A flat histogram stochastic growth algorithm

(with application to polymers and proteins)

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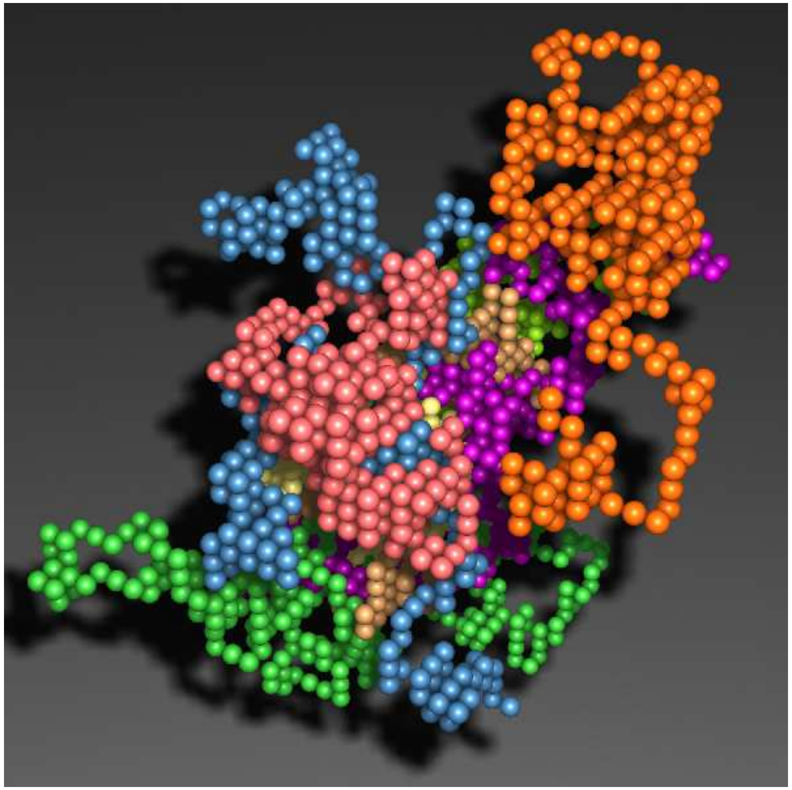
Joint work with Jaroslaw Krawczyk, TU Clausthal

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
- Consequence:
  chains clump together



Eight polymers in a bad solvent
(Grassberger, FZ Jülich)

Lattice Model

Self-Avoiding Walks with Interactions

- Physical space $\rightarrow$ lattice $\mathbb{Z}^3$ (or $\mathbb{Z}^d$)
- Polymer in solution $\rightarrow$ random walk with self-avoidance
- Quality of solvent $\rightarrow$ short-range interaction ϵ
- Properties of monomers $i, j \rightarrow$ interaction $\epsilon = \epsilon_{i,j}$

