Simulation of polymers with a new Monte-Carlo algorithm

(flatPERM - a flat histogram stochastic growth algorithm)

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joint work with

J. Krawczyk, TU Clausthal

A. Rechnitzer and A.L. Owczarek, Uni Melbourne

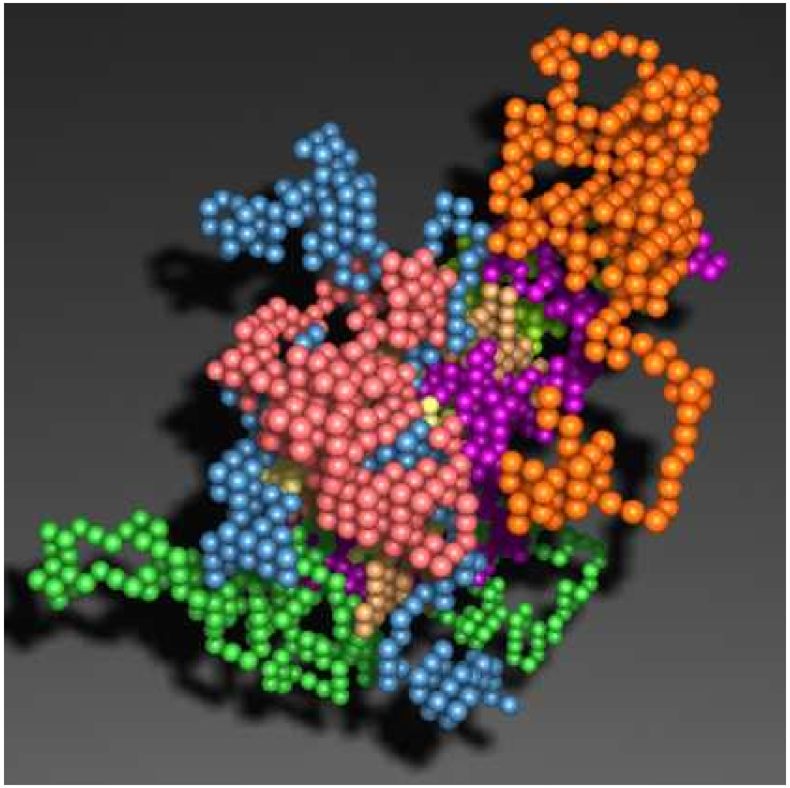
Content

- Polymers in solution:
  - Equilibrium statistical mechanics, lattice model
- Algorithm:
  - Stochastic growth & flat histogram (flatPERM)
- Applications:
  - Bulk phenomena
    - polymer collapse, protein groundstates
  - Surface phenomena
    - confined polymers, force-induced desorption, interplay of collapse and adsorption
- Outlook:
  - continuum models, branched polymers, . . .

Introduction

Modelling of Polymers in Solution

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



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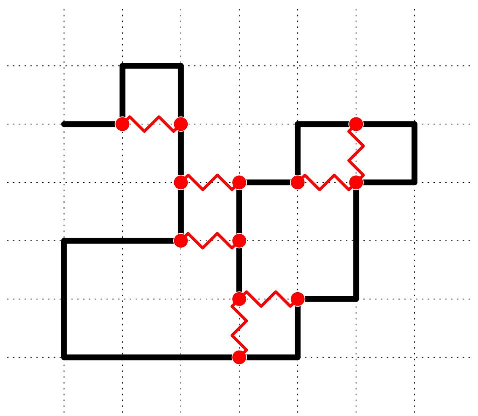
Pedagogical Setting: Lattice Model



Self-Avoiding Walks with Interactions

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

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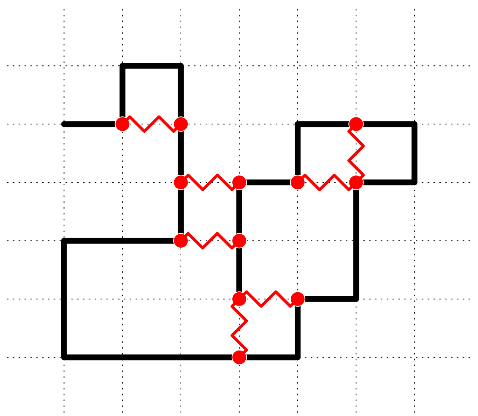

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  - ISAW model: homopolymer, interaction $\epsilon = -1$

    of interest: thermodynamic limit ($V = \infty$ and $n \rightarrow \infty$)

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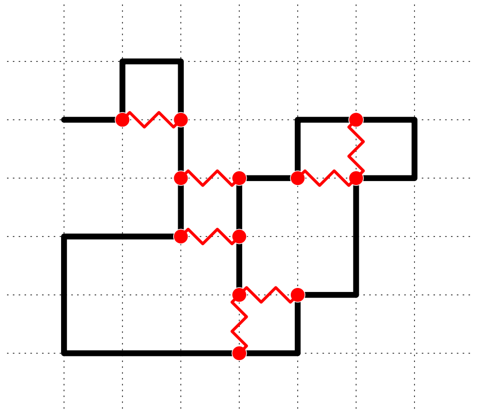

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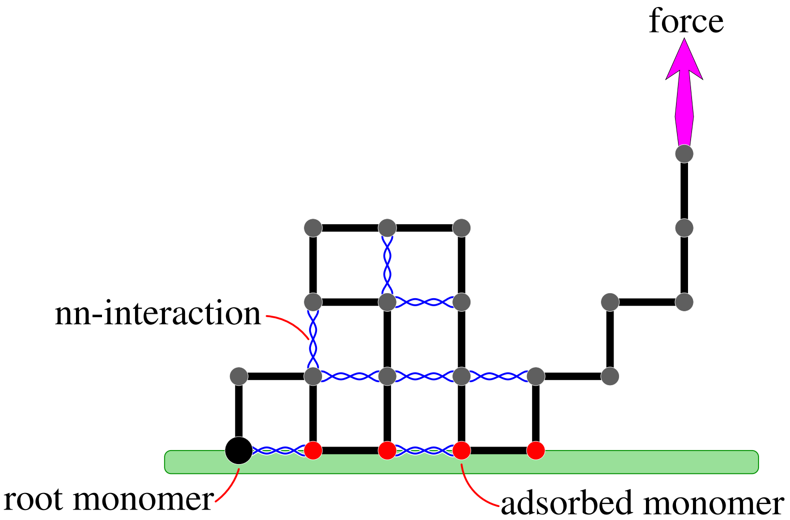
- Extension: interaction matrix $\epsilon = \epsilon_{i,j}$, protein folding
  of interest: fixed finite sequence, density of states

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



Why Simulations?

- Most interesting open questions for dense and geometrically restricted configurations

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- Most interesting open questions for dense and geometrically restricted configurations
- There is little theory and

$\boxed{\text{this is notoriously difficult to simulate}}$

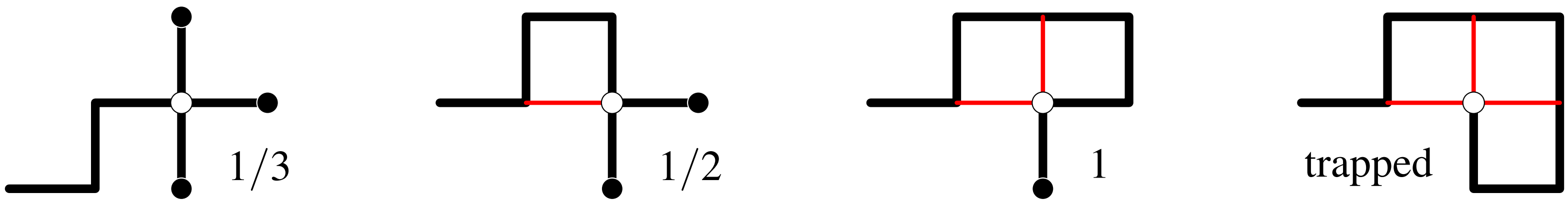
Stochastic Growth Algorithm

PERM: “Go With The Winners”

PERM = Pruned and Enriched Rosenbluth Method

Grassberger, Phys Rev E 56 (1997) 3682

- Rosenbluth Method: kinetic growth



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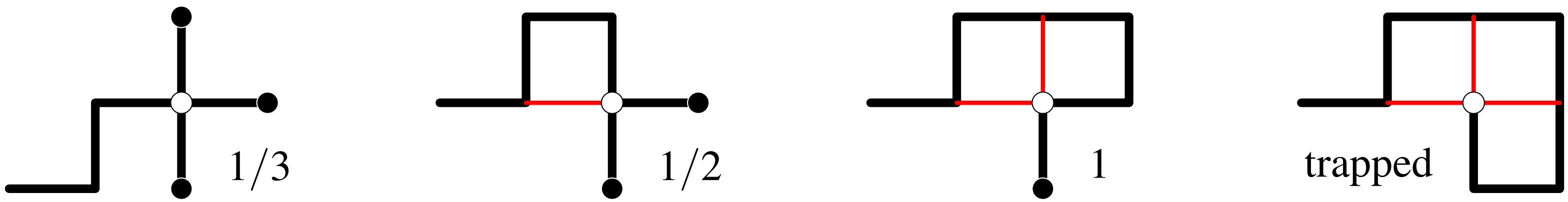

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- Pruning: weight too small → remove configuration occasionally

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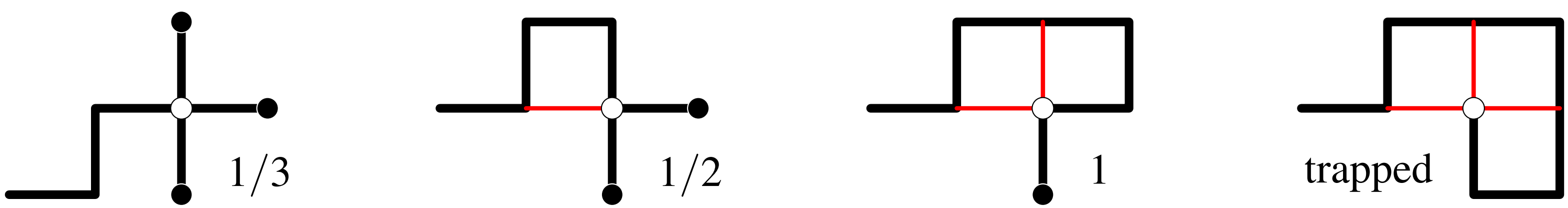

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Current work: flatPERM = flat histogram PERM

TP and JK, PRL 92 (2004) 120602, TP, JK, and AR, cond-mat/0402549

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

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Algorithm details

View kinetic growth as *approximate enumeration*

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$$W = \prod_{k=0}^{n-1} a_k$$

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  - S growth chains with weights $W_n^{(i)}$ give an estimate of the total number of configurations, $C_n^{est} = \langle W \rangle_n = \frac{1}{S} \sum_i W_n^{(i)}$

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

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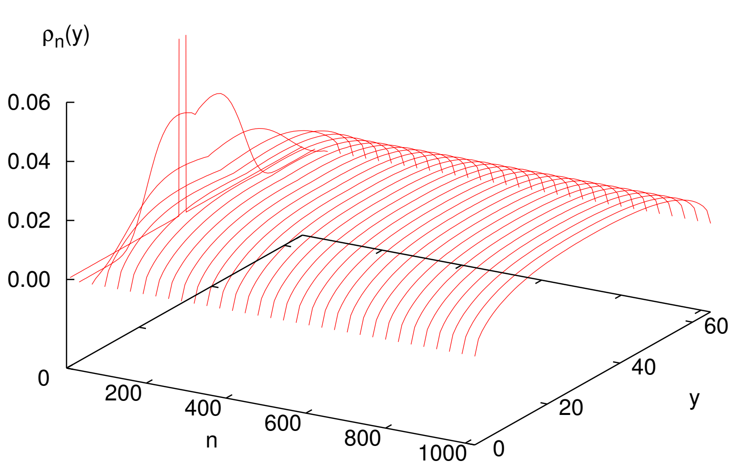
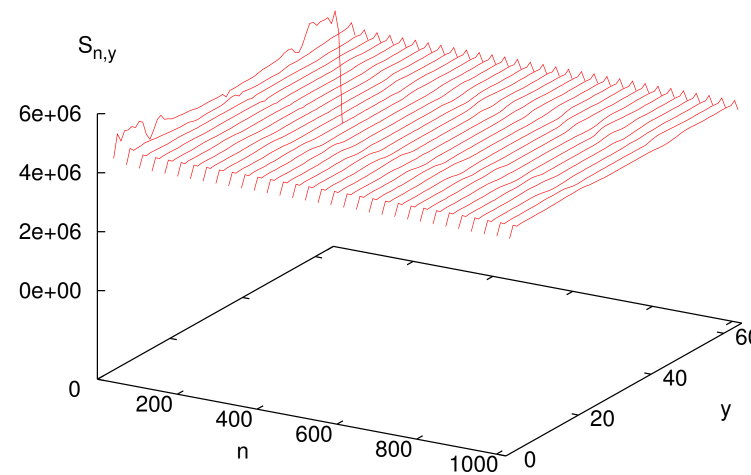
Simulation Results

