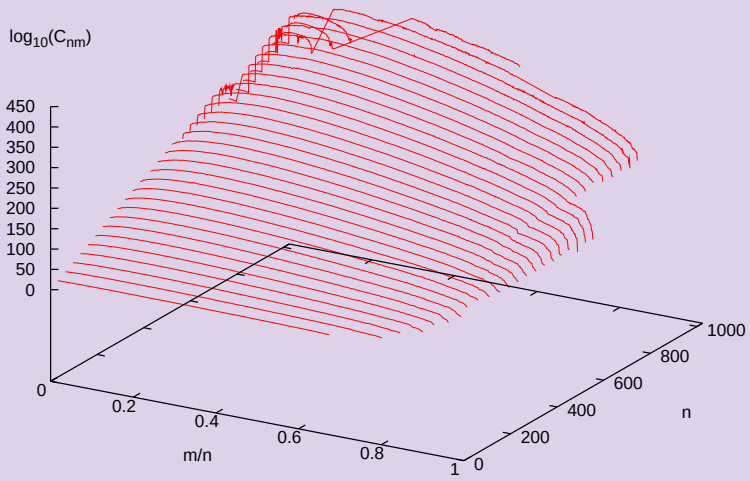
Total sample size: $120,000,000$

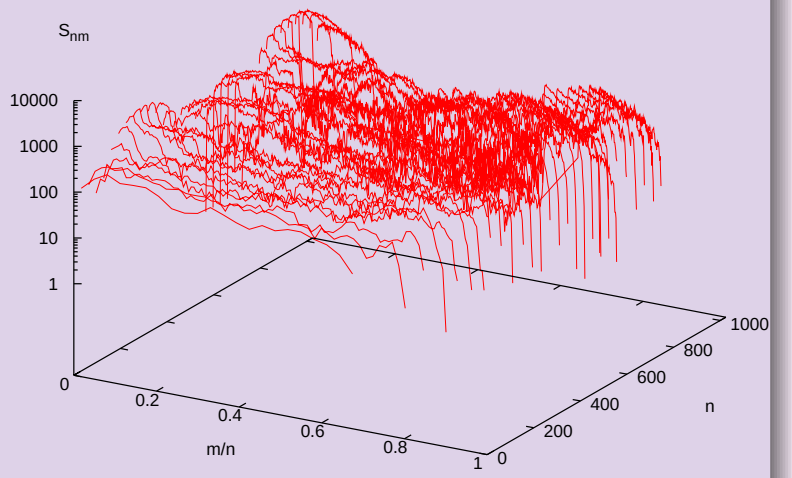




2d ISAW simulation up to $N = 1024$

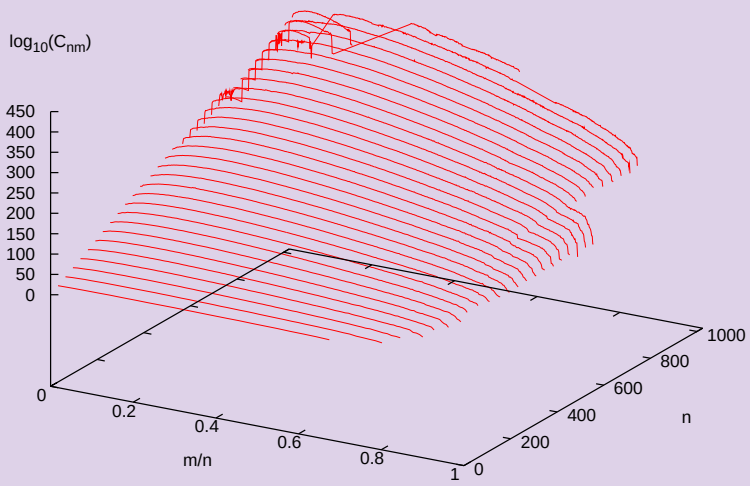
Total sample size: $130,000,000$

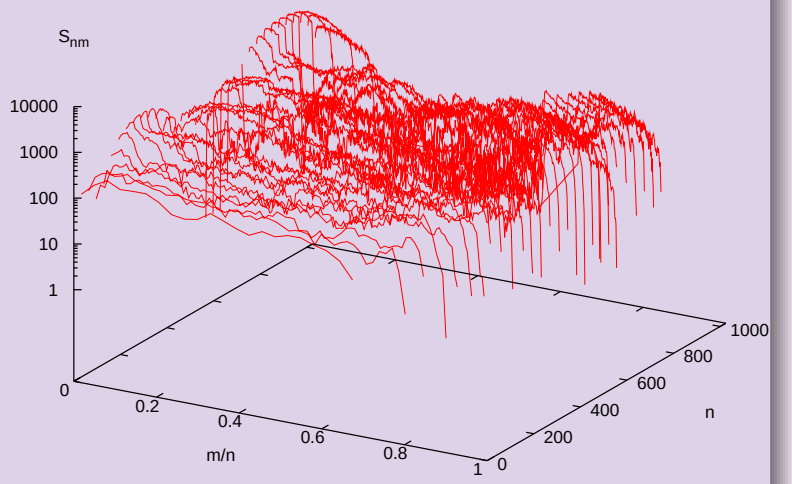




2d ISAW simulation up to $N = 1024$

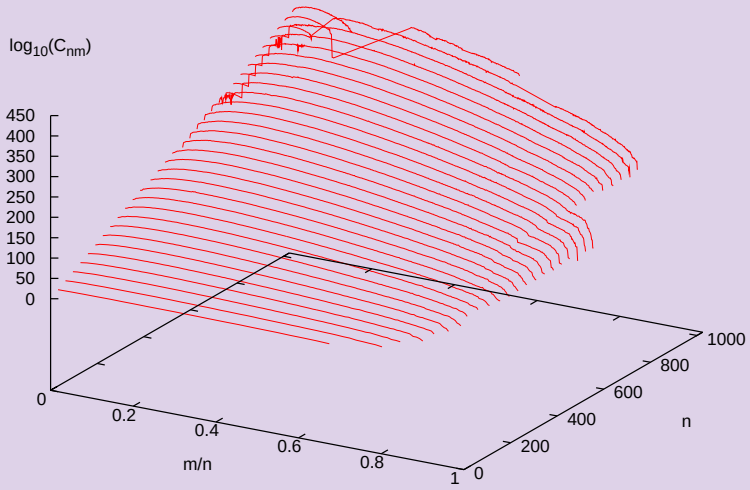
Total sample size: $140,000,000$

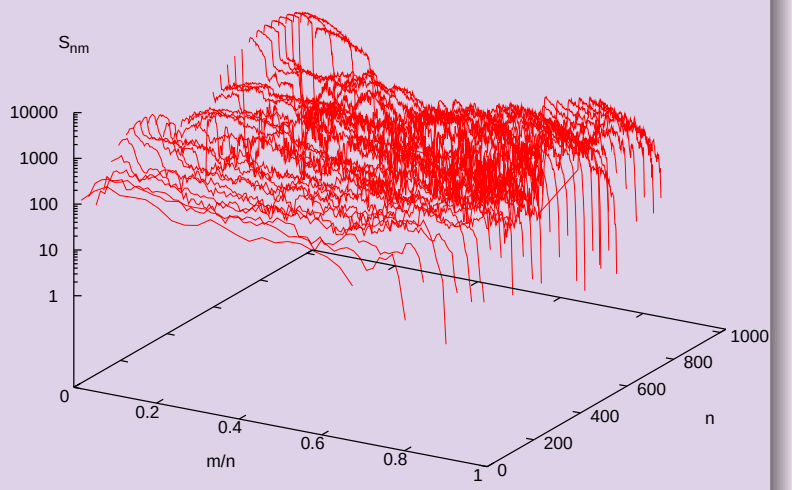




2d ISAW simulation up to $N = 1024$

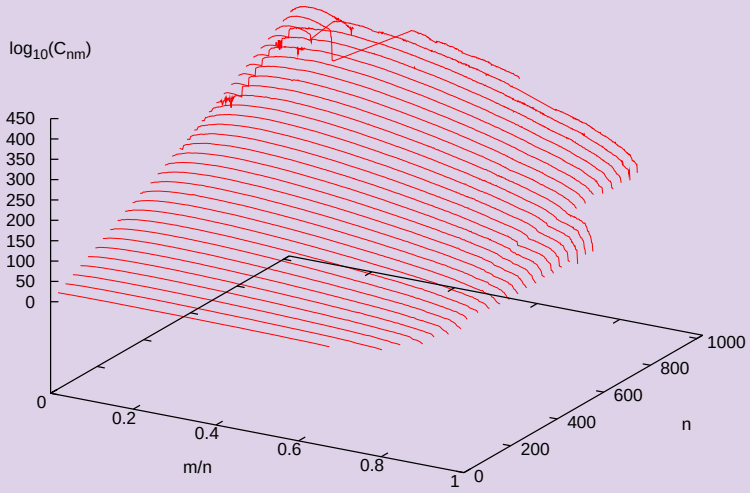
Total sample size: $150,000,000$

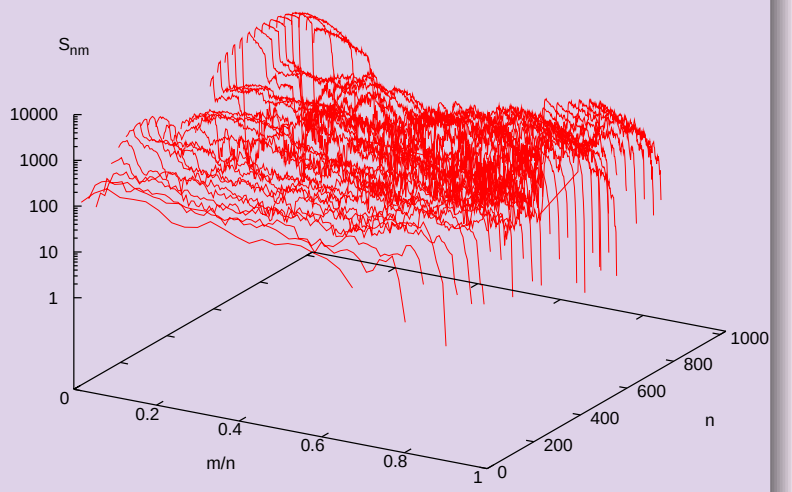




2d ISAW simulation up to $N = 1024$

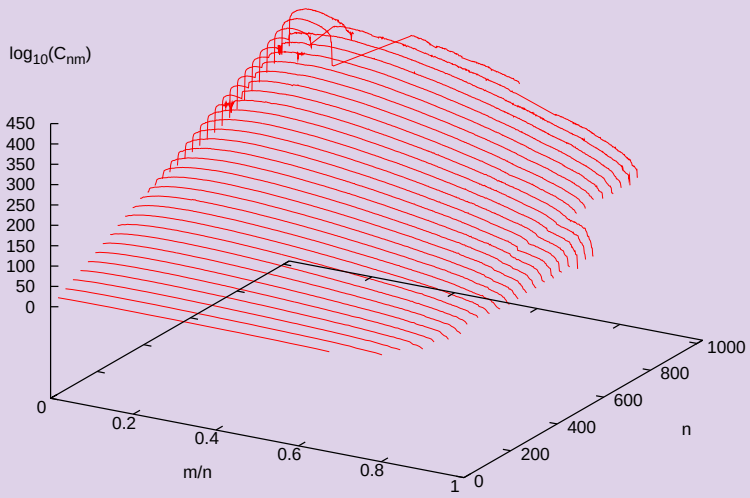
Total sample size: $160,000,000$

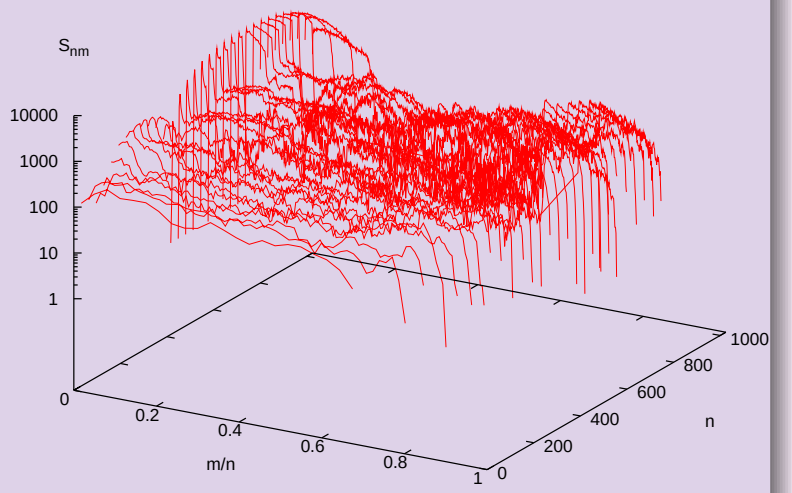




2d ISAW simulation up to $N = 1024$

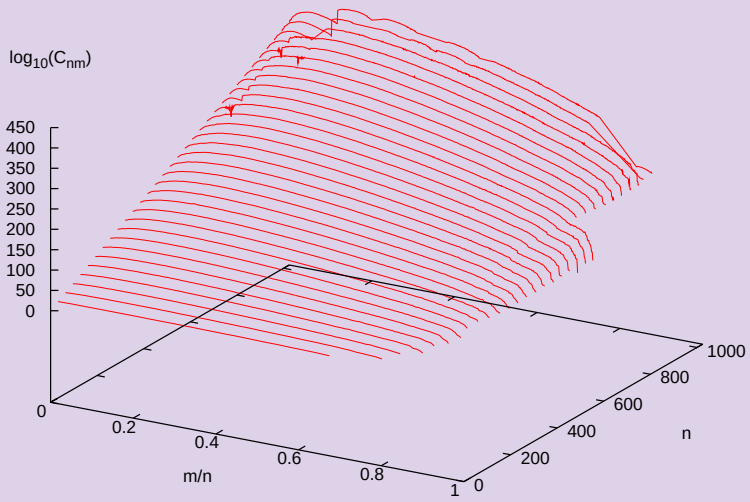
Total sample size: $170,000,000$

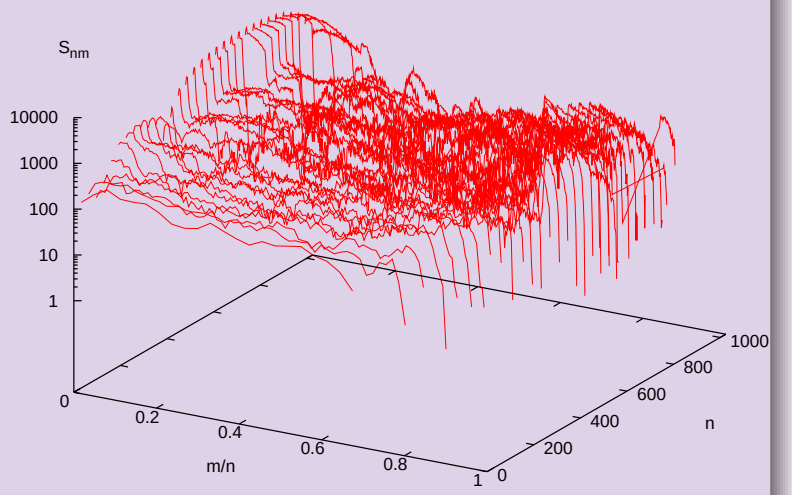