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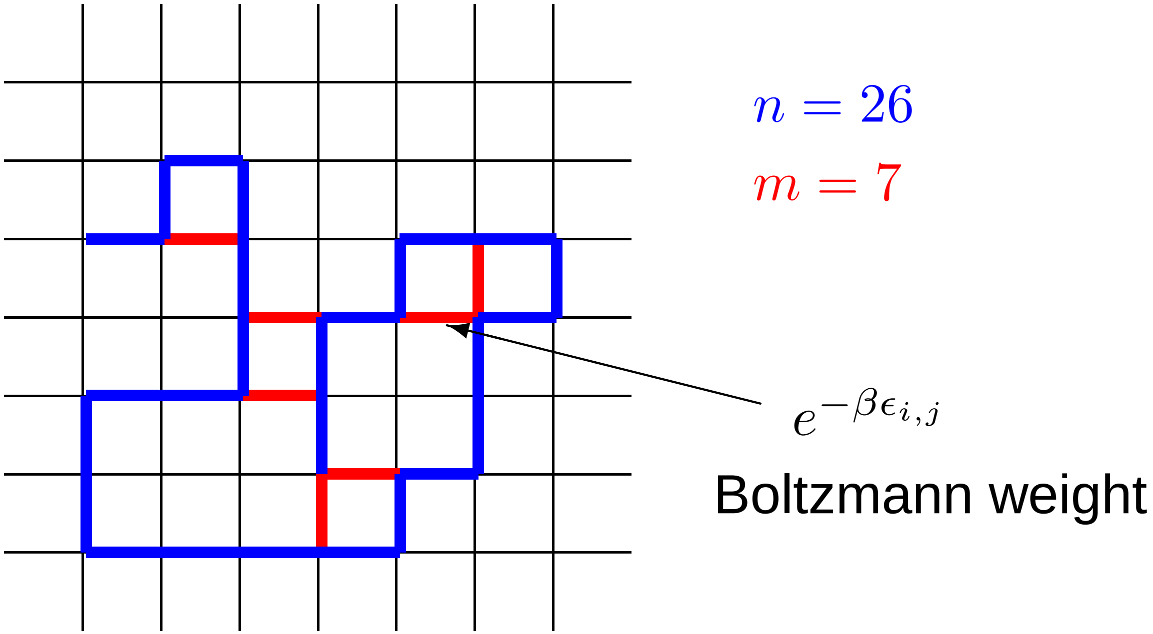
- Properties of monomers $i, j \rightarrow$ interaction $\epsilon = \epsilon_{i,j}$
- Two examples:
  - ISAW model: interaction $\epsilon_{i,j} = -1$
    of interest: thermodynamic limit ($V = \infty$ and $n \rightarrow \infty$)
  - HP model: two types of monomers H and P
    $\epsilon_{HH} = -1$, $\epsilon_{HP} = \epsilon_{PH} = \epsilon_{PP} = 0$
    of interest: fixed finite sequence, density of states

Lattice Model: ISAW



- ISAW model: interaction $\epsilon_{i,j} = -1$, $\omega = e^{\beta}$
- Partition function: $Z_n(\omega) = \sum_m C_{n,m}\omega^m$
- $C_{n,m}$ number of SAW with length n and m interactions

Lattice Model: HP model

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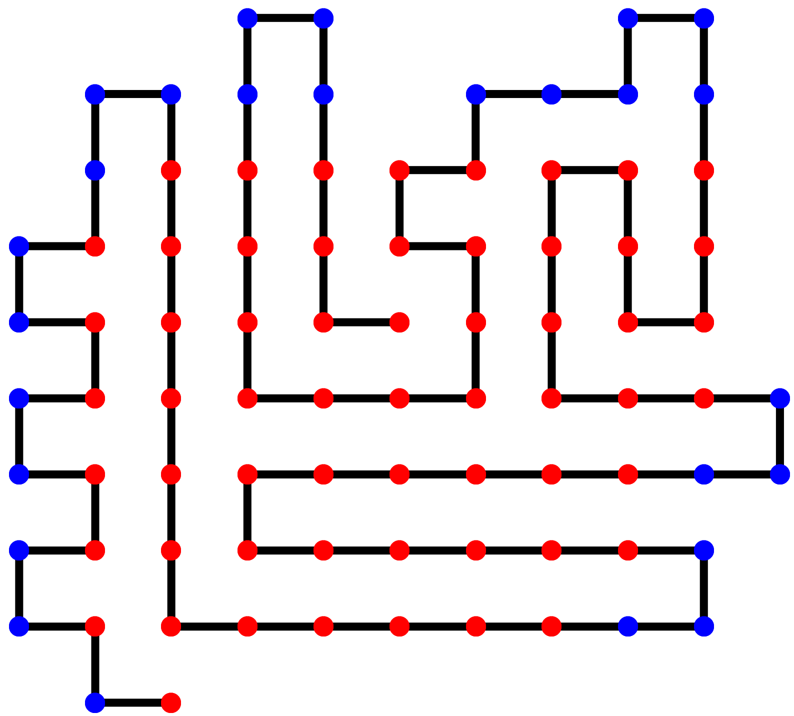
Hydrophobic

Polar



- Groundstate of sequence with 85 monomers ($d = 2$)

Why Simulations?