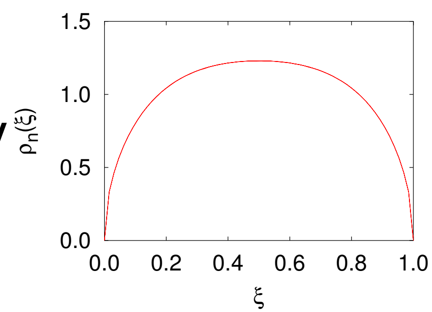
Simulation results: SAW in a strip

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





- Scaled endpoint density



- Compares favorably with “Markovian anticipation”–PERM

Hsu and Grassberger, Eur Phys J 36 (2003) 209

Simulation: dynamics of the algorithm

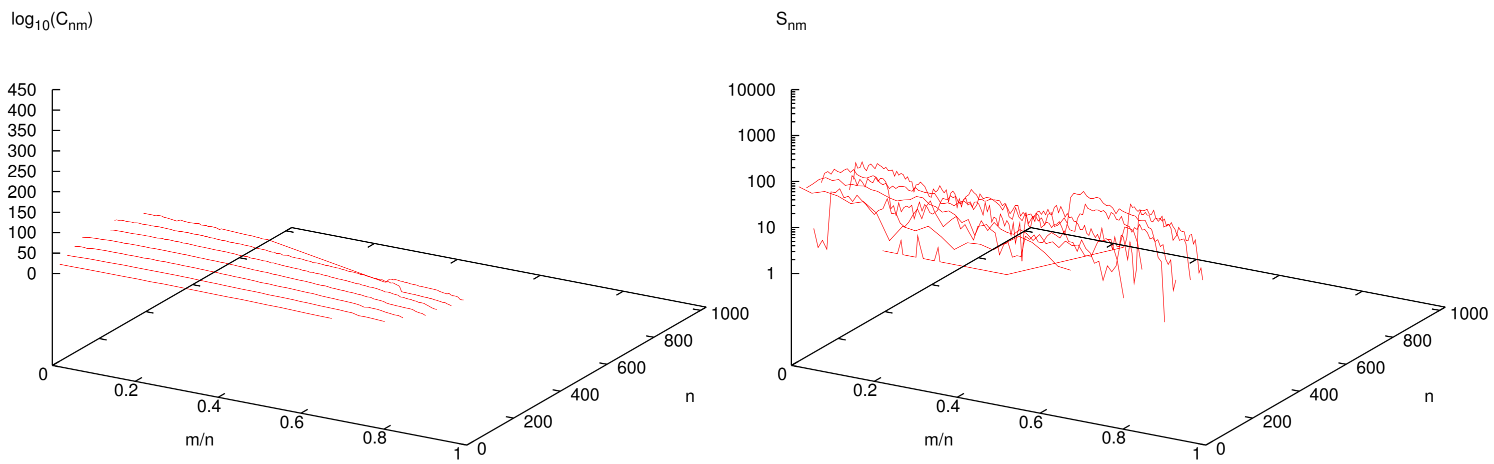
2d ISAW simulation up to $n = 1024$

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

Simulation: dynamics of the algorithm

2d ISAW simulation up to $n = 1024$

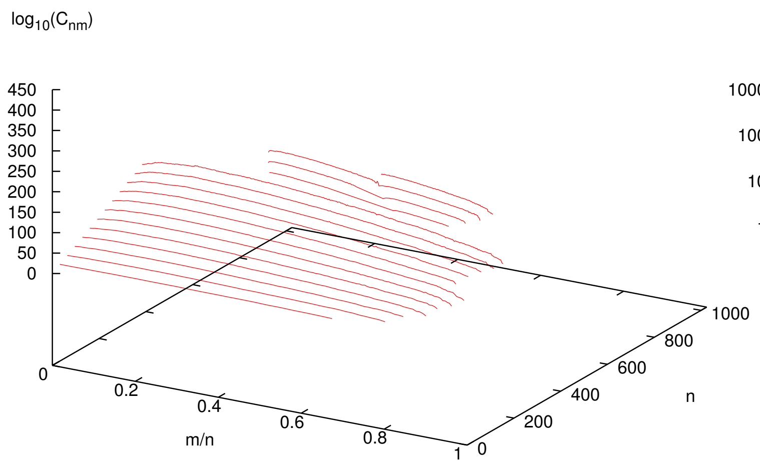
- Total sample size: $1,000,000$

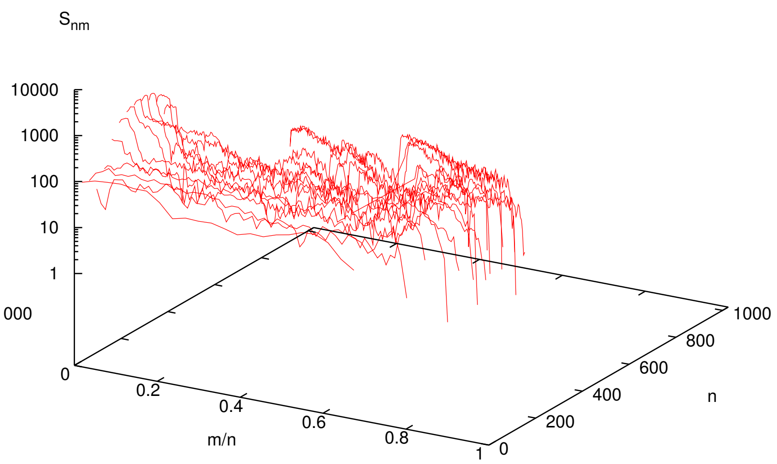


Simulation: dynamics of the algorithm

2d ISAW simulation up to $n = 1024$

- Total sample size: $10,000,000$

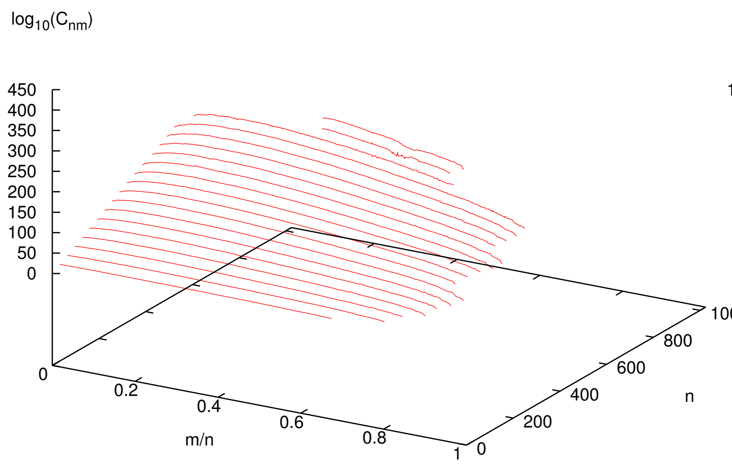


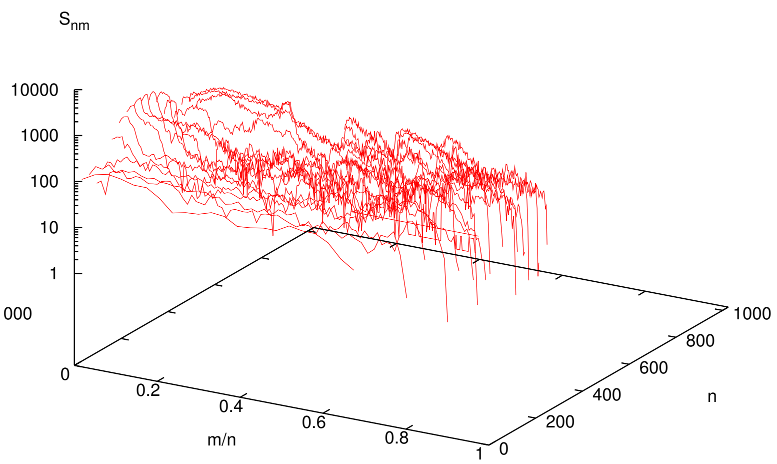


Simulation: dynamics of the algorithm

2d ISAW simulation up to $n = 1024$

- Total sample size: $20,000,000$

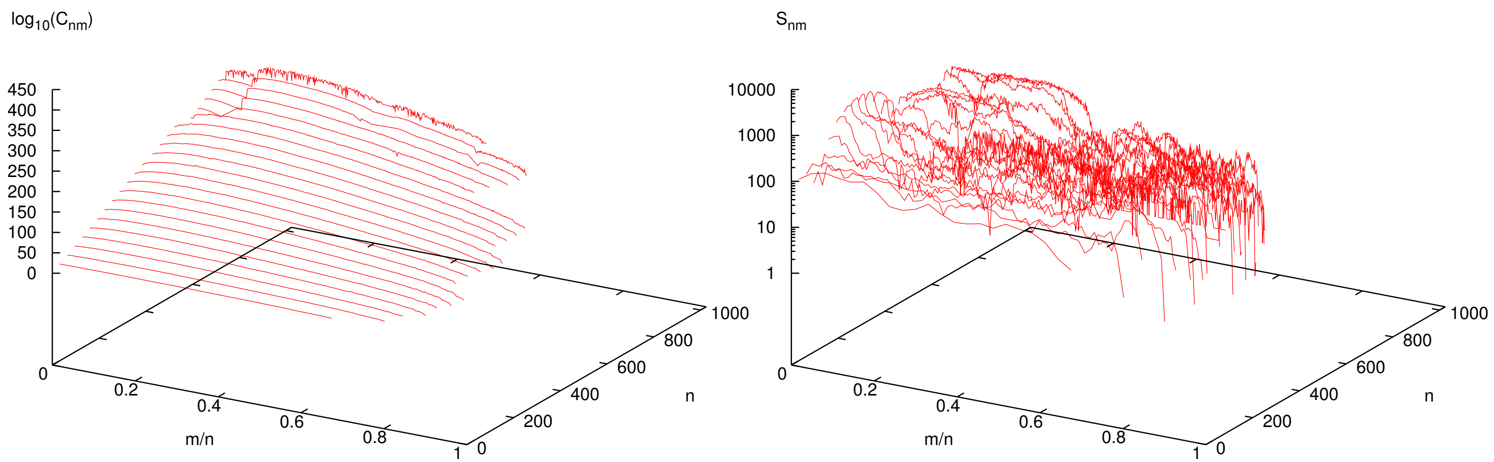




Simulation: dynamics of the algorithm

2d ISAW simulation up to $n = 1024$

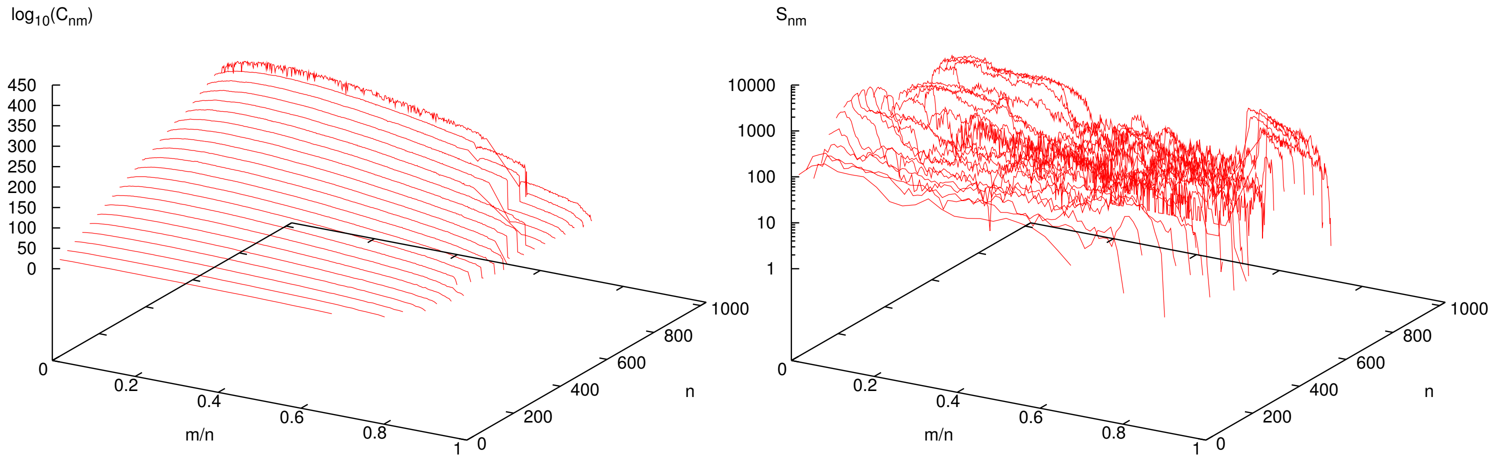
- Total sample size: $30,000,000$