2d ISAW simulation up to $N = 1024$

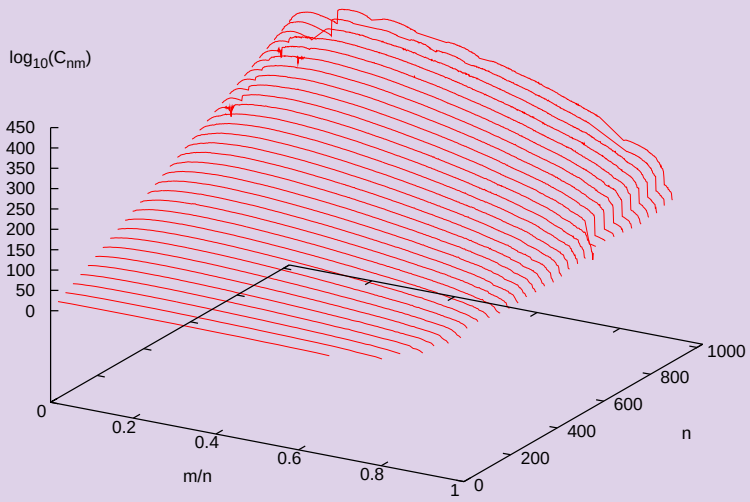
Total sample size: $180,000,000$

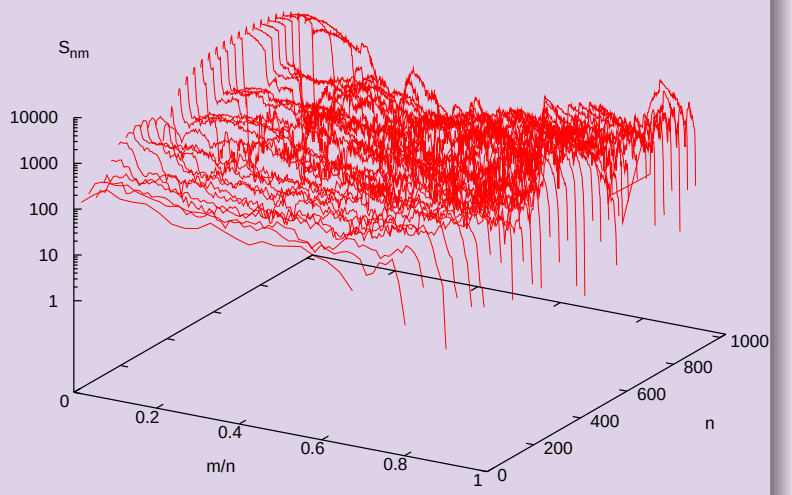




2d ISAW simulation up to $N = 1024$

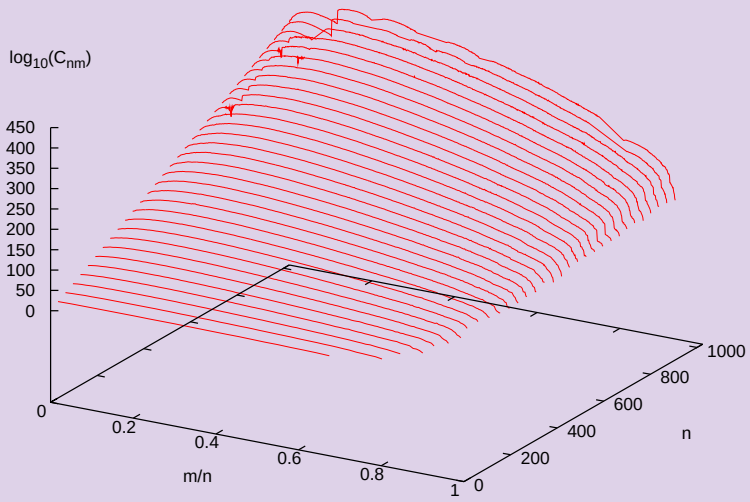
Total sample size: $190,000,000$

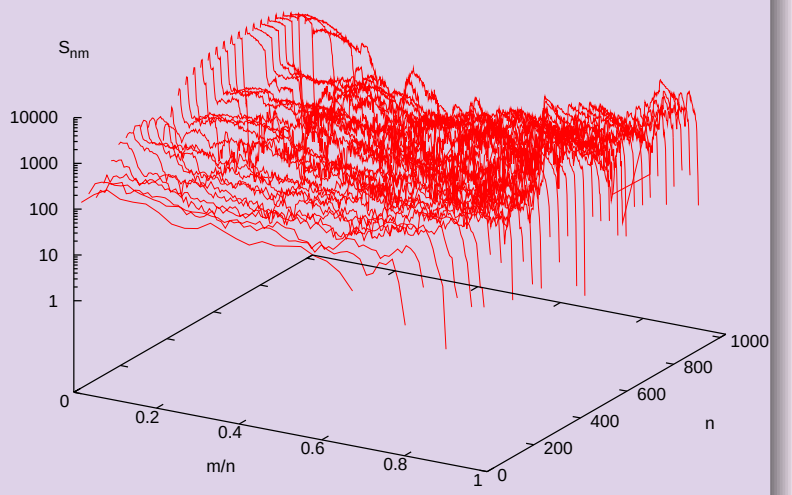




2d ISAW simulation up to $N = 1024$

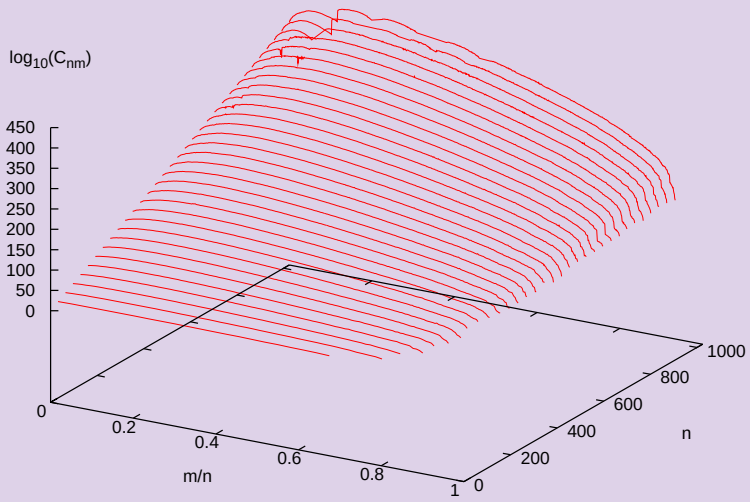
Total sample size: $200,000,000$

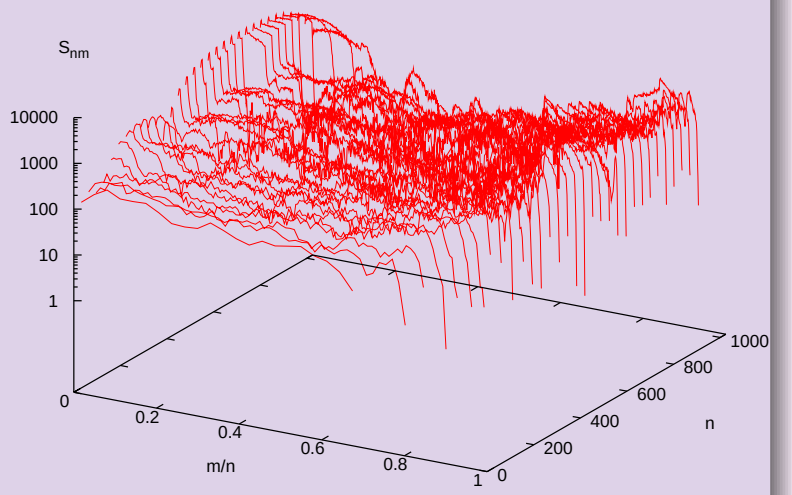




2d ISAW simulation up to $N = 1024$

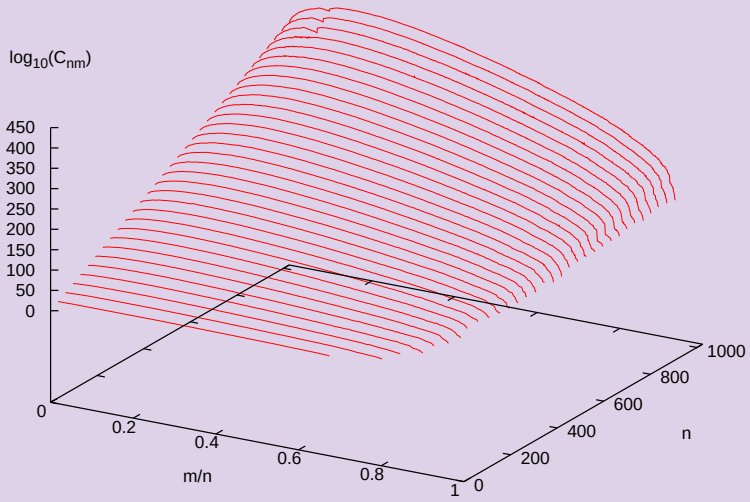
Total sample size: $210,000,000$

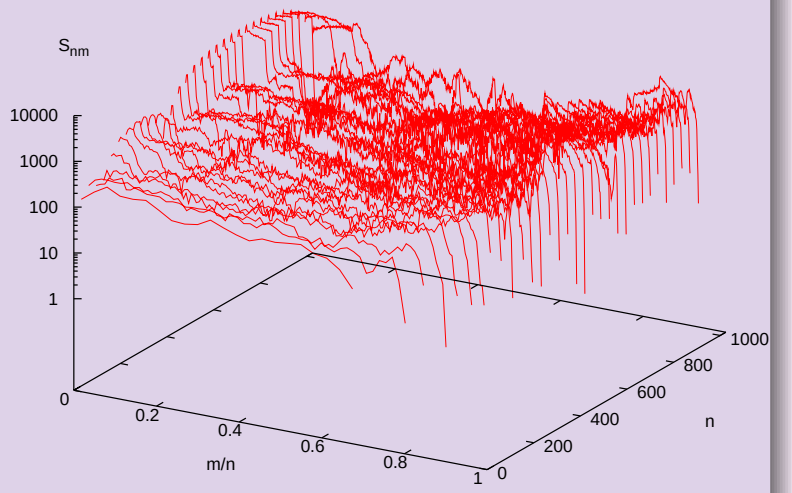




2d ISAW simulation up to $N = 1024$

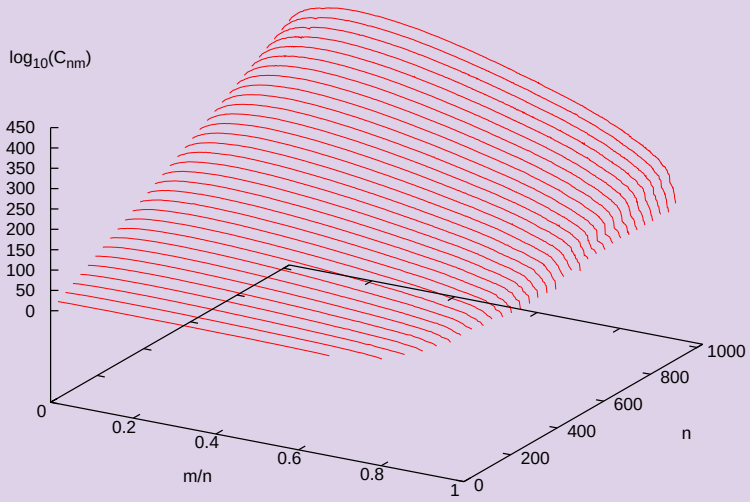
Total sample size: $220,000,000$

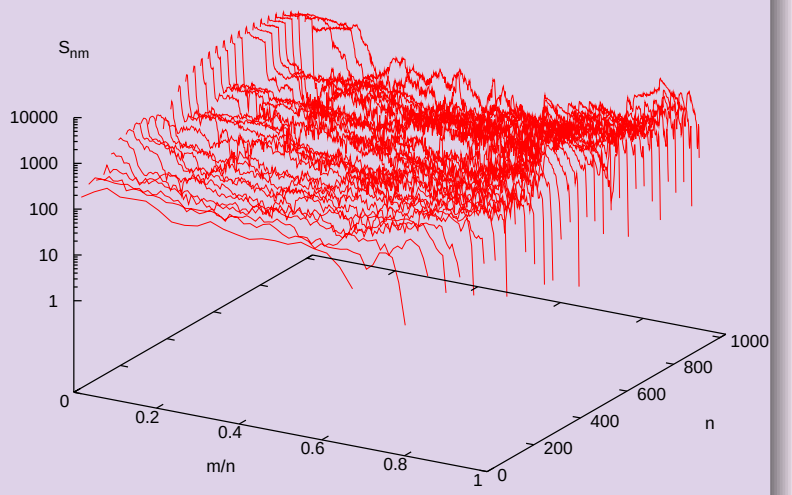




2d ISAW simulation up to $N = 1024$

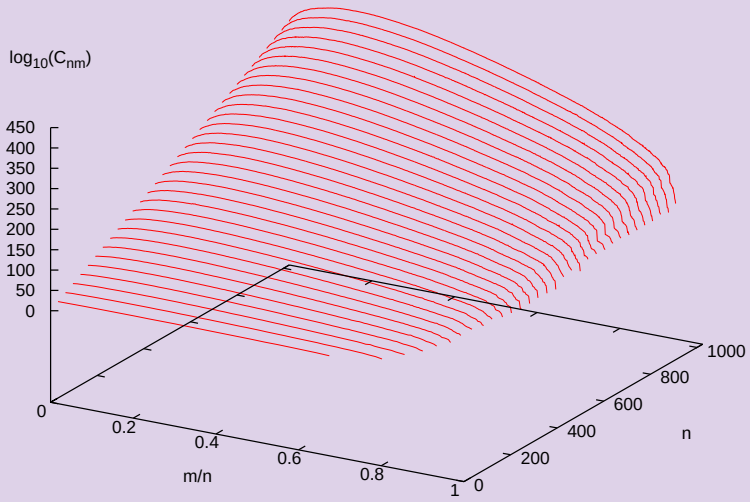