- ISAW model:
  - Tricritical phase transition, $d_u = 3$
  - In principle understood, however surprising details
    e.g. “pseudo-first-order transition” for $d > 3$
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- Most interesting open questions in collapsed regime

Collapsed regime is notoriously difficult to simulate

Stochastic Growth Algorithms

PERM: “Go With The Winners”

PERM = Pruned and Enriched Rosenbluth Method

Grassberger, Phys Rev E 56 (1997) 3682

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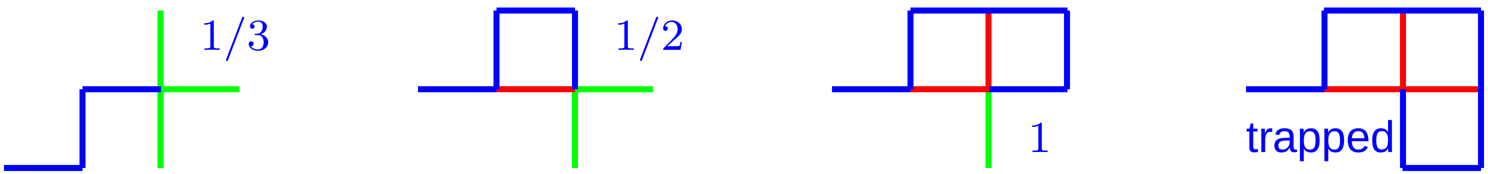
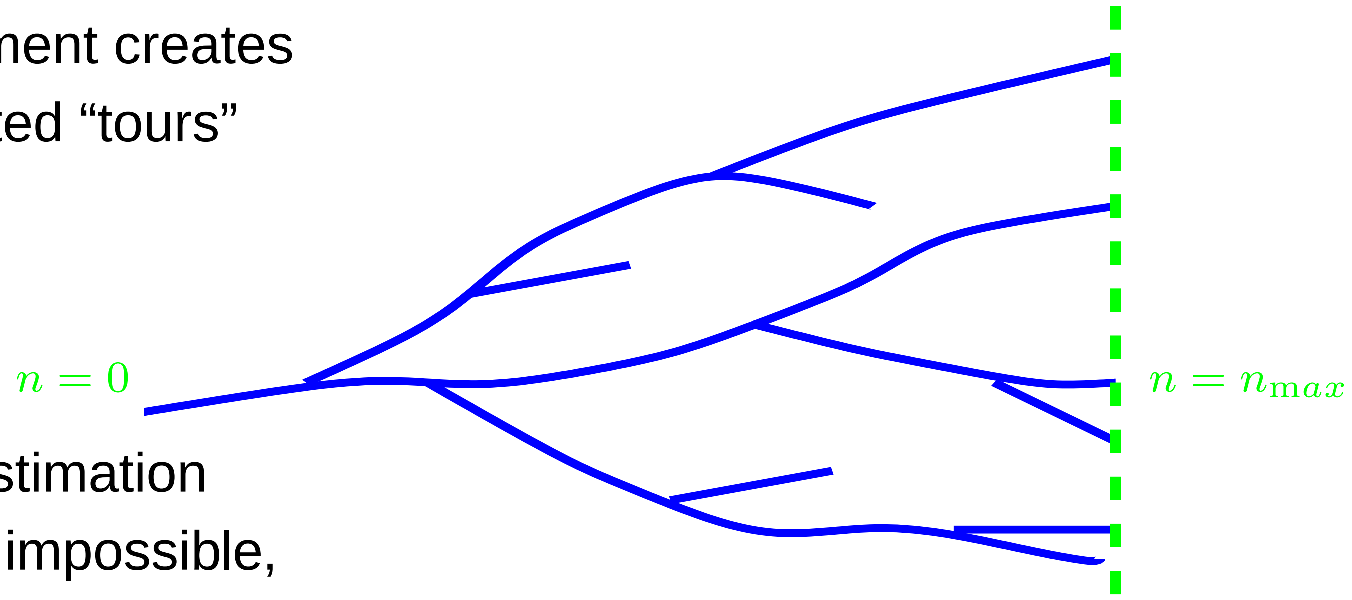


- Enrichment: weight too large $\rightarrow$ make copies of configuration
- Pruning: weight too small $\rightarrow$ remove configuration occasionally

Observation: kinetic growth weights and interactions balance each other at suitable temperatures (in the collapse region)