Simulation: dynamics of the algorithm

2d ISAW simulation up to $n = 1024$

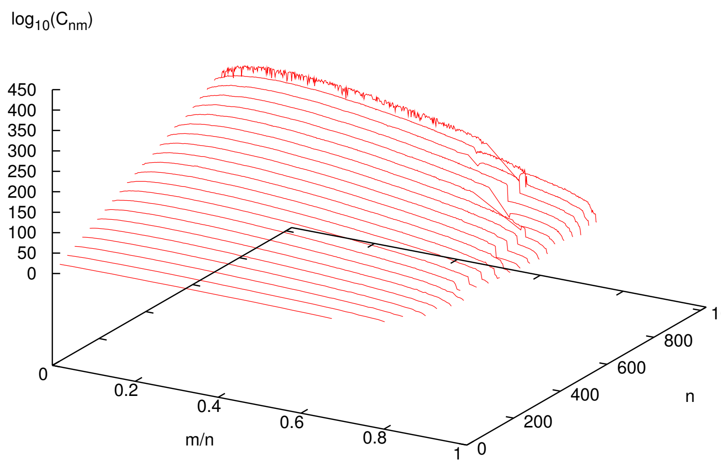
- Total sample size: $40,000,000$

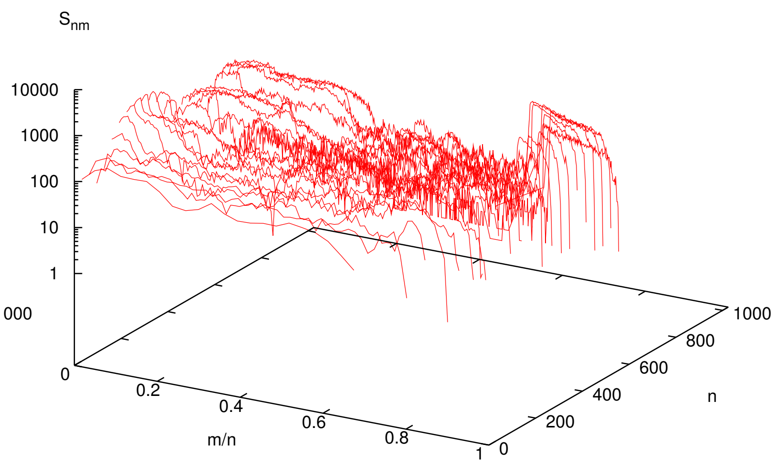


Simulation: dynamics of the algorithm

2d ISAW simulation up to $n = 1024$

- Total sample size: $50,000,000$

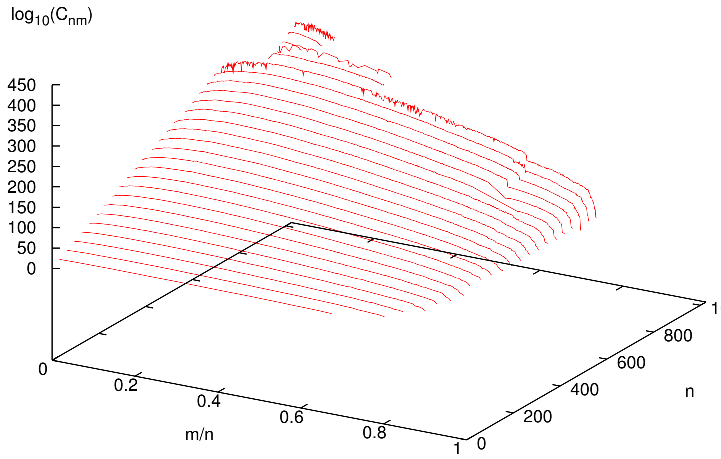


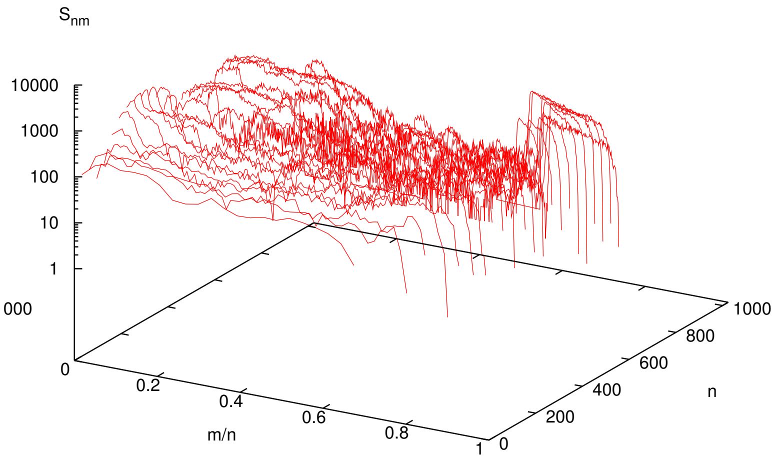


Simulation: dynamics of the algorithm

2d ISAW simulation up to $n = 1024$

- Total sample size: $60,000,000$

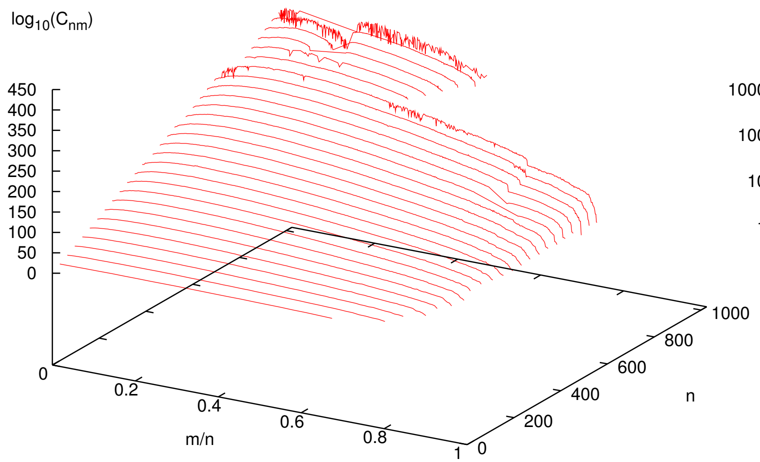


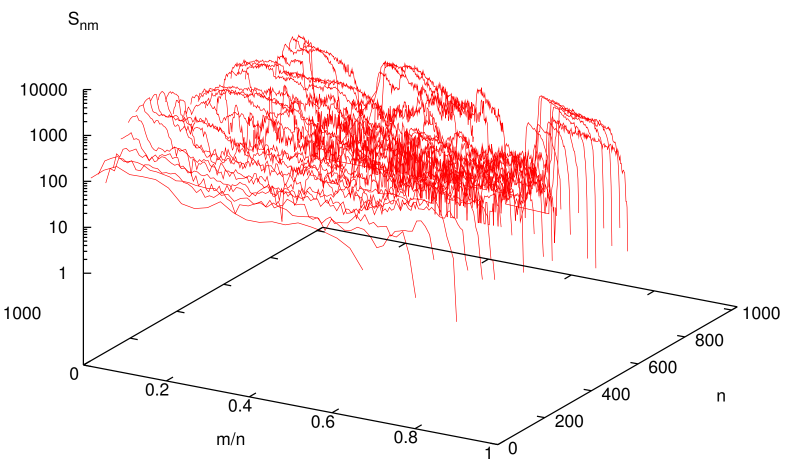


Simulation: dynamics of the algorithm

2d ISAW simulation up to $n = 1024$

- Total sample size: $70,000,000$

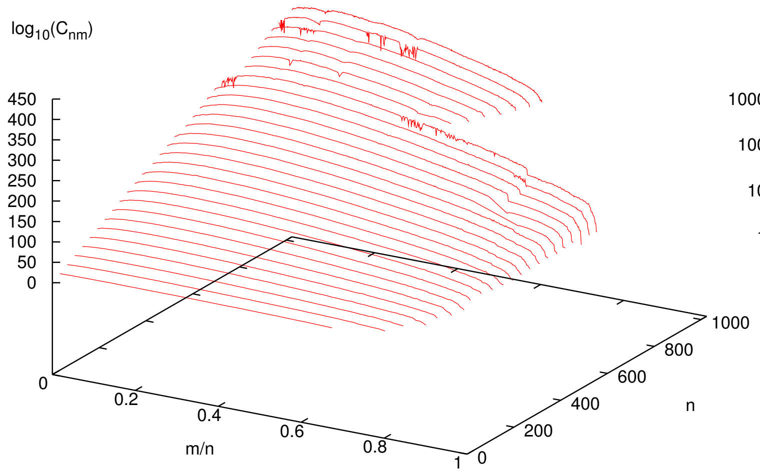


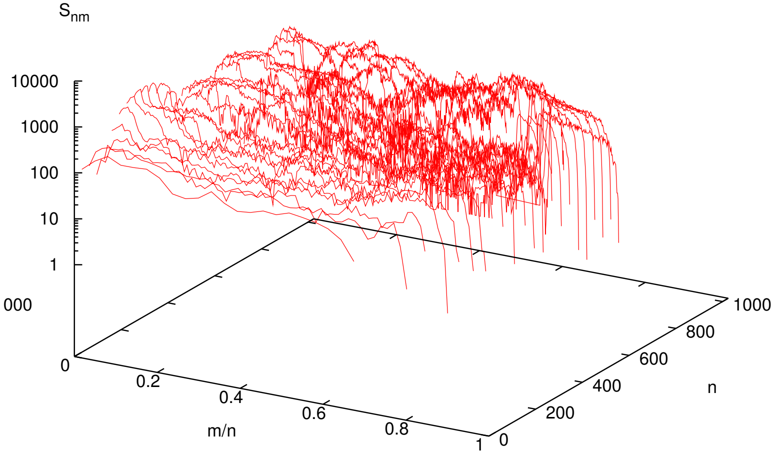


Simulation: dynamics of the algorithm

2d ISAW simulation up to $n = 1024$

- Total sample size: $80,000,000$

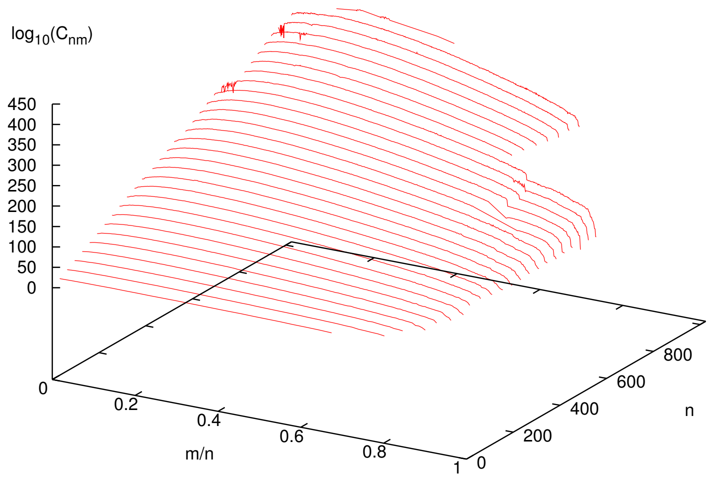


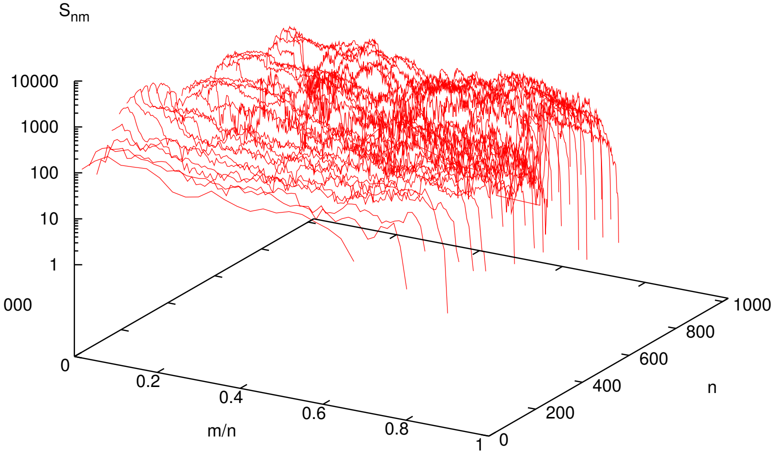


Simulation: dynamics of the algorithm

2d ISAW simulation up to $n = 1024$

- Total sample size: $90,000,000$