Total sample size: $230,000,000$

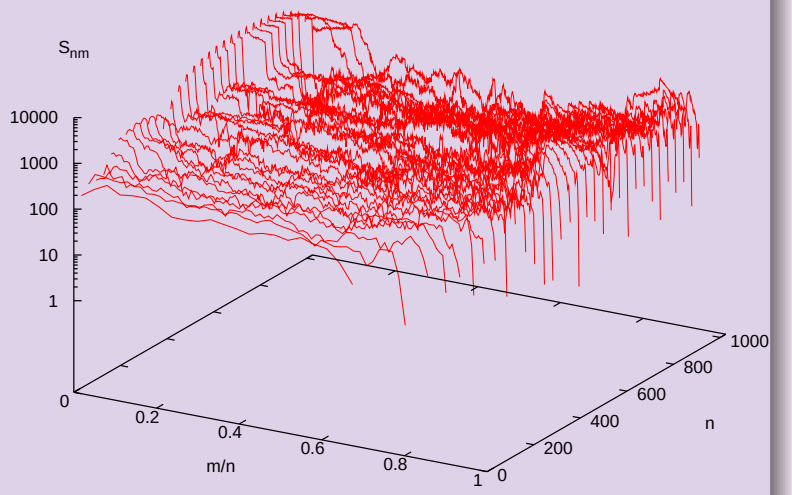




2d ISAW simulation up to $N = 1024$

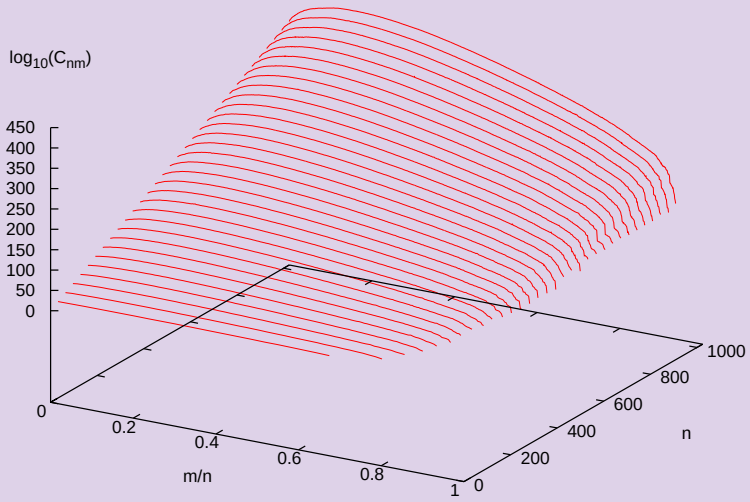
Total sample size: $240,000,000$

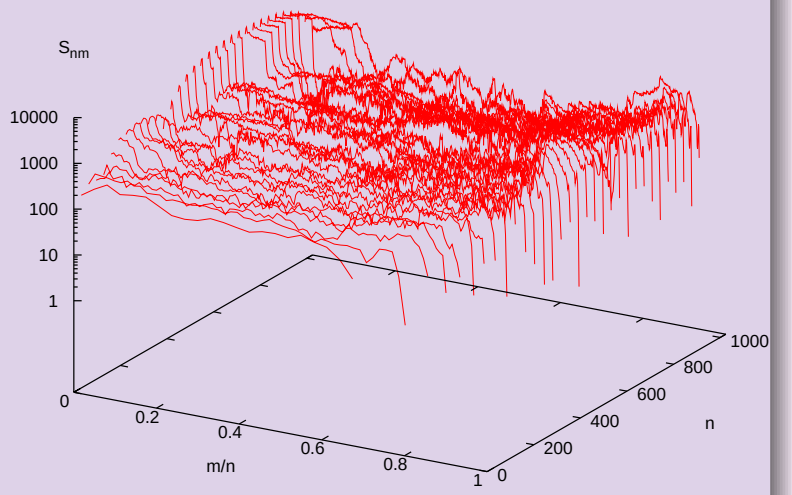




2d ISAW simulation up to $N = 1024$

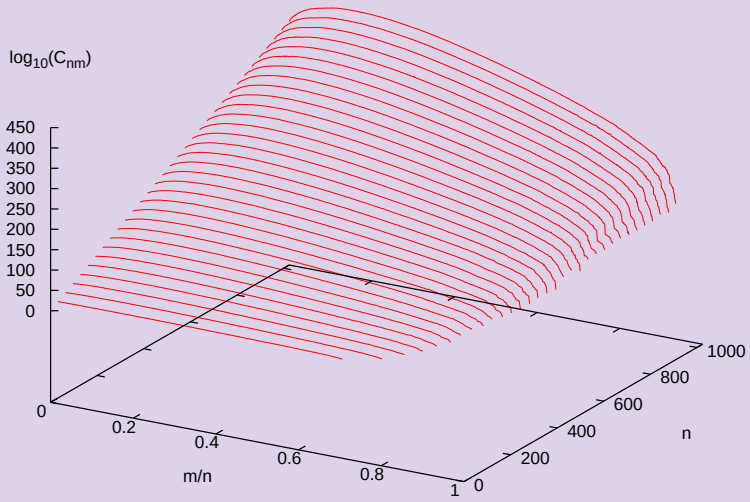
Total sample size: $250,000,000$

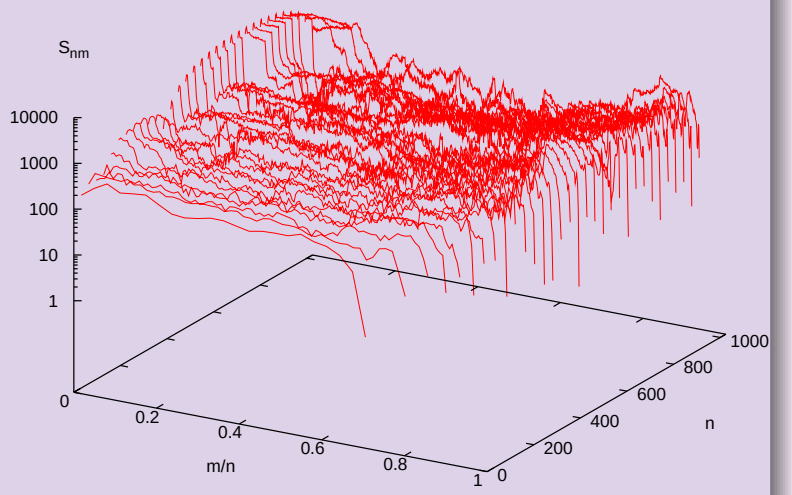




2d ISAW simulation up to $N = 1024$

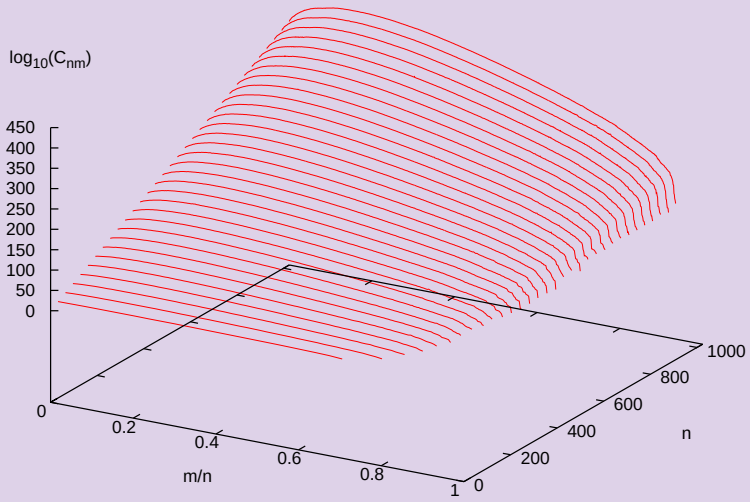
Total sample size: $260,000,000$

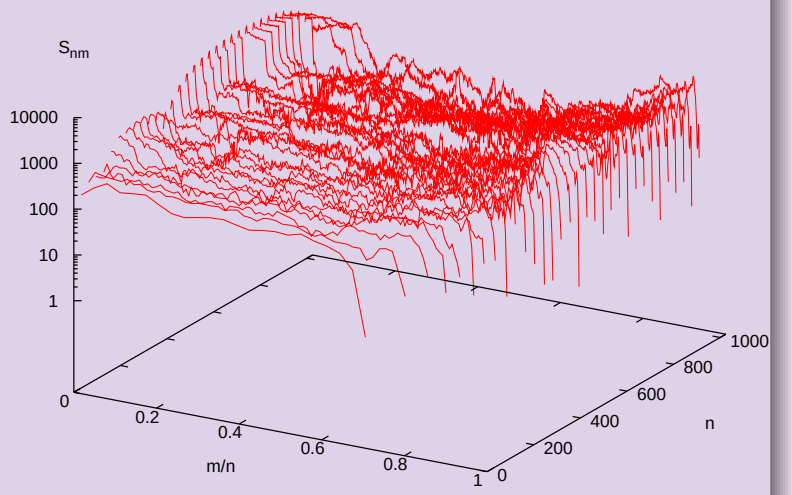




2d ISAW simulation up to $N = 1024$

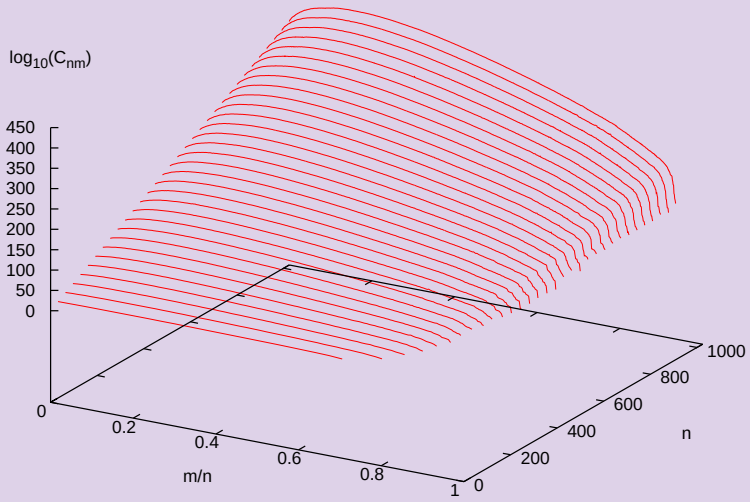
Total sample size: $270,000,000$

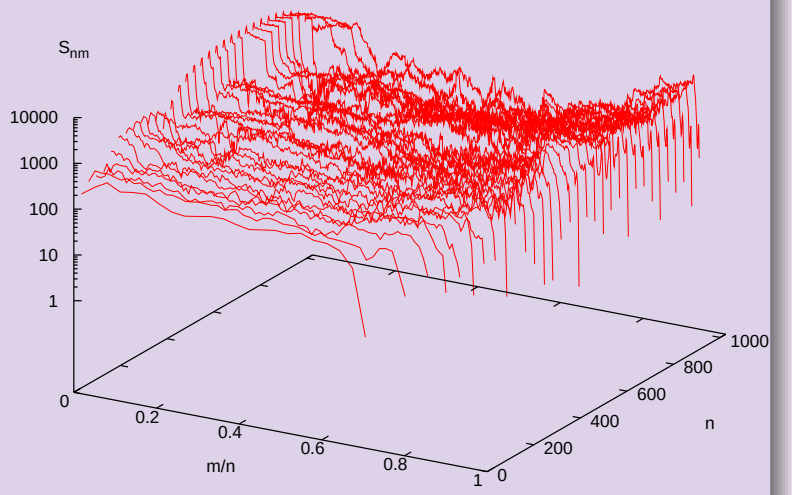




2d ISAW simulation up to $N = 1024$

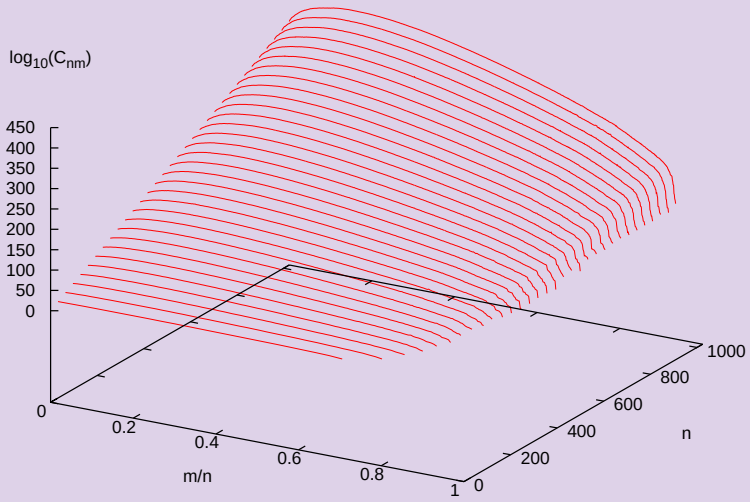
Total sample size: $280,000,000$

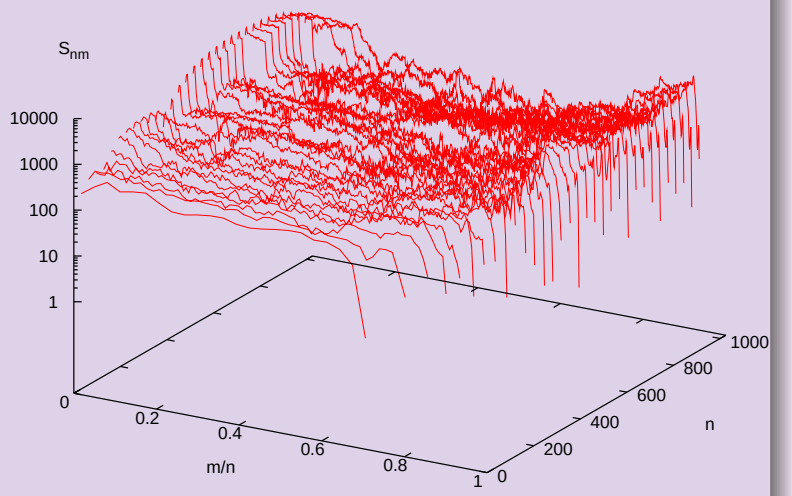