PERM – continued

- PERM well suited for simulation of collapsing polymers
- Enrichment creates correlated “tours”



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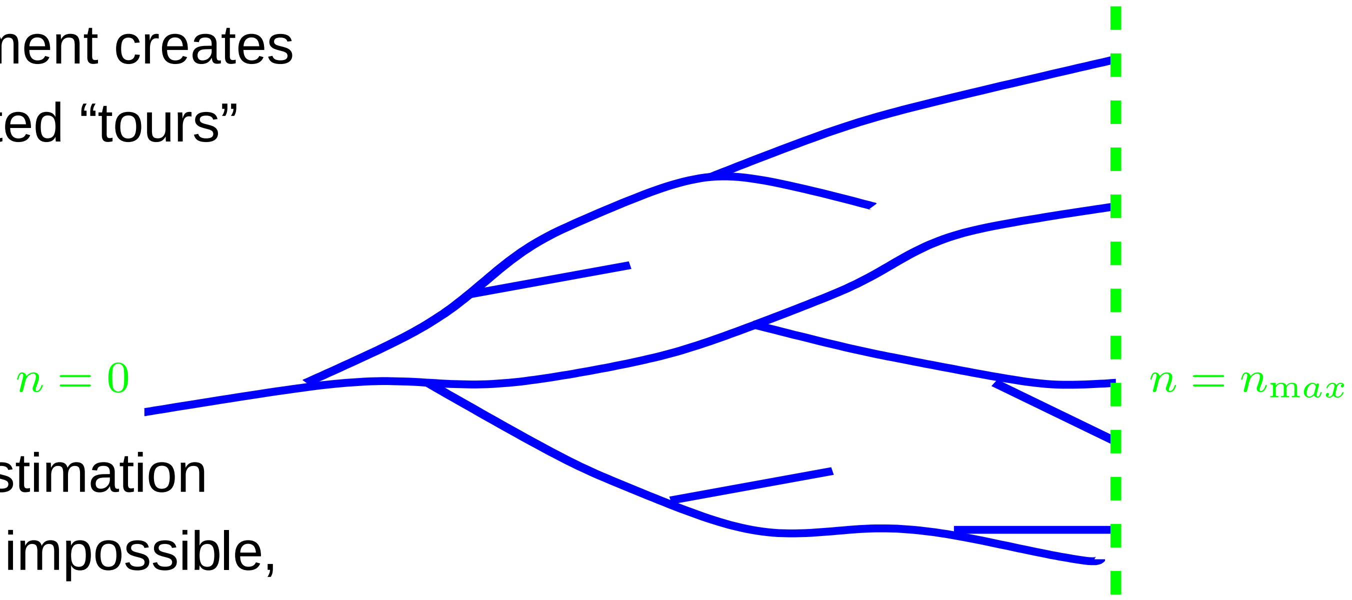

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PERM is “blind” - it benefits from “visual aids”, such as

- Markovian anticipation (learning from experience)

PERM – further developments

- A significant improvement: nPERM = “new” PERM

  Hsu et al, J Chem Phys 118 (2003) 444

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- Current work: flatPERM = “flat histogram” PERM

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  - flatPERM samples a generalised multicanonical ensemble
  - Covers the whole temperature range in *one* simulation!

Related: multicanonical chain growth algorithm

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Applications:

- linear and branched polymers, proteins, percolation, . . .

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- Exact enumeration: choose *all* a continuations with equal weight
- Kinetic growth: chose *one* continuation with a-fold weight (a may be zero).
  - An n step configuration gets assigned a weight

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

  - S growth chains with weights $W_n^{(i)}$ give estimate

$$C_n^{est} = \langle W \rangle_n = \frac{1}{S} \sum_i W_n^{(i)}$$

Algorithm details - pruning/enrichment

- $W_n^{(i)}$ is estimate of C_n
- Consider ratio $r = W_n^{(i)} / C_n^{est}$
  - $r > 1 \rightarrow$ enrichment step:
    make $c = \min(\lfloor r \rfloor, a_n)$ distinct copies with weight $\frac{1}{c} W_n^{(i)}$
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- Consequences
  - Number of samples generated for each n is roughly constant
  - Ideally, unbiased random walk in configuration size
  - We have a **flat histogram algorithm**