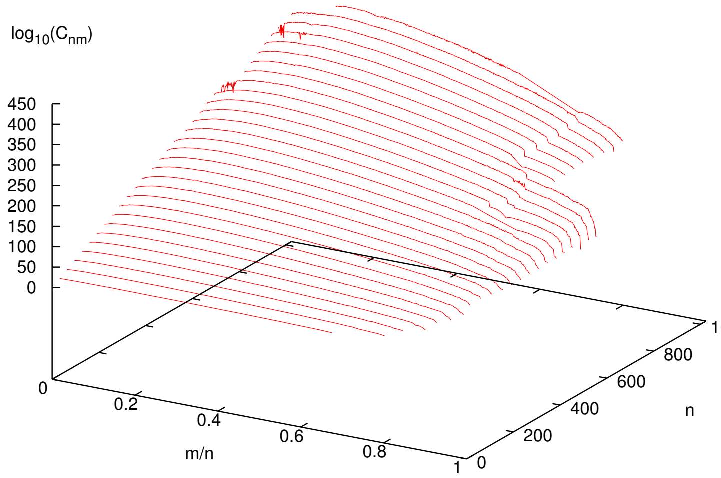


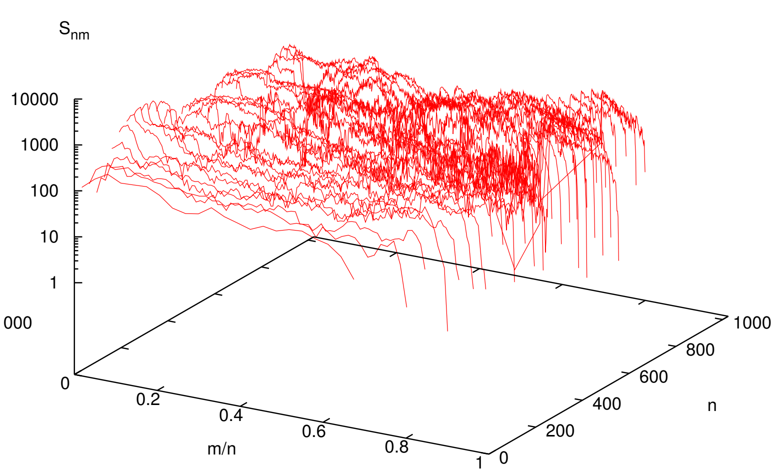


Simulation: dynamics of the algorithm

2d ISAW simulation up to $n = 1024$

- Total sample size: $100, 000, 000$

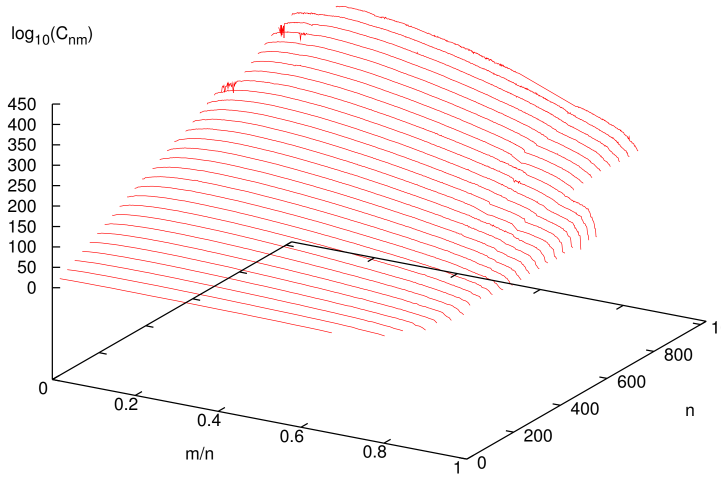


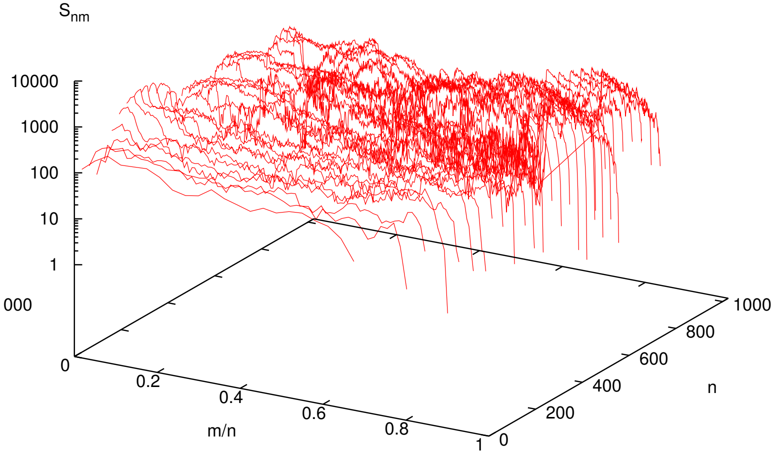


Simulation: dynamics of the algorithm

2d ISAW simulation up to $n = 1024$

- Total sample size: $110,000,000$





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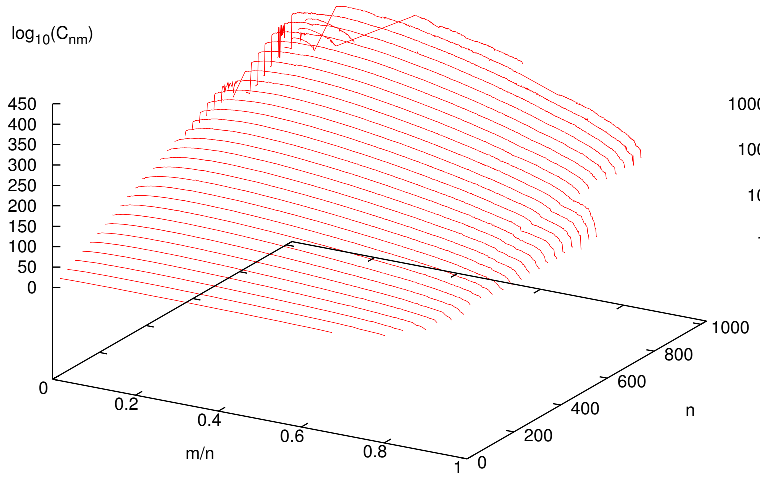
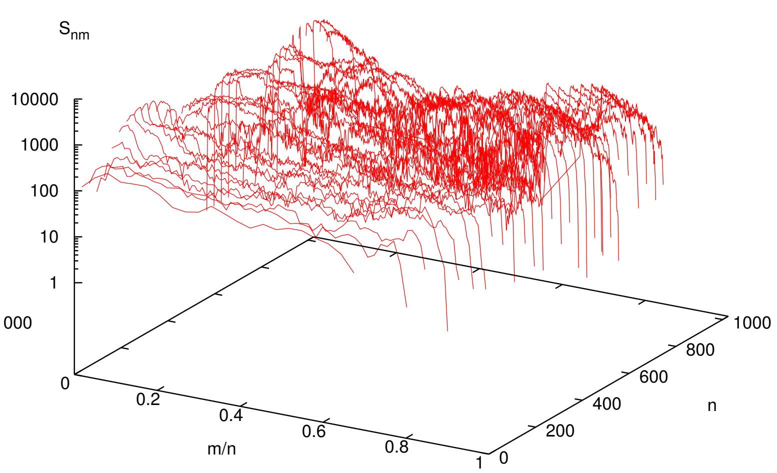
Simulation: dynamics of the algorithm

2d ISAW simulation up to $n = 1024$

- Total sample size: $120,000,000$

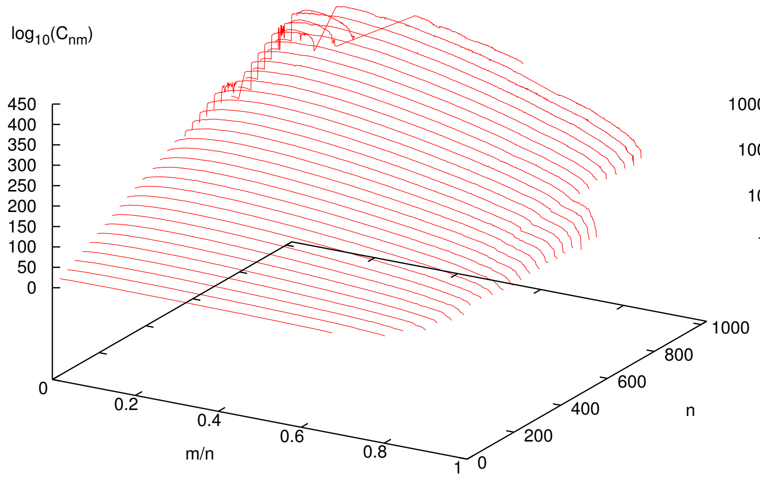


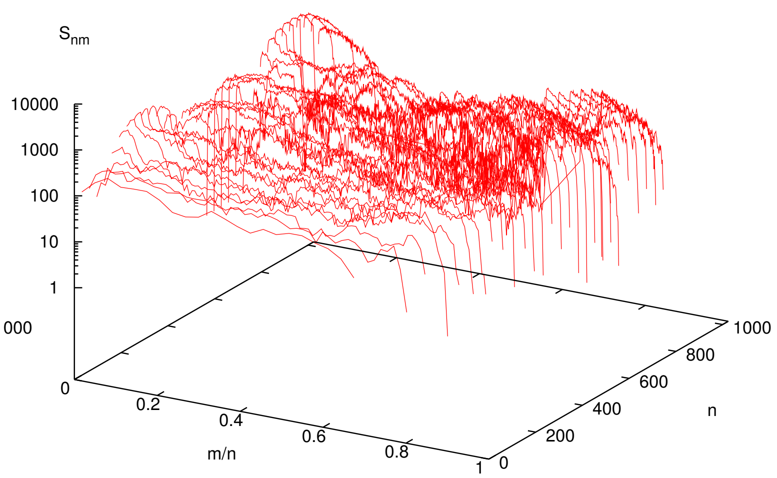


Simulation: dynamics of the algorithm

2d ISAW simulation up to $n = 1024$

- Total sample size: $130,000,000$

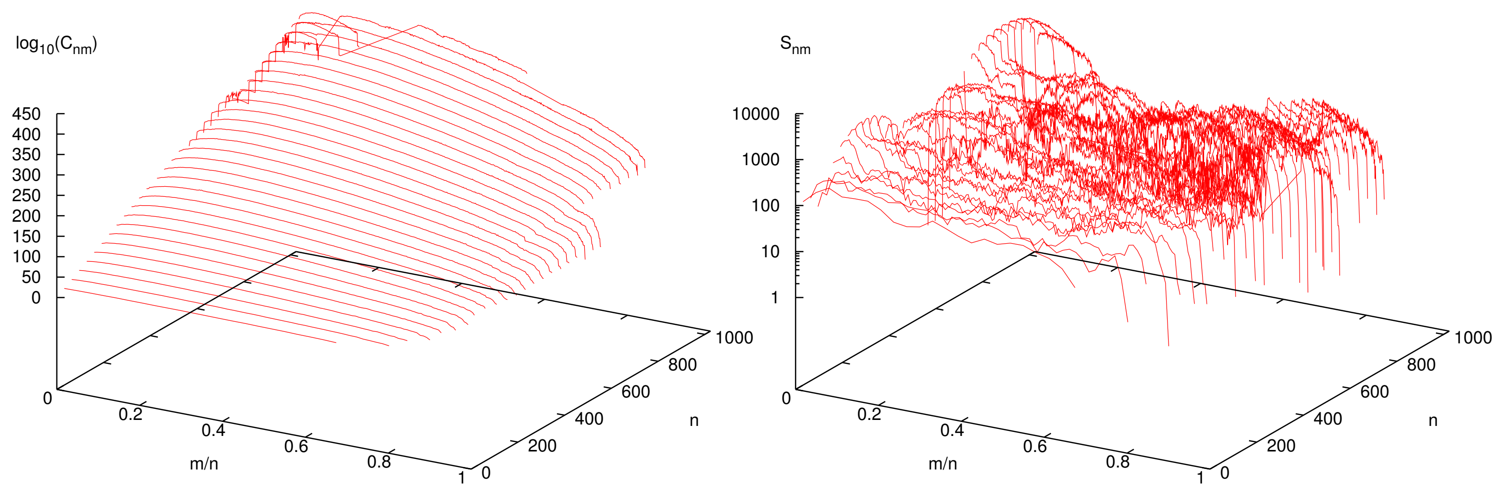




Simulation: dynamics of the algorithm

2d ISAW simulation up to $n = 1024$

- Total sample size: $140,000,000$



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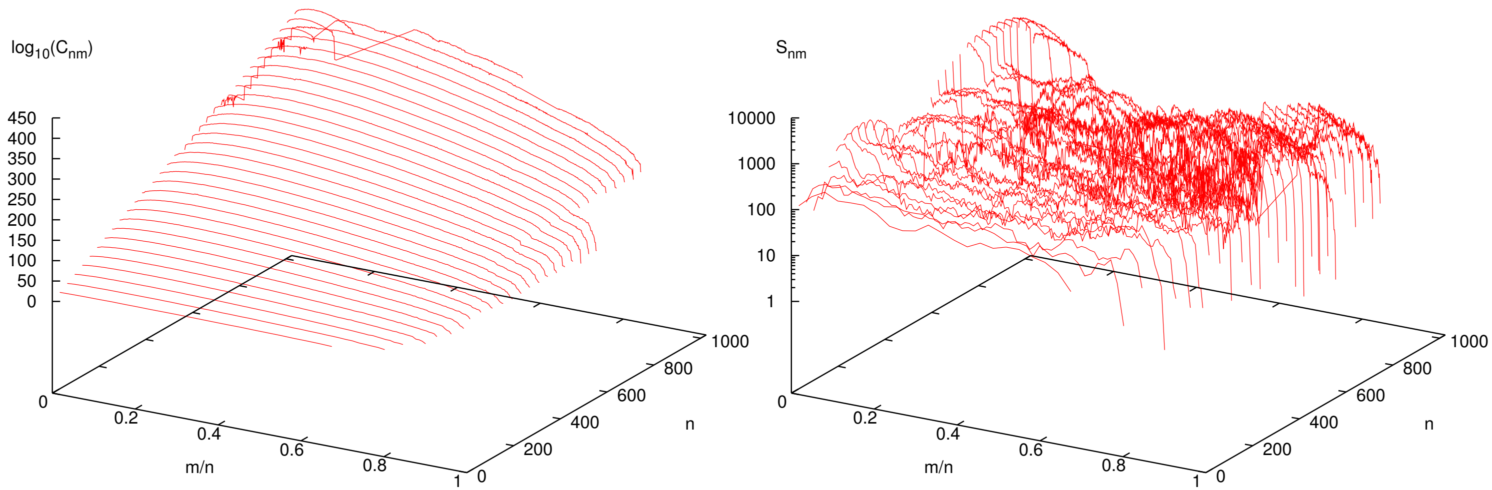
Simulation: dynamics of the algorithm