2d ISAW simulation up to $N = 1024$

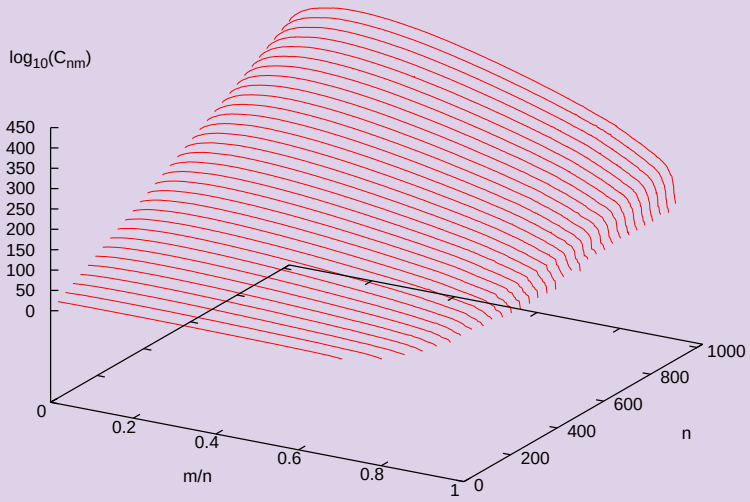
Total sample size: $290,000,000$

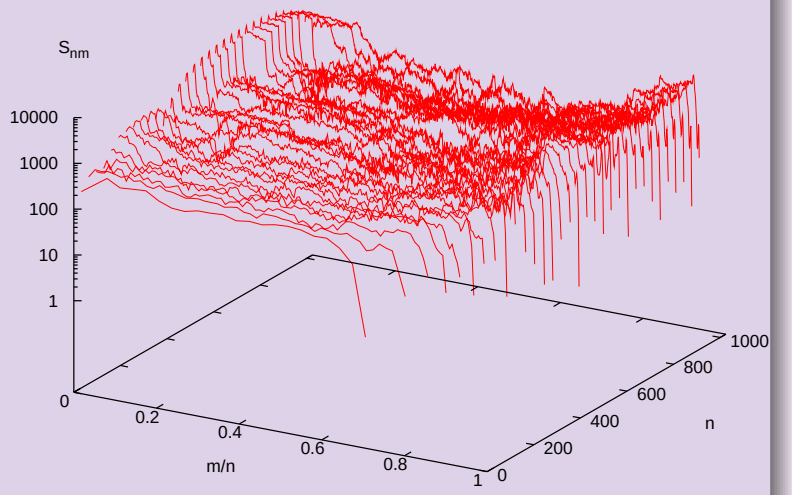




2d ISAW simulation up to $N = 1024$

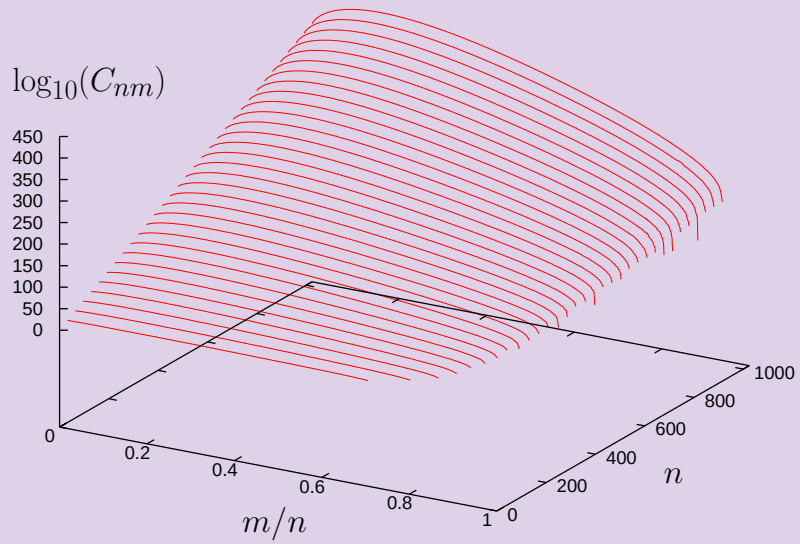
Total sample size: $300,000,000$

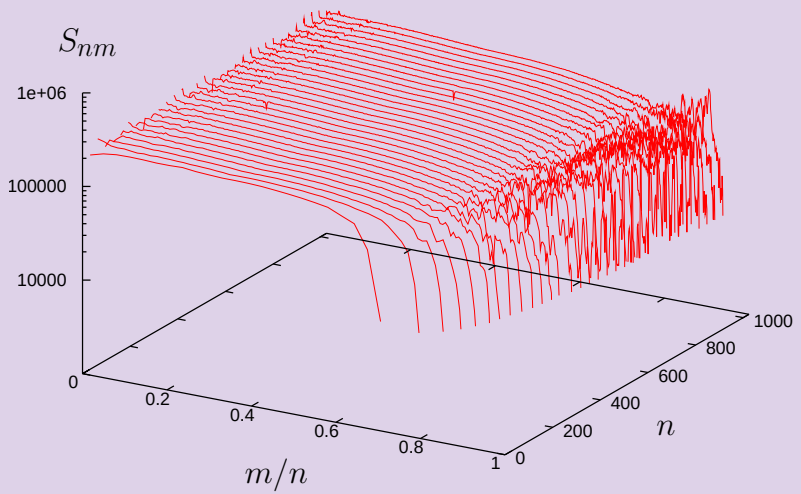




ISAW simulations

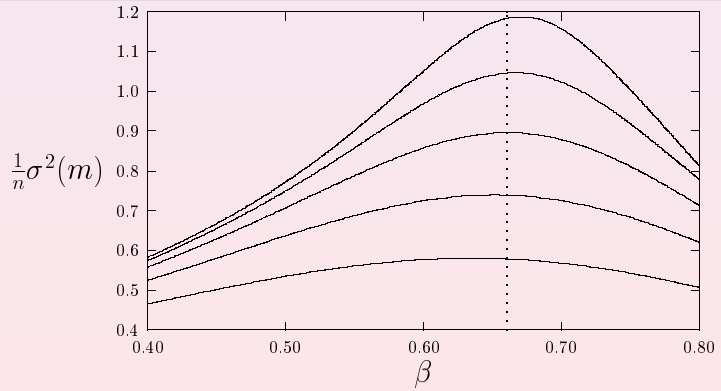
T Prellberg and J Krawczyk, PRL 92 (2004) 120602





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

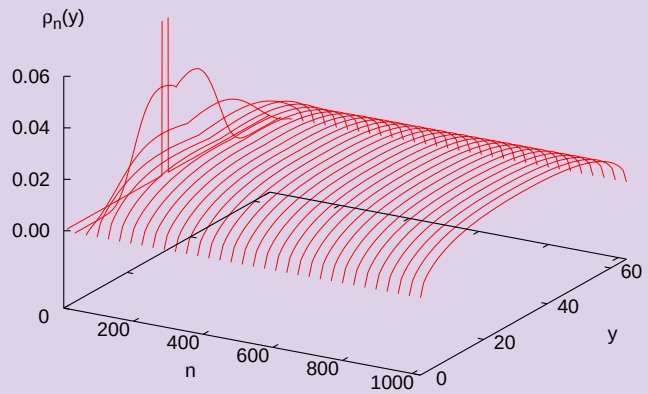
(only 2d shown, 3d similar)

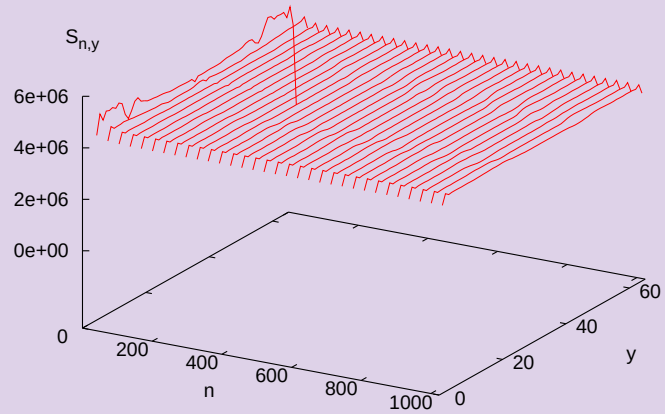


Simulation results: SAW in a strip

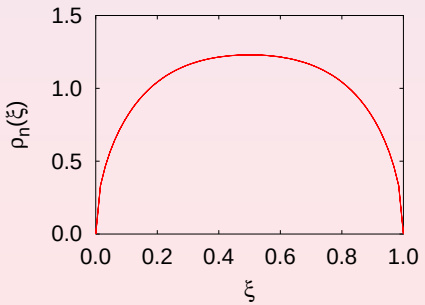
T Prellberg et al, in: Computer Simulation Studies in Condensed Matter Physics XVII, Springer Verlag, 2006

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





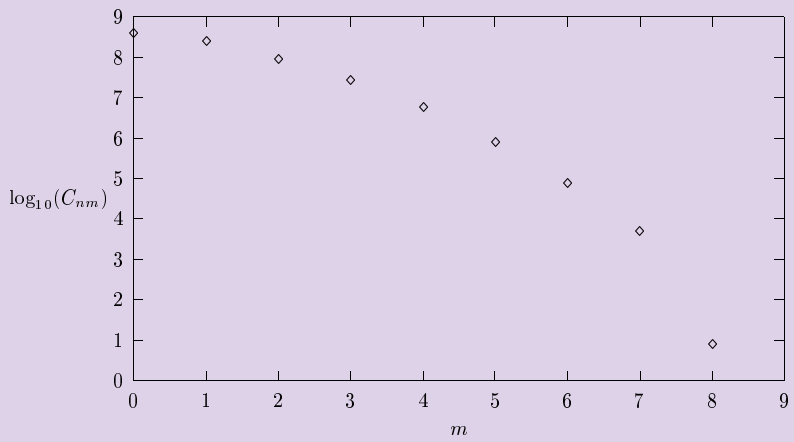
- Scaled endpoint density