2d ISAW simulation up to $n = 1024$

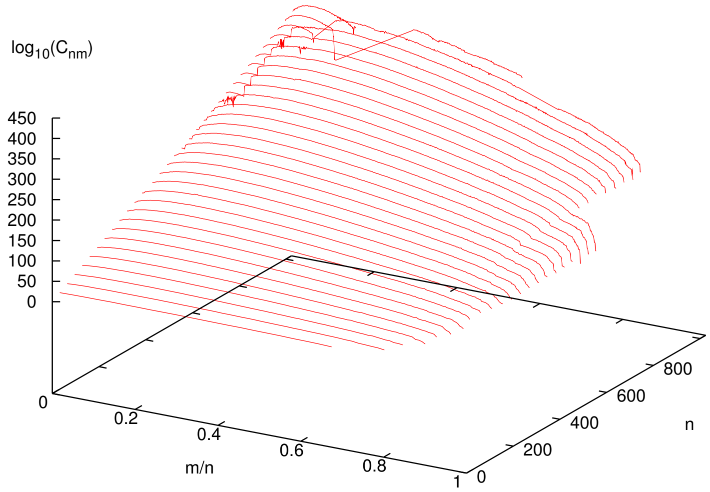
- Total sample size: $150,000,000$

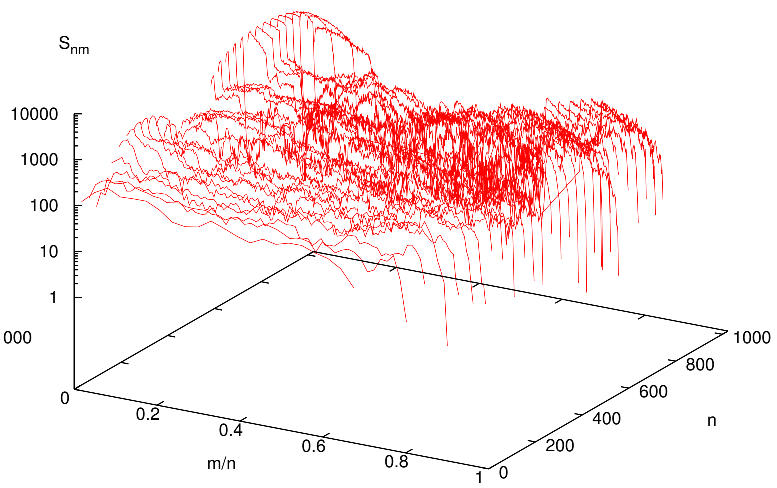


Simulation: dynamics of the algorithm

2d ISAW simulation up to $n = 1024$

- Total sample size: $160,000,000$

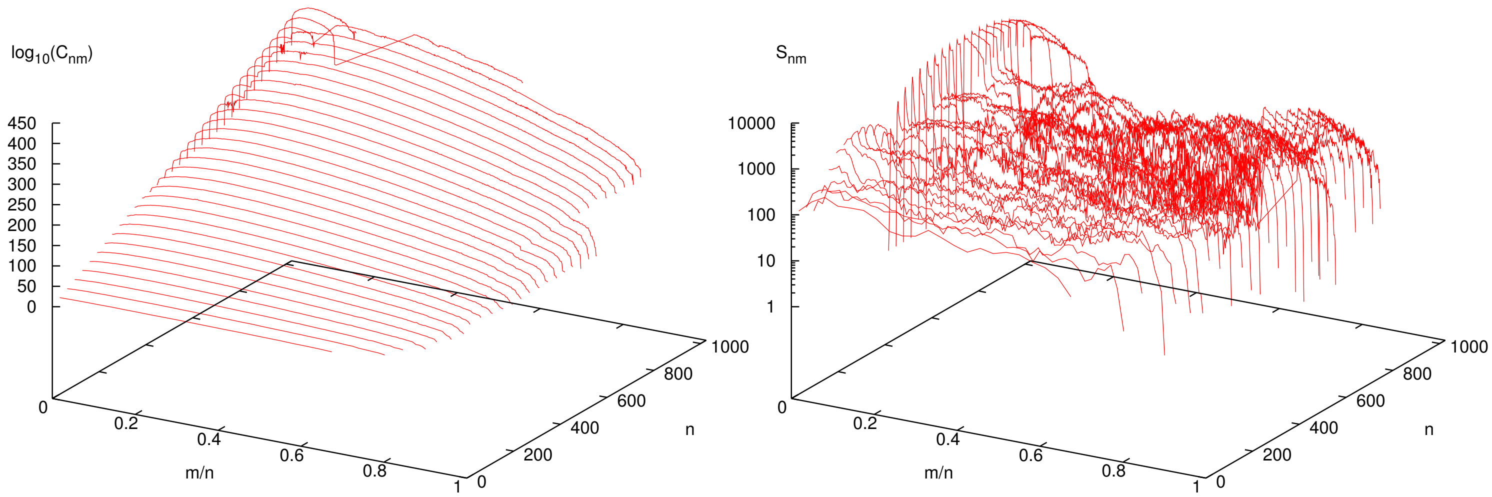




Simulation: dynamics of the algorithm

2d ISAW simulation up to $n = 1024$

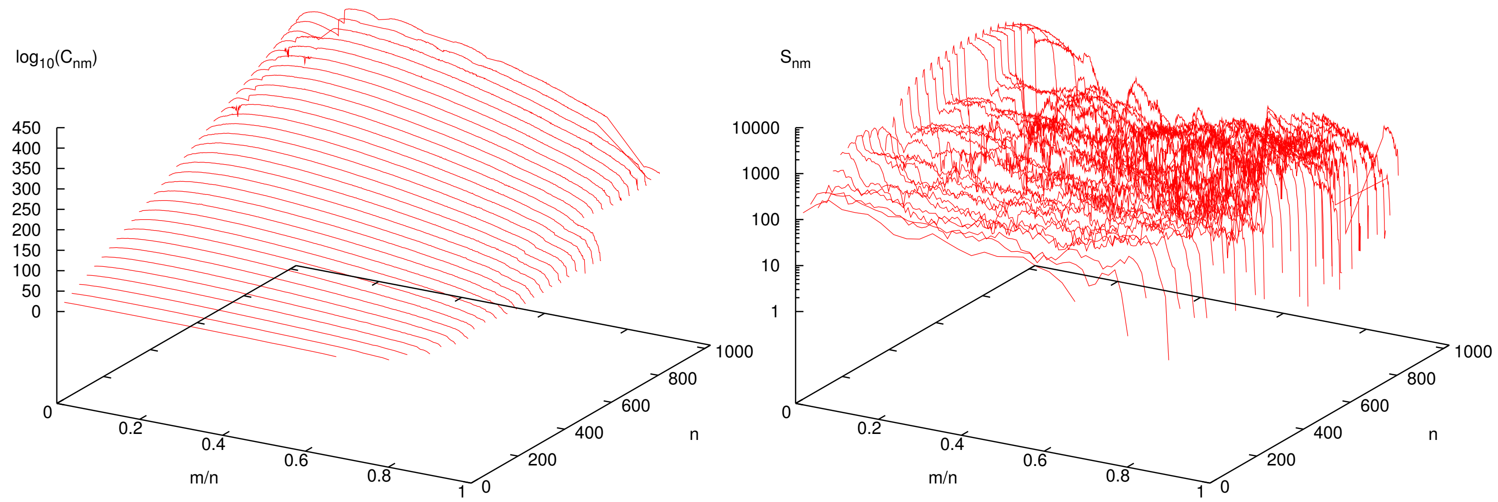
- Total sample size: $170,000,000$



Simulation: dynamics of the algorithm

2d ISAW simulation up to $n = 1024$

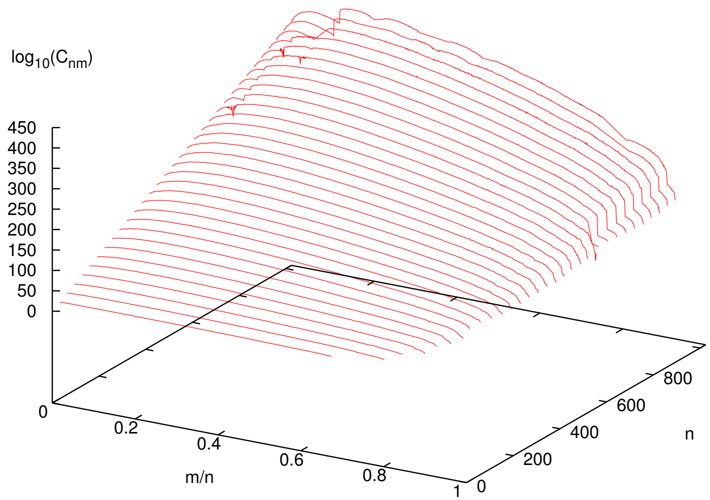
- Total sample size: $180,000,000$

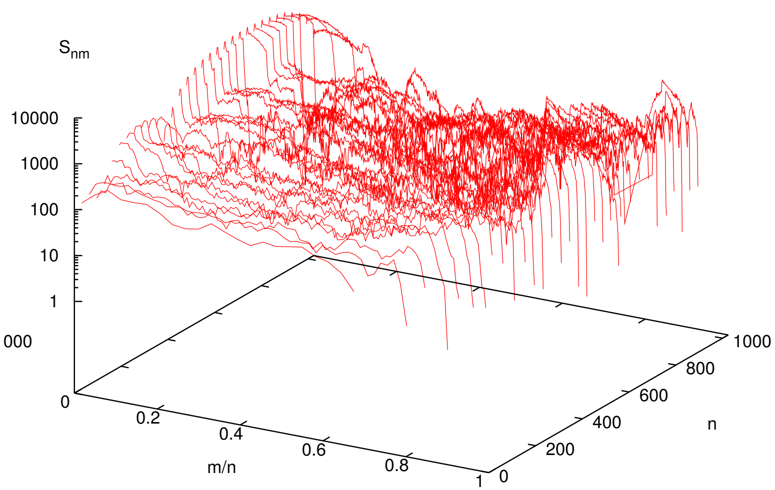


Simulation: dynamics of the algorithm

2d ISAW simulation up to $n = 1024$

- Total sample size: $190,000,000$

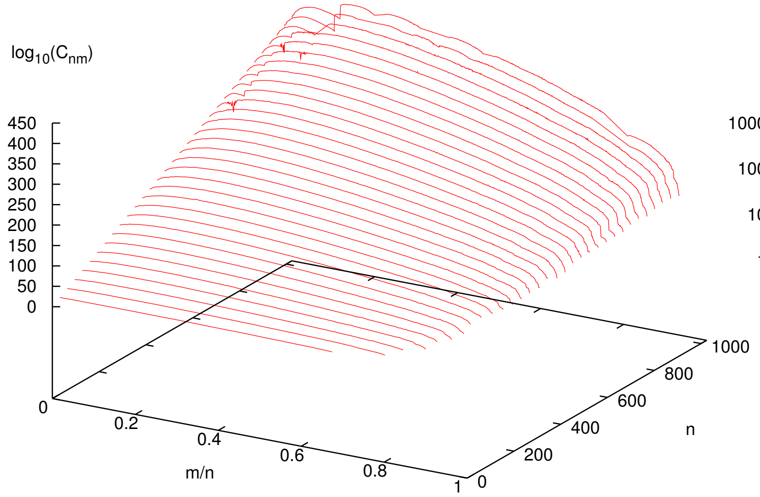


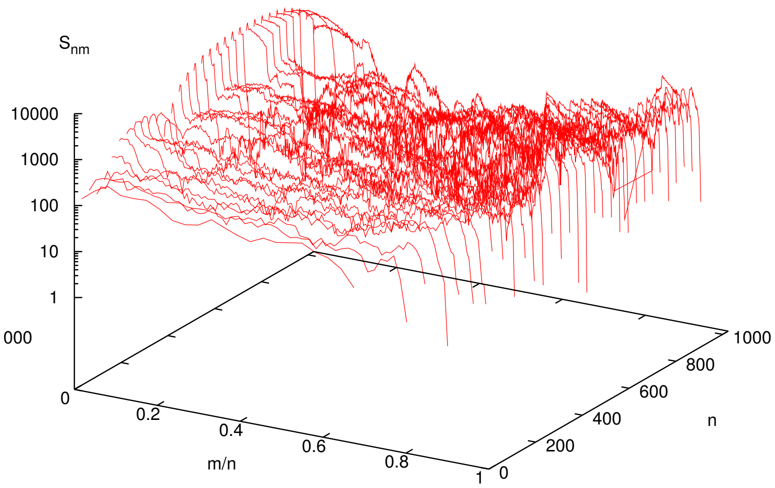


Simulation: dynamics of the algorithm

2d ISAW simulation up to $n = 1024$

- Total sample size: $200,000,000$





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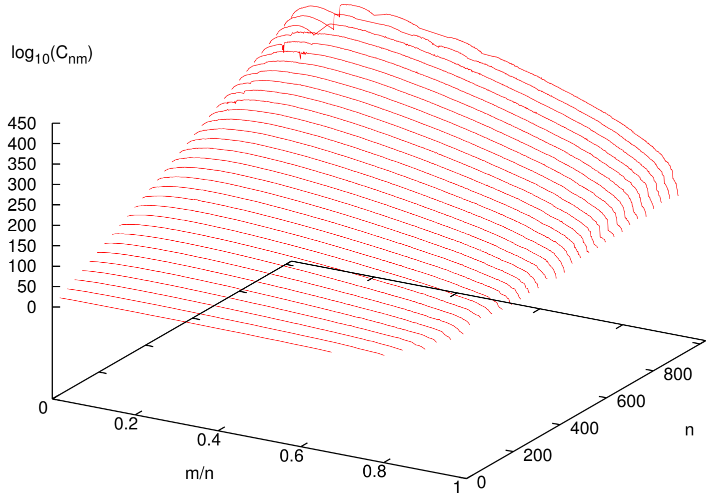
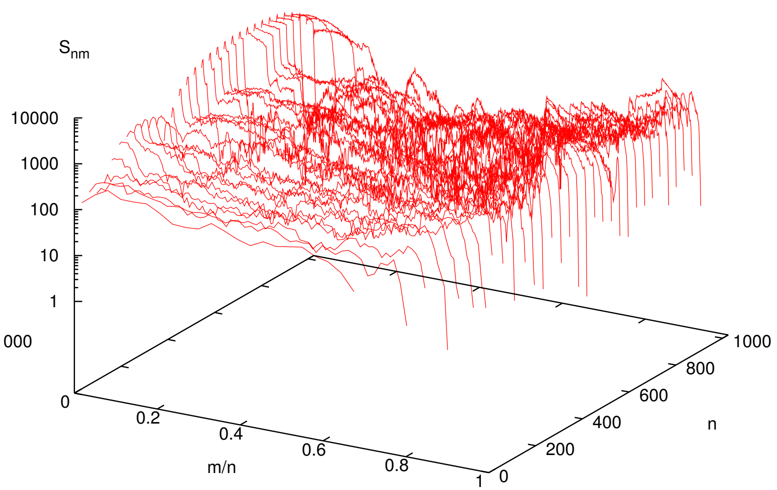
Simulation: dynamics of the algorithm

2d ISAW simulation up to $n = 1024$

- Total sample size: $210,000,000$

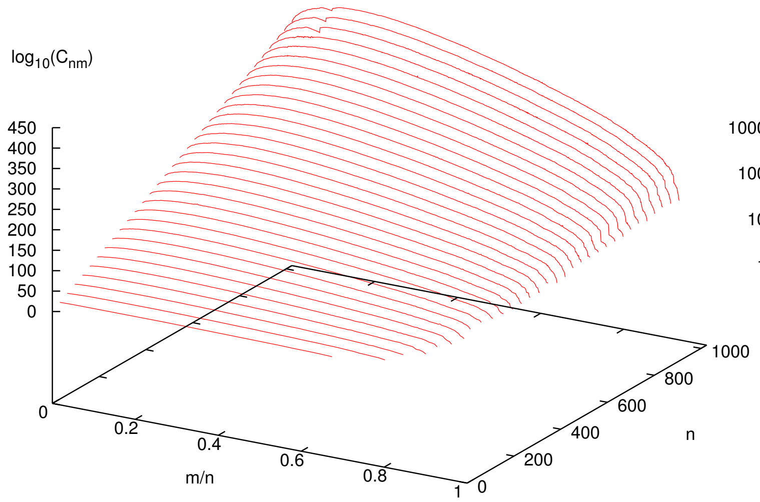


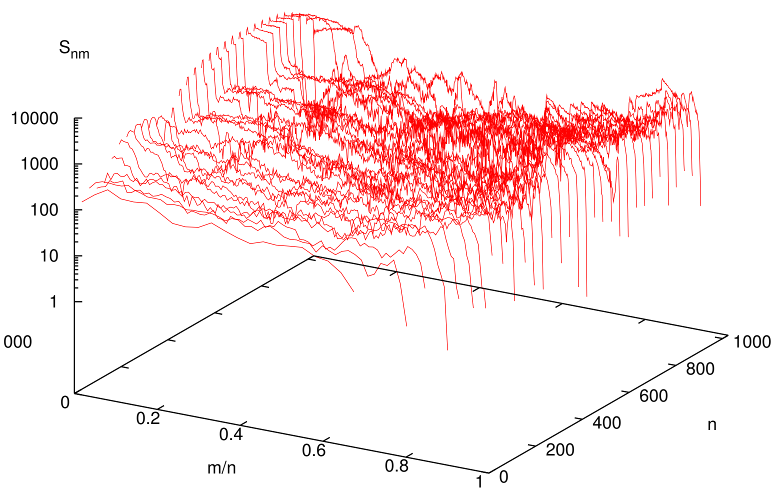


Simulation: dynamics of the algorithm

2d ISAW simulation up to $n = 1024$

- Total sample size: $220,000,000$

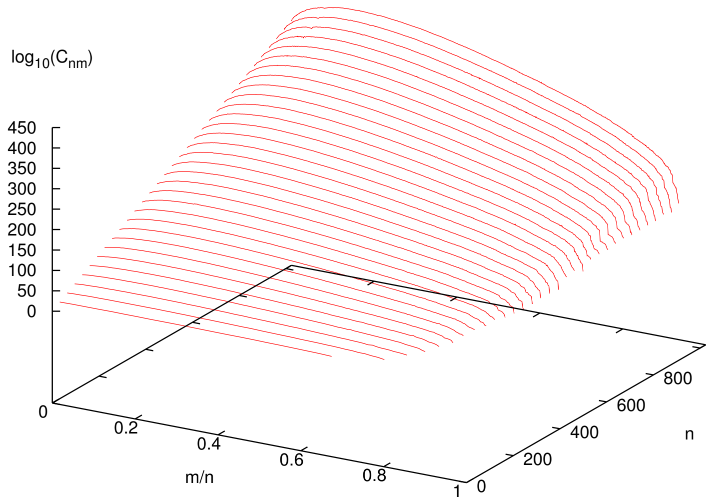


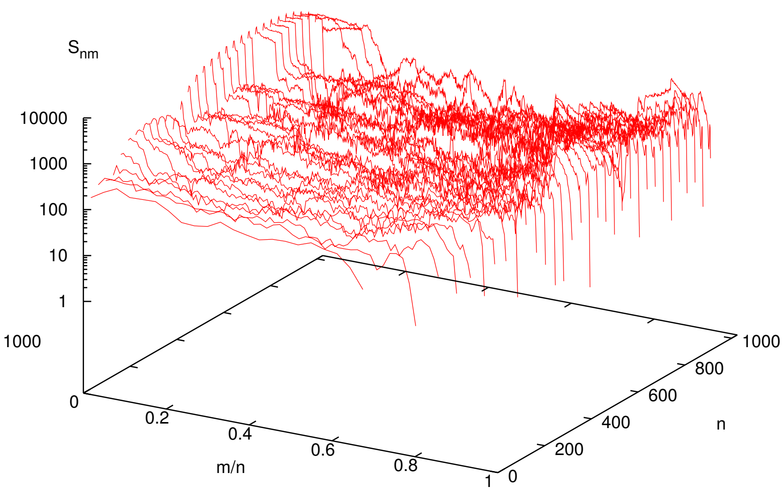


Simulation: dynamics of the algorithm

2d ISAW simulation up to $n = 1024$

- Total sample size: $230,000,000$

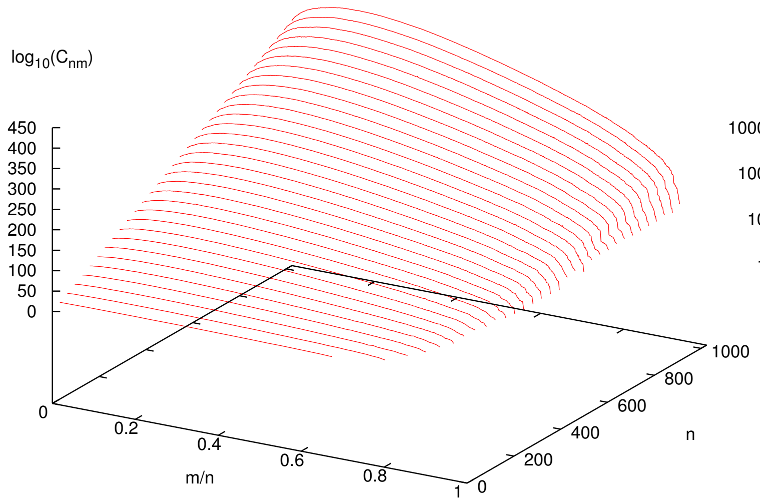


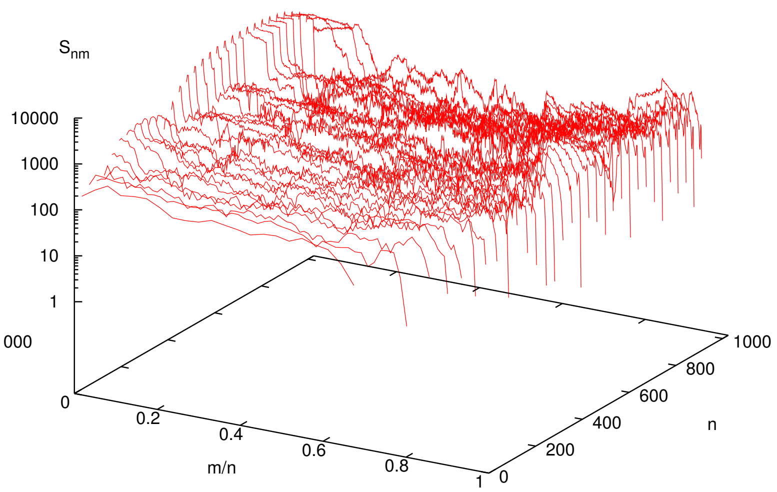


Simulation: dynamics of the algorithm

2d ISAW simulation up to $n = 1024$

- Total sample size: $240,000,000$

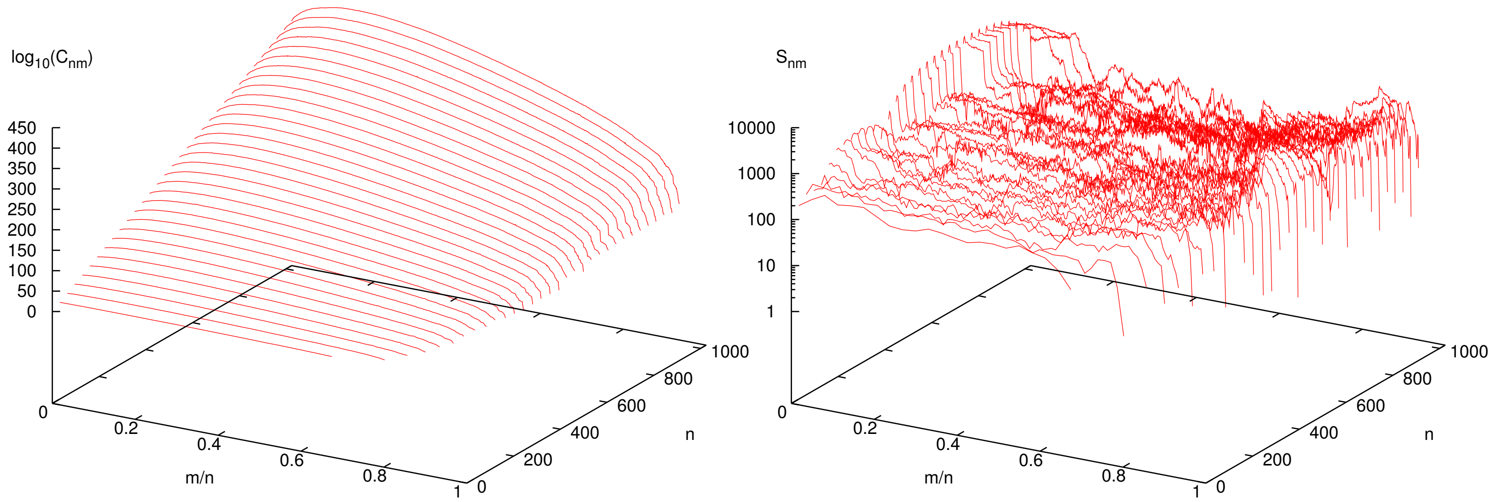




Simulation: dynamics of the algorithm

2d ISAW simulation up to $n = 1024$

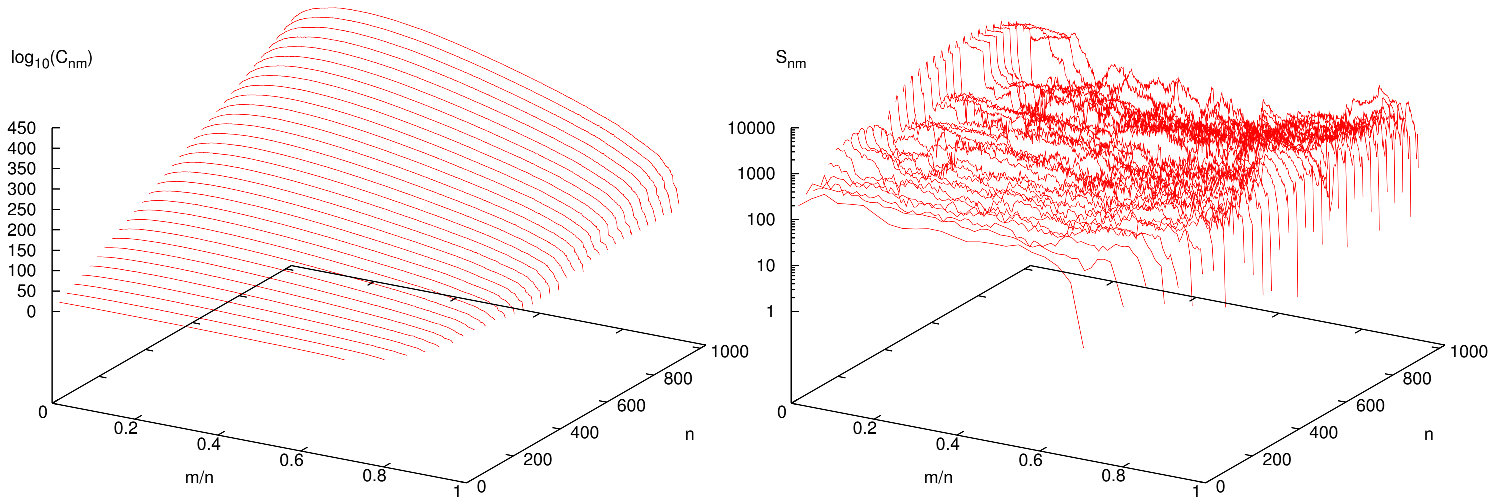
- Total sample size: $250,000,000$



Simulation: dynamics of the algorithm

2d ISAW simulation up to $n = 1024$

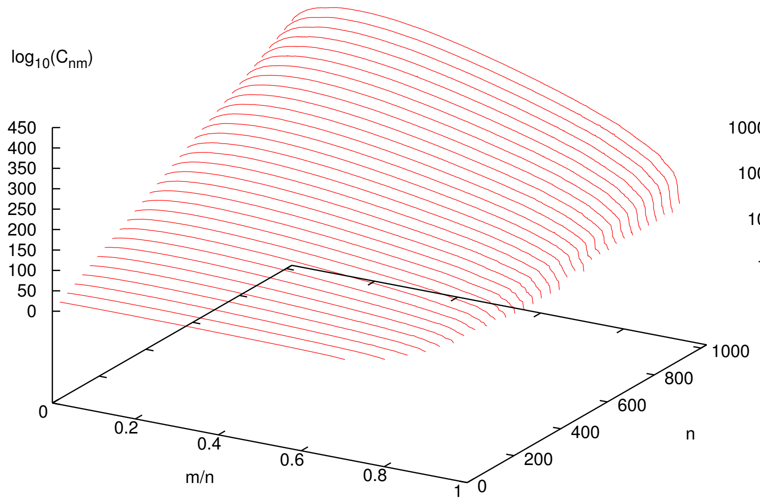
- Total sample size: $260,000,000$

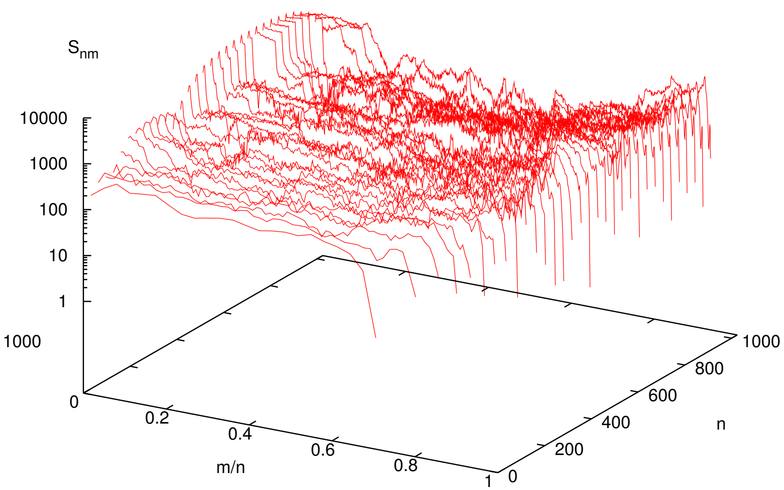


Simulation: dynamics of the algorithm

2d ISAW simulation up to $n = 1024$

- Total sample size: $270,000,000$

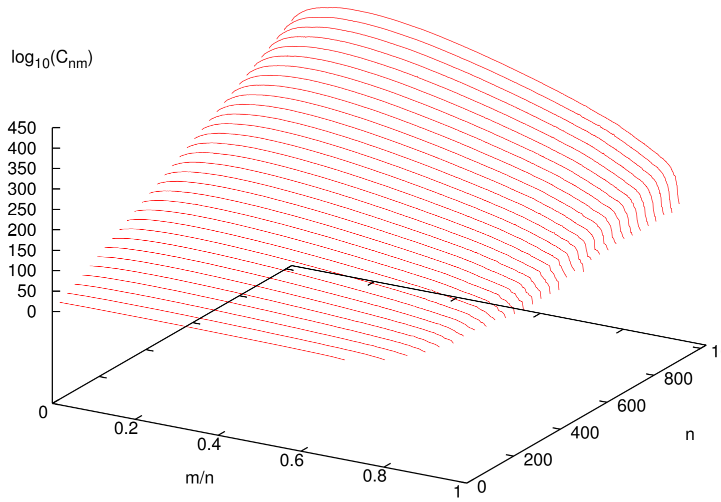


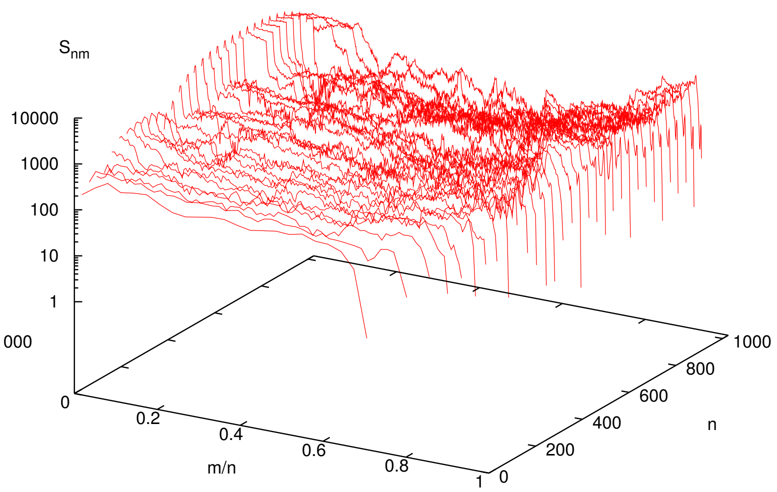


Simulation: dynamics of the algorithm