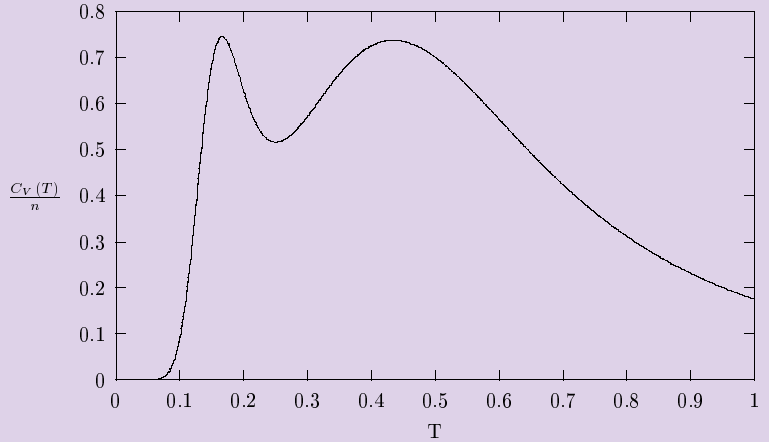


HP model simulations

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

- Engineered sequence HPHPHHPHPHHPPH in $d = 3$:



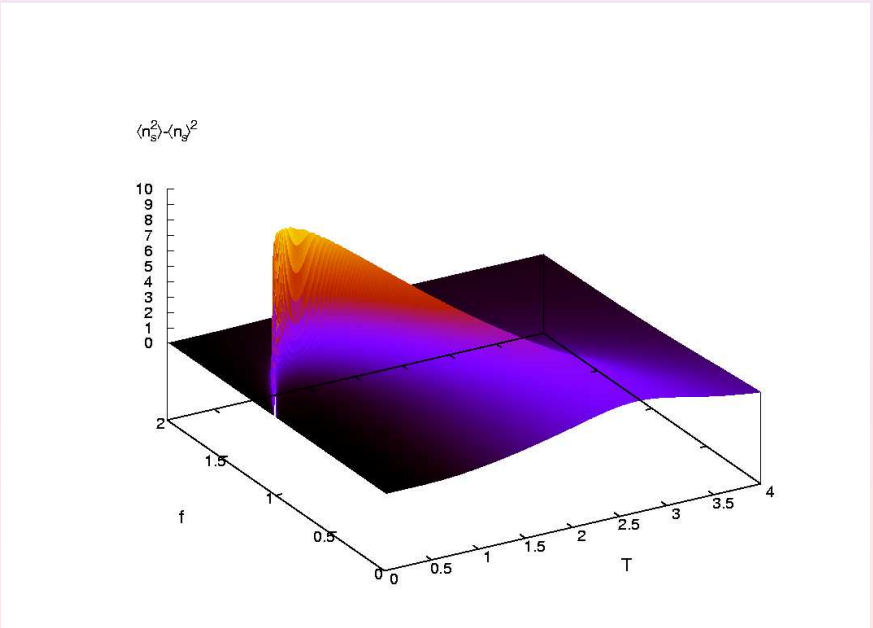


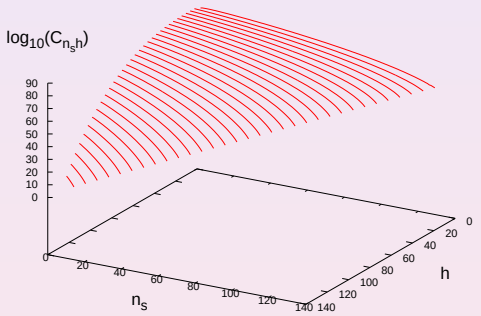
- Investigated other sequences up to $N \approx 100$ in $d = 2$ and $d = 3$
- Collapsed regime accessible
- Reproduced known ground state energies
- Obtained density of states $C_{n,m}$ over large range ($\approx 10^{30}$)

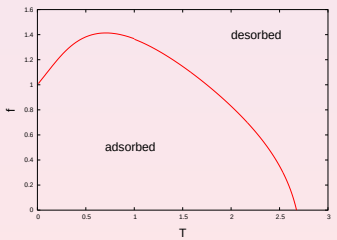
2-Dimensional Density of States

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





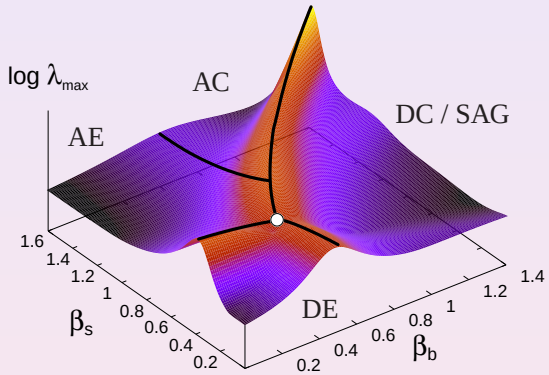


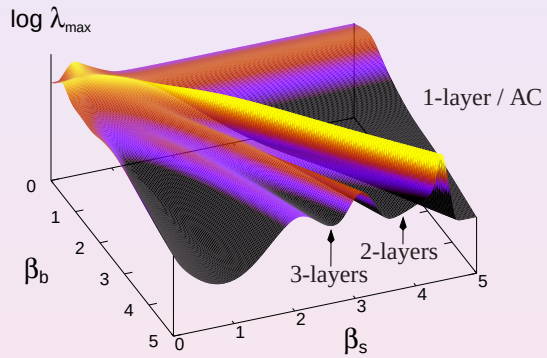
2-Dimensional Density of States

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

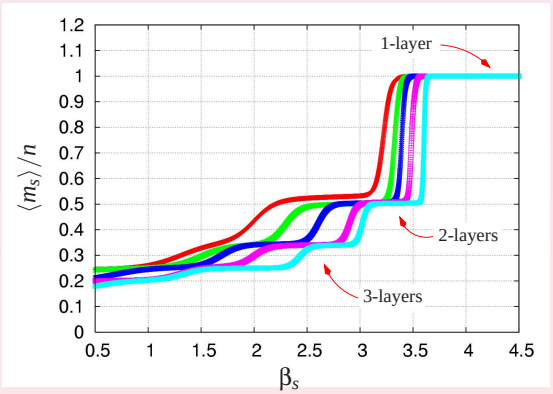
AL Owczarek et al, J Phys A 40 (2007) 13257-13267

- Layering transitions of adsorbed polymers in poor solvents





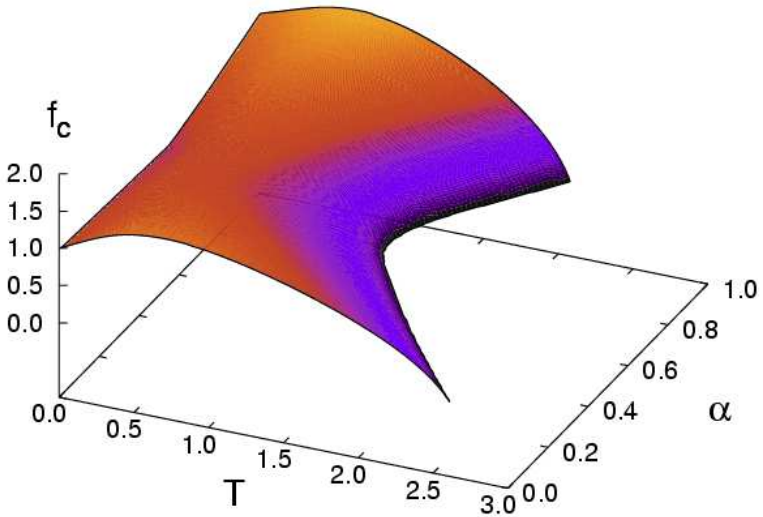
- whole phase diagram at once
- low temperatures accessible
- hierarchy of layering transitions
- resolved controversy over "surface attached globule"

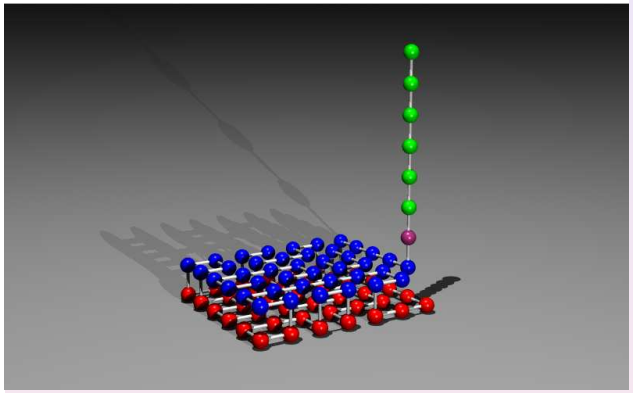


3-Dimensional Density of States

J Krawczyk et al, JSTAT (2005) P05008

- Pulling adsorbing and collapsing polymers off a surface





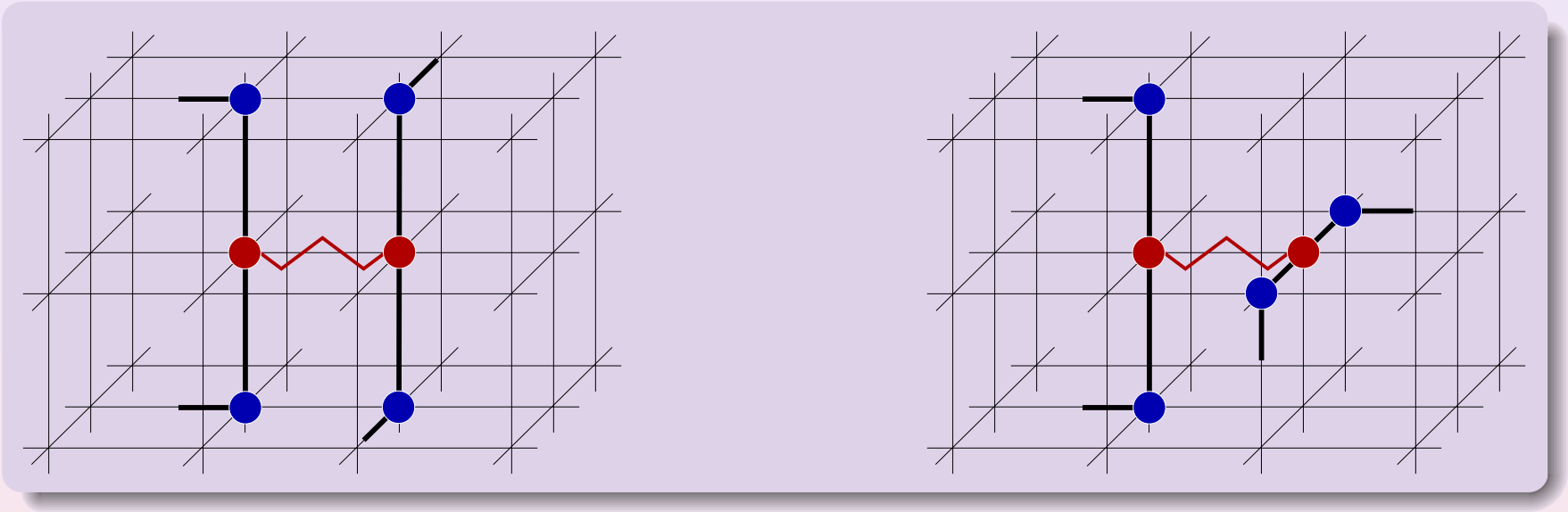
$\epsilon_s = \alpha$, $\epsilon_b = 1 - \alpha$

- 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

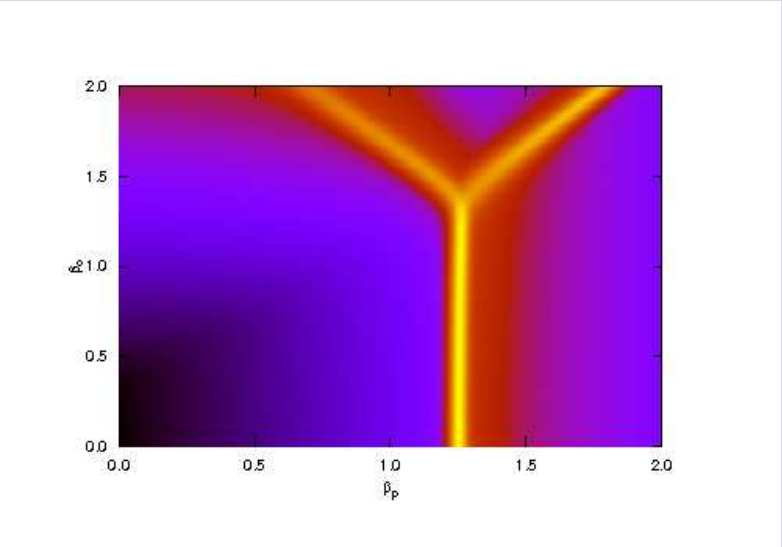
J Krawczyk et al, Phys. Rev. E 76 (2007) 051904

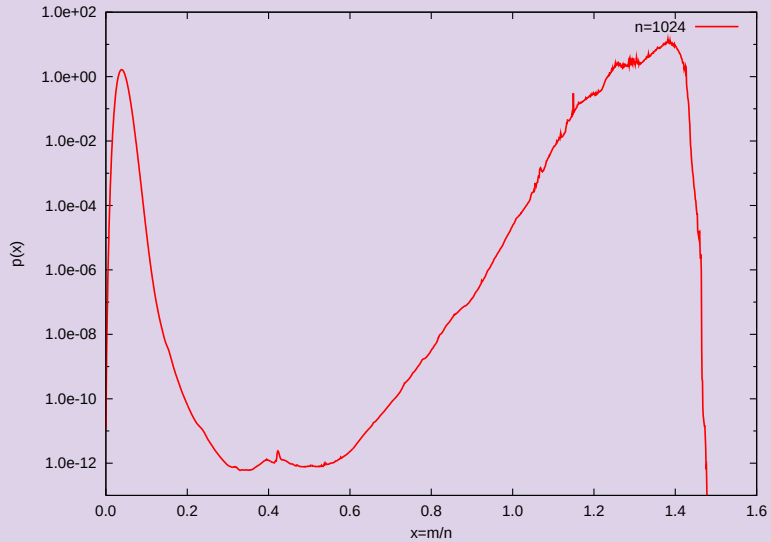
Hydrogen-like interactions between *straight* segments of the walk



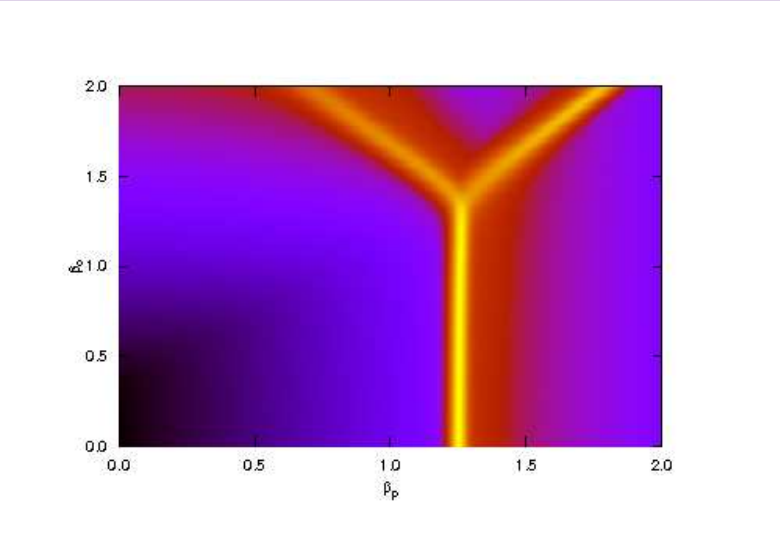
Distinguish parallel and orthogonal interactions: layering of β-sheets

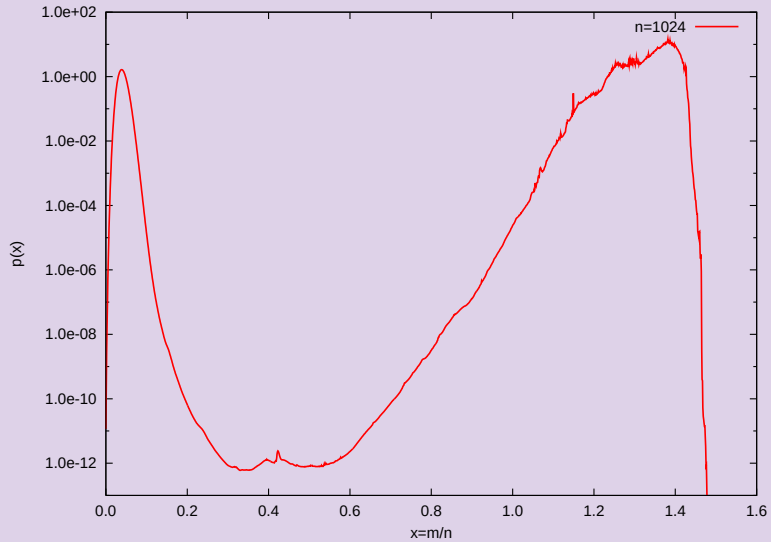
Hydrogen-bond type interactions (ctd.)

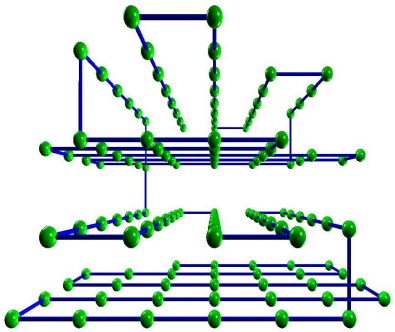


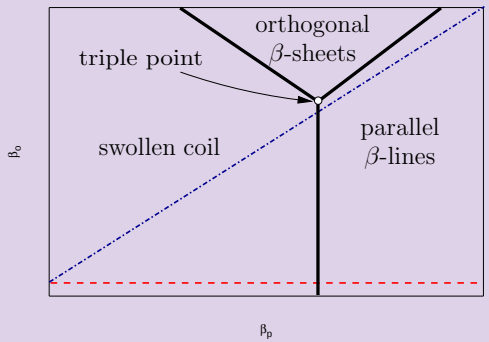


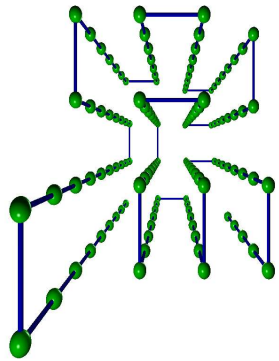
Hydrogen-bond type interactions (ctd.)