2d ISAW simulation up to $n = 1024$

- Total sample size: $280,000,000$

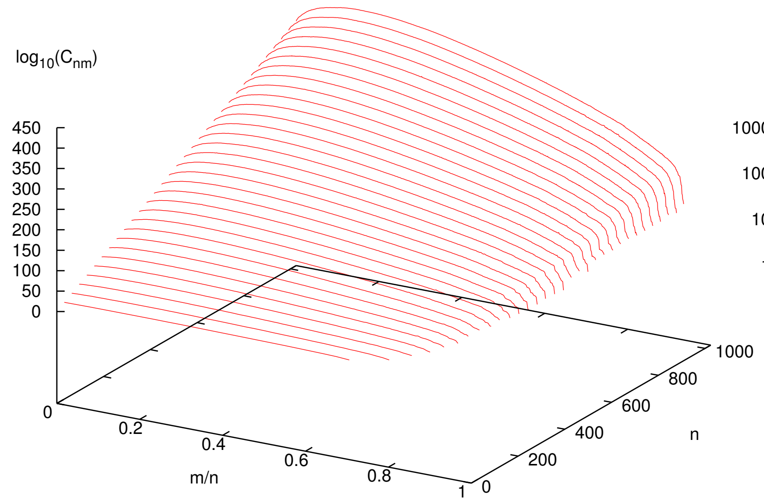


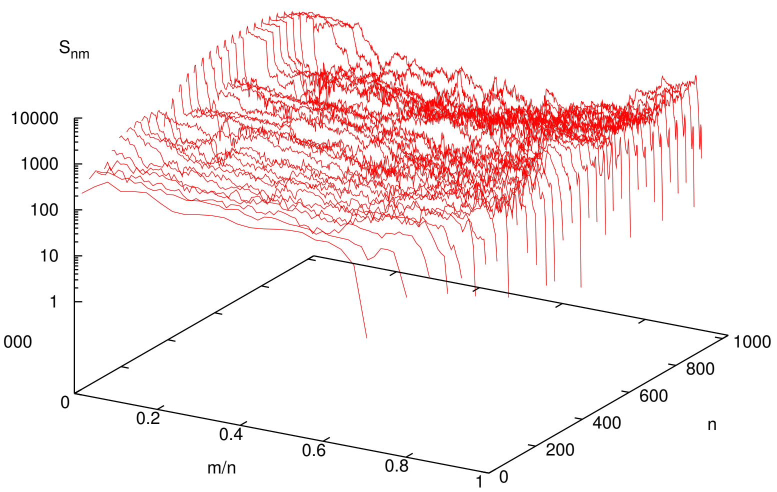


Simulation: dynamics of the algorithm

2d ISAW simulation up to $n = 1024$

- Total sample size: $290,000,000$

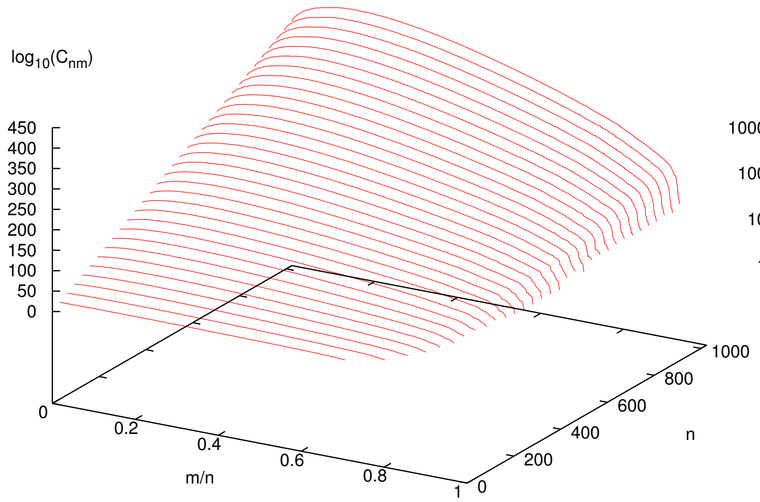


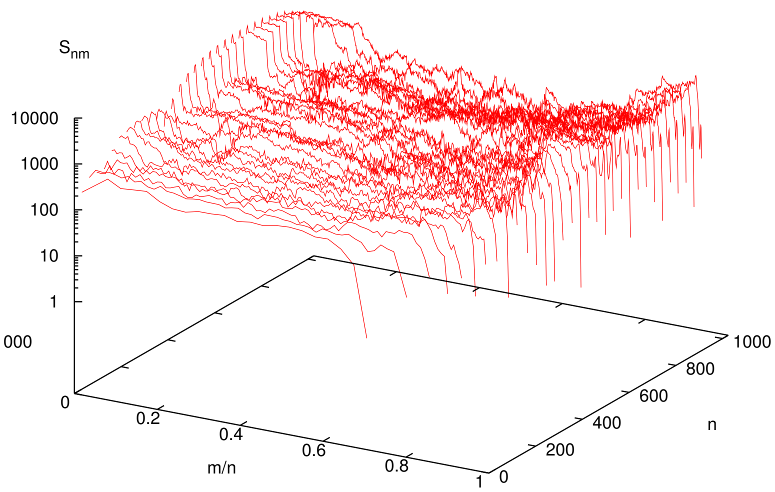


Simulation: dynamics of the algorithm

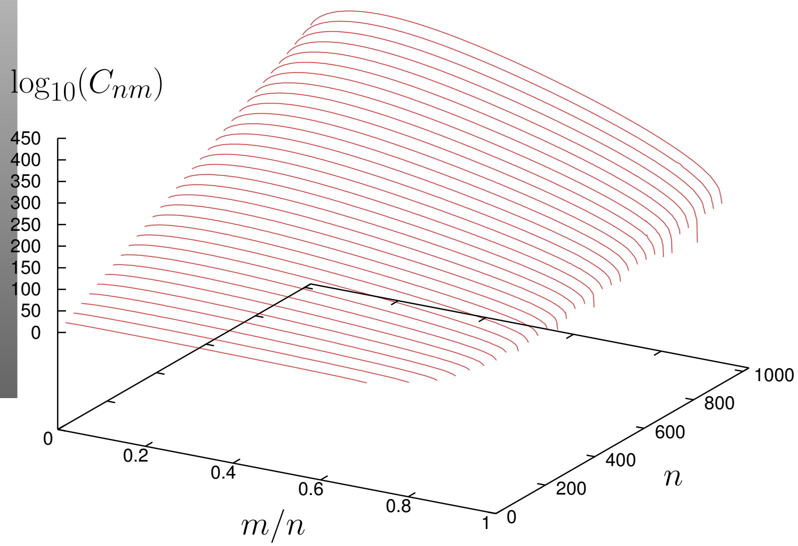
2d ISAW simulation up to $n = 1024$

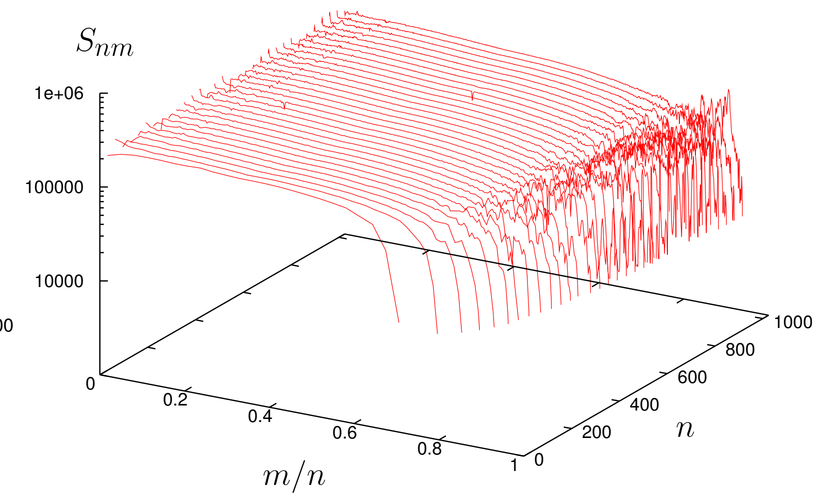
- Total sample size: $300,000,000$





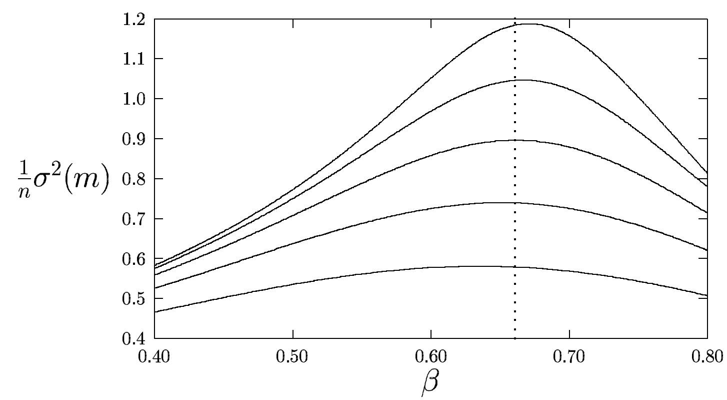
Simulation results: ISAW





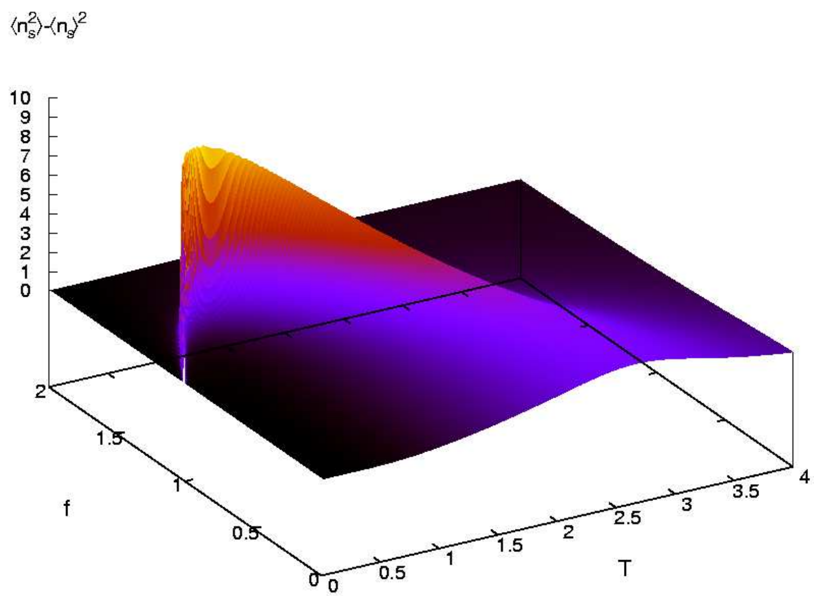
- 2d ISAW up to $n = 1024$
- One simulation suffices
- 400 orders of magnitude

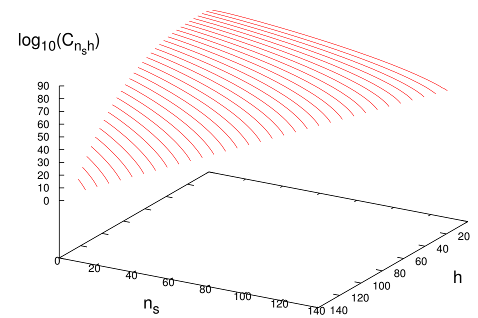
(only 2d shown, 3d similar)

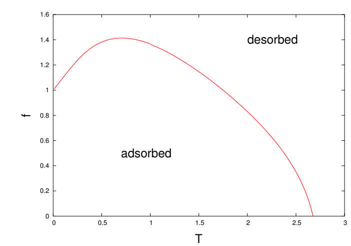


2-Dimensional Density of States

- 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 $n = 256$



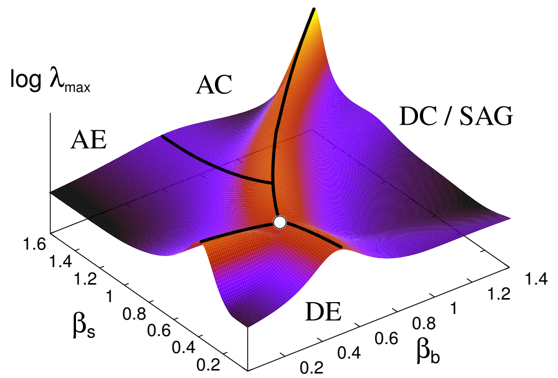


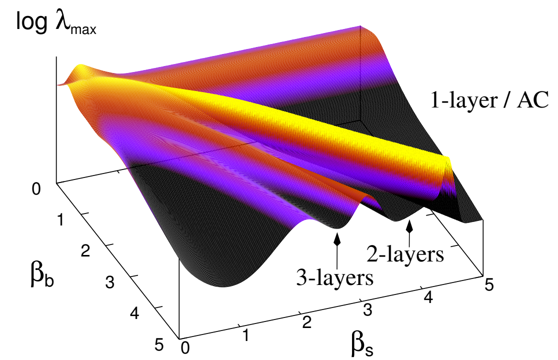


JK et al, JSTAT (2004) P10004

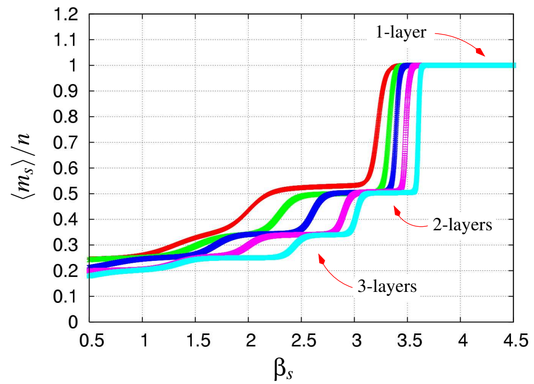
2-Dimensional Density of States

- Layering transitions of adsorbed polymers in poor solvents





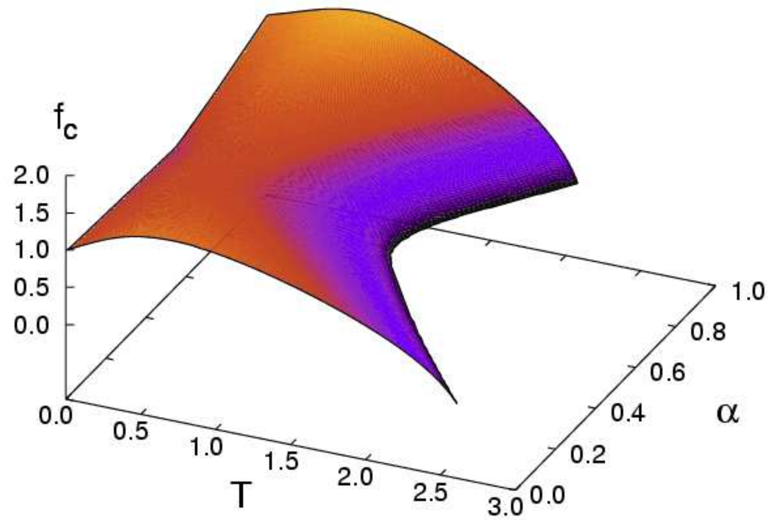
- whole phase diagram at once
- low temperatures accessible
- hierarchy of layering transitions
- resolved controversy over "surface attached globule"

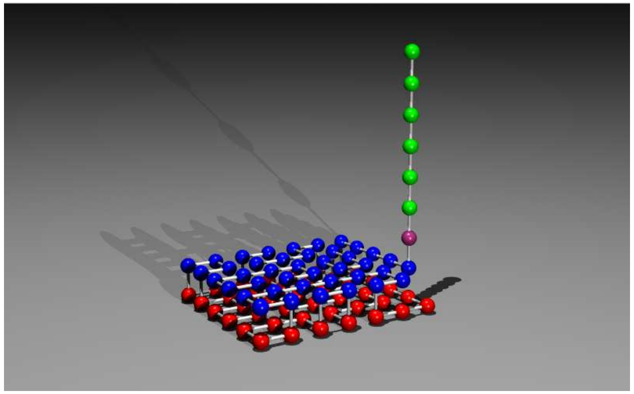


JK et al, cond-mat/0408310

3-Dimensional Density of States

- 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 ($\alpha = 0$)

JK et al, cond-mat/0410189

Summary and Outlook

Conclusion: A Promising New Algorithm

- Presented “flat histogram” version of PERM
  - *One* simulation for complete density of states!
    (the range can also be selectively restricted)

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Conclusion: A Promising New Algorithm

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- Simulations:
  - SAW in a strip, HP model, ISAW
  - force-induced desorption
  - adsorbed, collapsed polymers

Conclusion: A Promising New Algorithm

- Presented “flat histogram” version of PERM
  - *One* simulation for complete density of states!
    (the range can also be selectively restricted)
- Simulations:
  - SAW in a strip, HP model, ISAW
  - force-induced desorption
  - adsorbed, collapsed polymers
- Outlook: applications to further models, e.g.
  - branched polymers in wedges
  - extended Domb-Joyce model
  - more realistic models, off-lattice simulations

The End