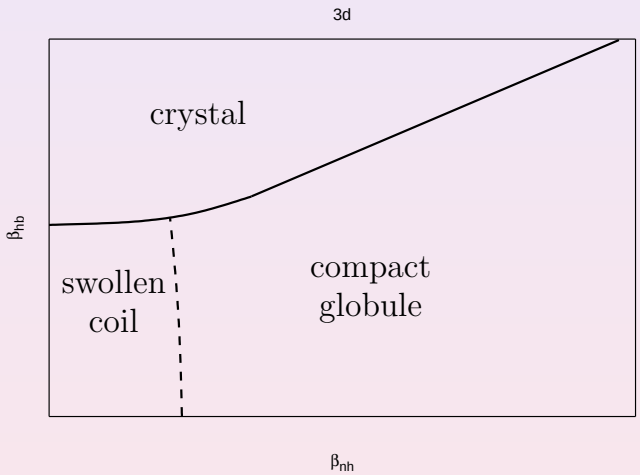


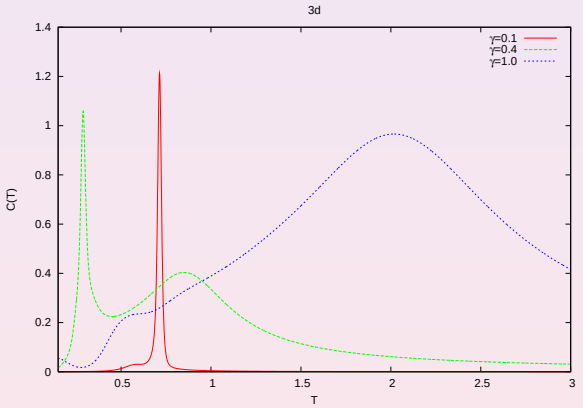


Hydrogen-bond vs. isotropic interactions

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

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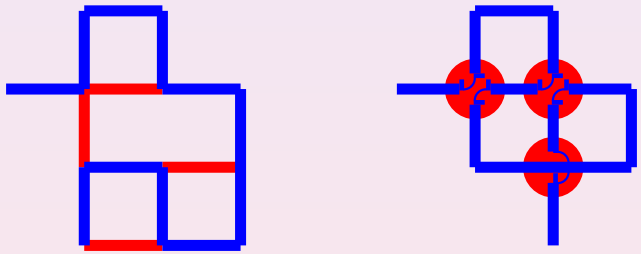
- Canonical model: interacting self-avoiding walks (ISAW)
- Alternative model: interacting self-avoiding trails (ISAT)

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



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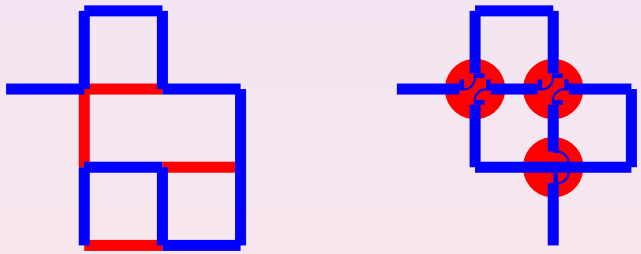

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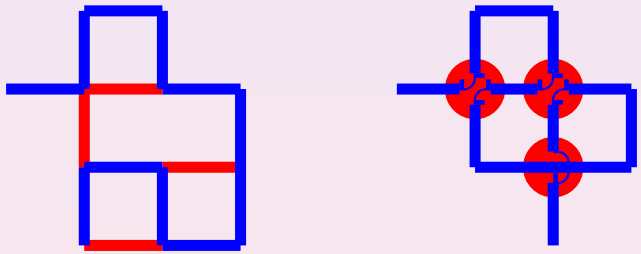


nearest-neighbour interaction $\Leftrightarrow$ contact interaction

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

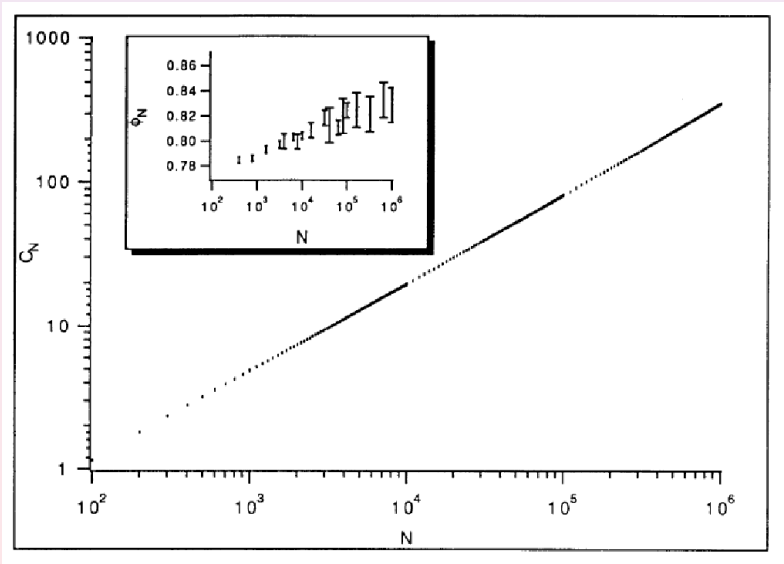
Simulations of ISAT

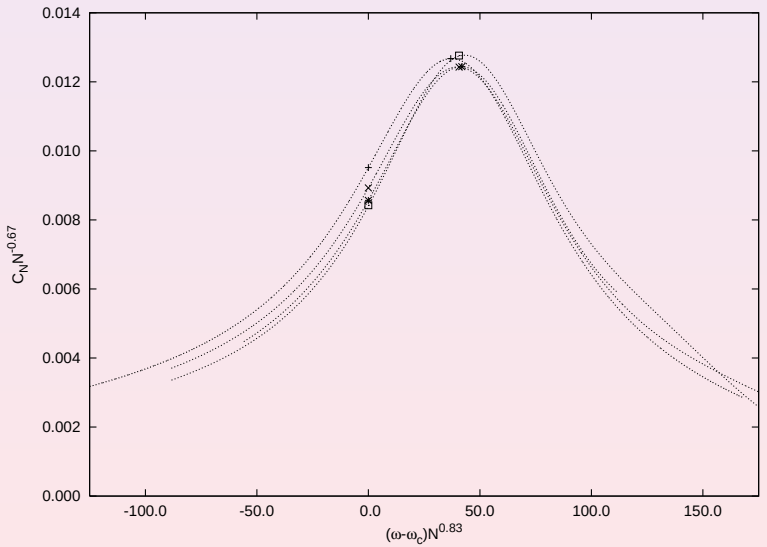
- At critical T_c, ISAT can be modelled as kinetic growth; simulations up to $N = 10^6$

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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- Site-weighted random walk:
  - lattice random walk weighted by multiple visits of sites
  - few visits to same site are favoured (attractive interaction)
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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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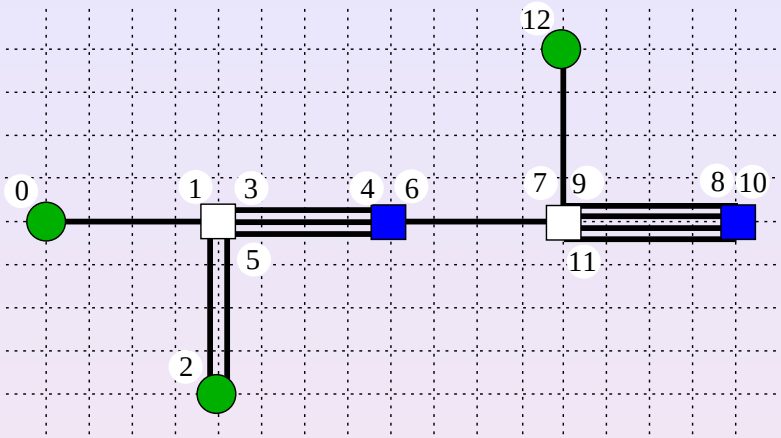
- Incorporate self-avoidance and attraction via choice of $f(t)$. For example, $f(0) = f(1) = 0$,

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

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

Site-Weighted Random Walk (ctd)



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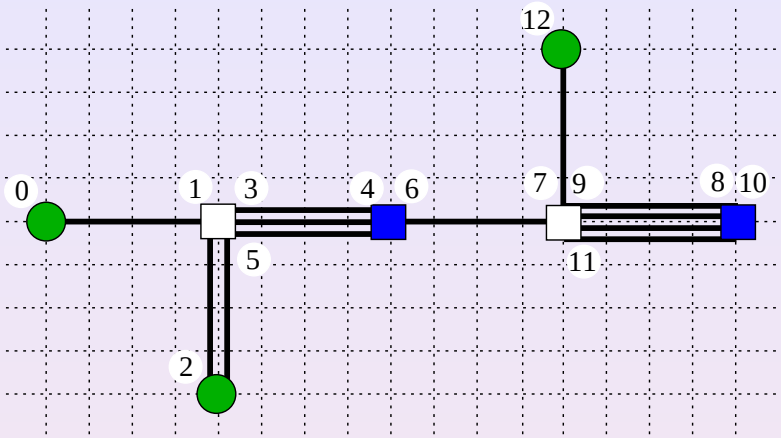

- Partition function

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

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

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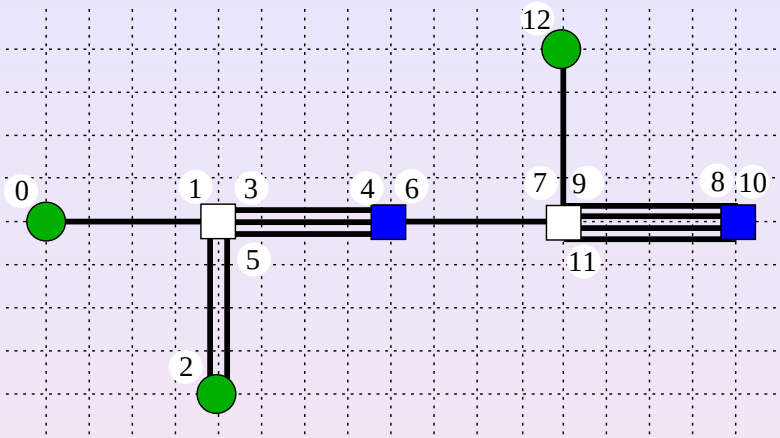

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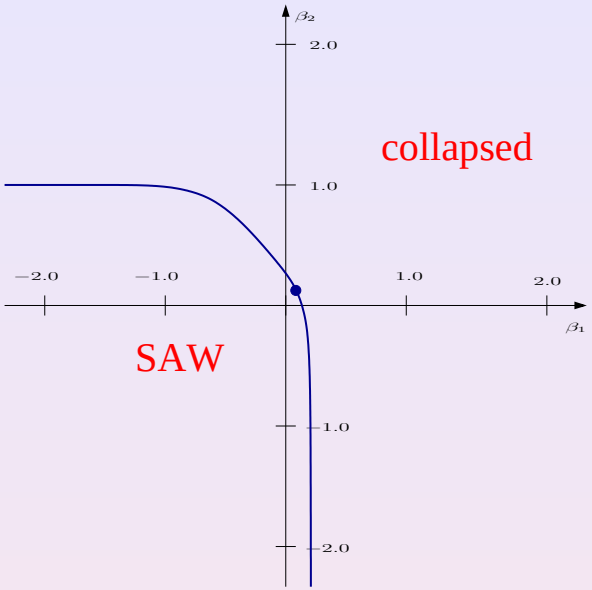
with density of states C_{N,m_1,m_2}

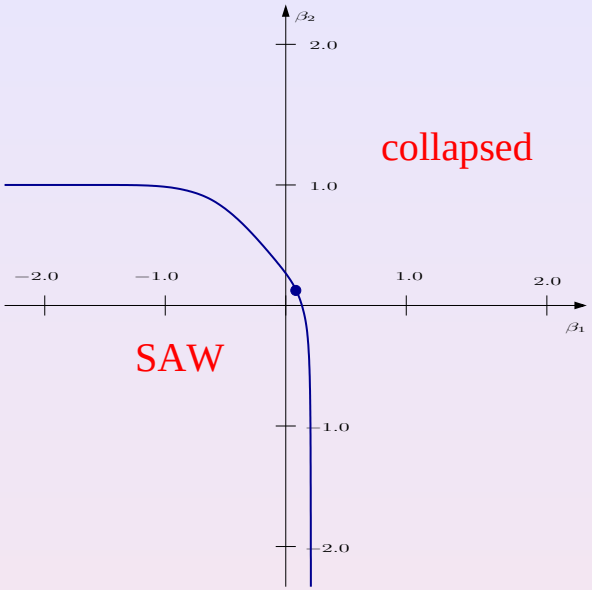
- Simulate two variants of the model on the square and simple cubic lattice
  - random walks with immediate reversal allowed (RA2, RA3)
  - random walks with immediate reversal forbidden (RF2, RF3)

SWRW in 3d, reversal forbidden (RF3)



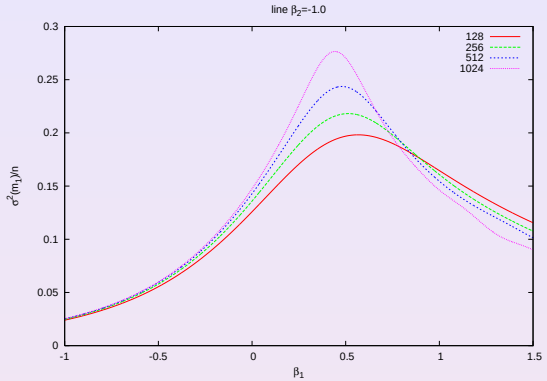
Phase diagram

SWRW in 3d, reversal forbidden (RF3)



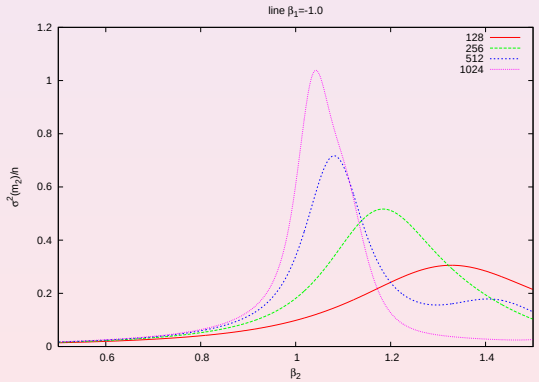
Phase diagram

$\beta_2 = -1.0$:



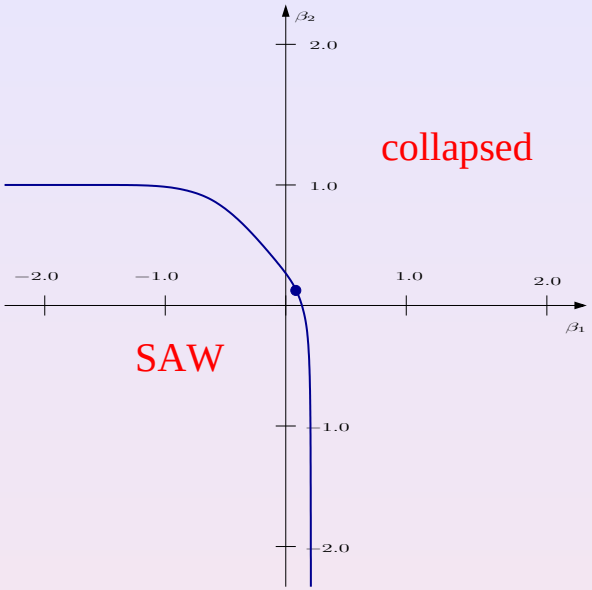
2nd order transition

$\beta_1 = -1.0$:



1st order transition

SWRW in 3d, reversal forbidden (RF3)



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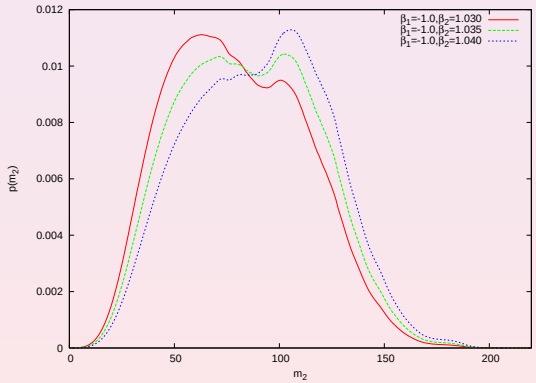

bimodal distribution

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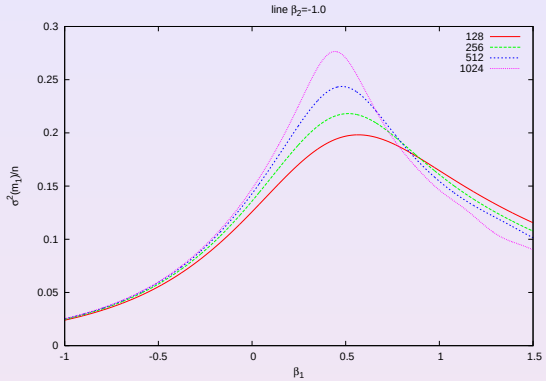

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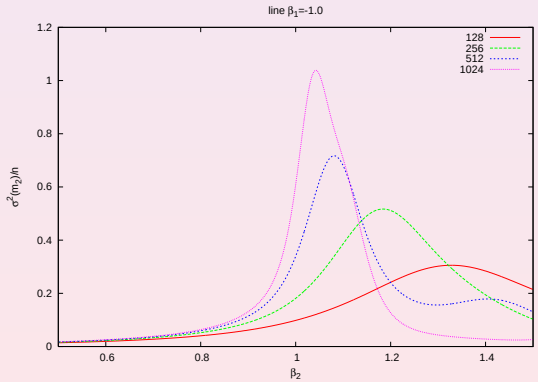
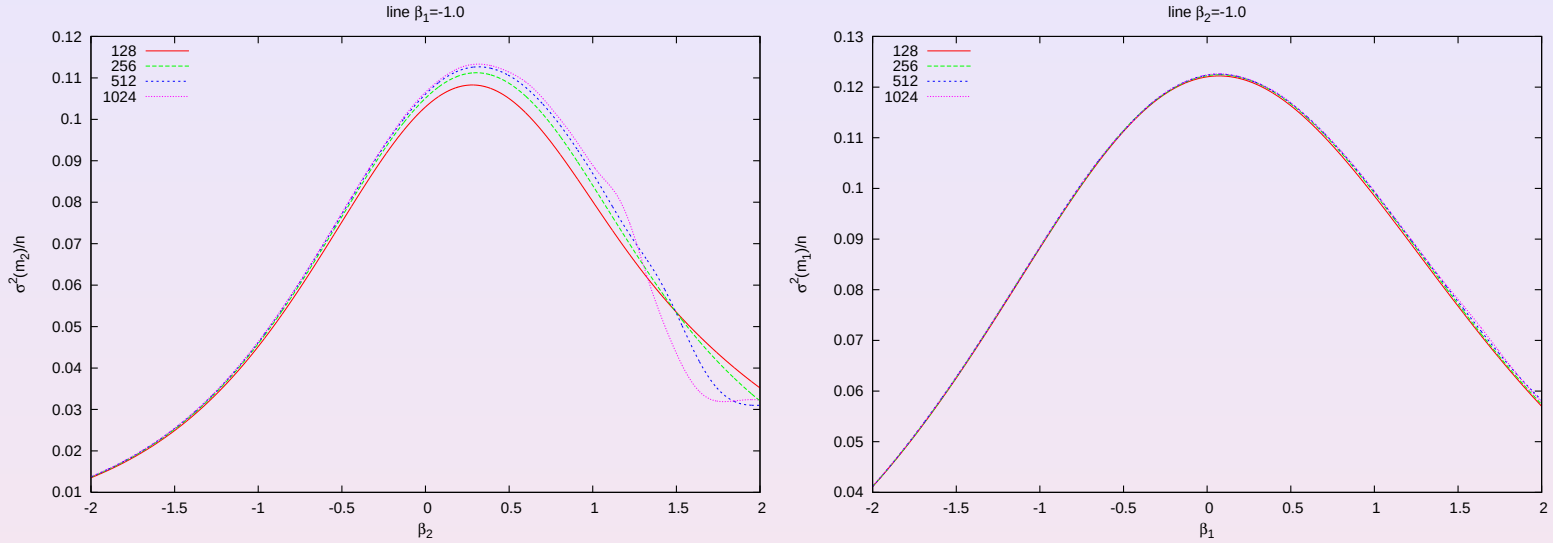


1st order transition

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)

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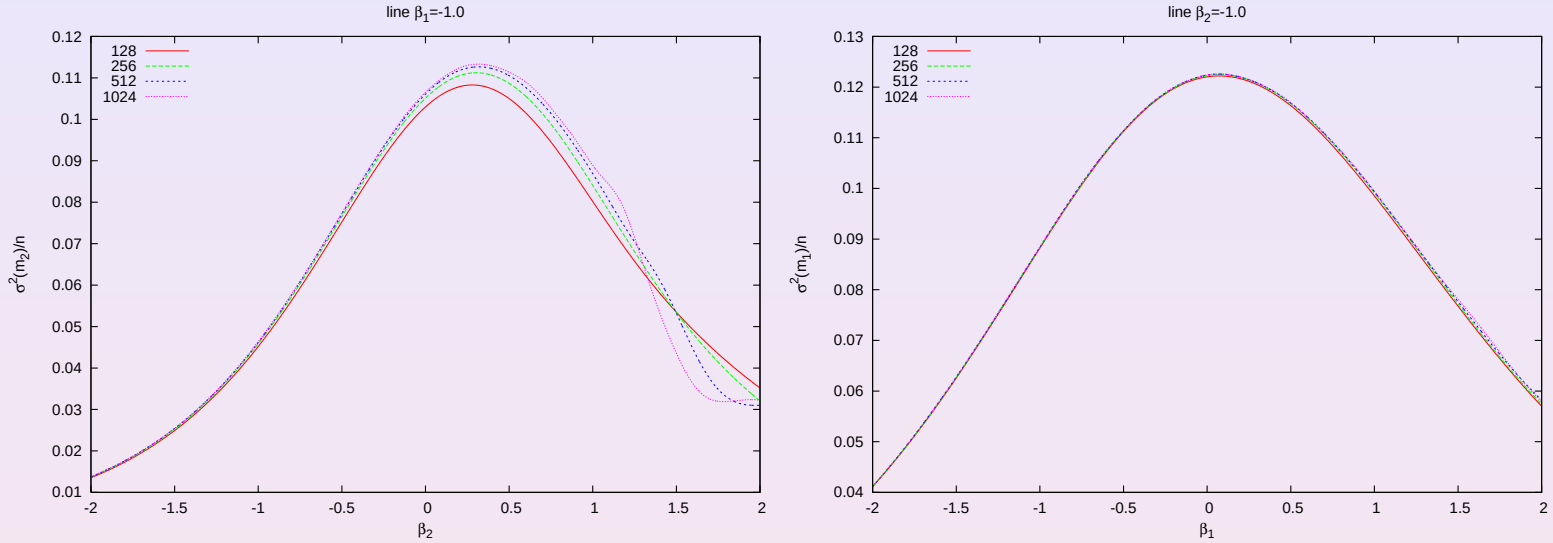

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RA3 and RF2

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

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Unexpected and intriguing behaviour

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

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Many open questions remain ...

References

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  - J. Krawczyk, T. Prellberg, A. L. Owczarek, and A. Rechnitzer, "On a type of self-avoiding random walk with multiple site weightings and restrictions," Phys. Rev. Lett. 96 (2006) 240603

The End