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- thermal PERM: estimate partition function $Z_n(\beta)$
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- Generalization to more microcanonical parameters possible

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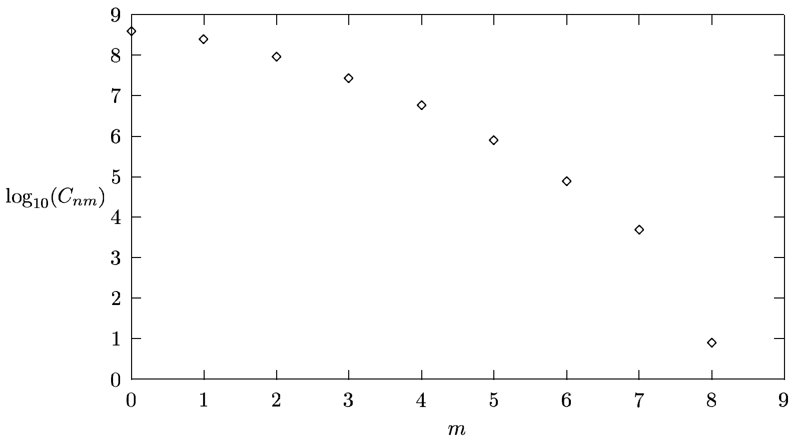
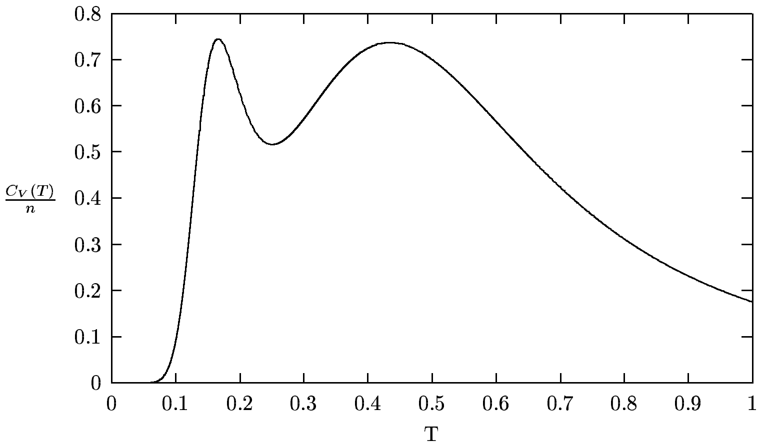
- What if we don’t need the whole histogram?
  - Restriction of histogram possible
  - e.g. impose internal energy restriction $m/n < u_{cutoff}$
- What if we don’t want a “flat” histogram?
  - Sample profile can be tuned
  - Selectively perform pruning/enrichment
    with respect to profile shape $f_{n,m}$

Simulation Results

Simulation results: HP model

- Sequence I (14 Monomers, HPHPHHPHPHHPPH, $d = 3$):

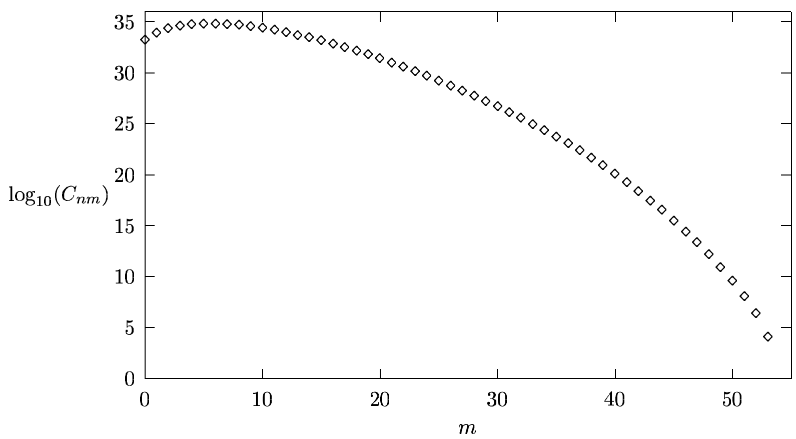


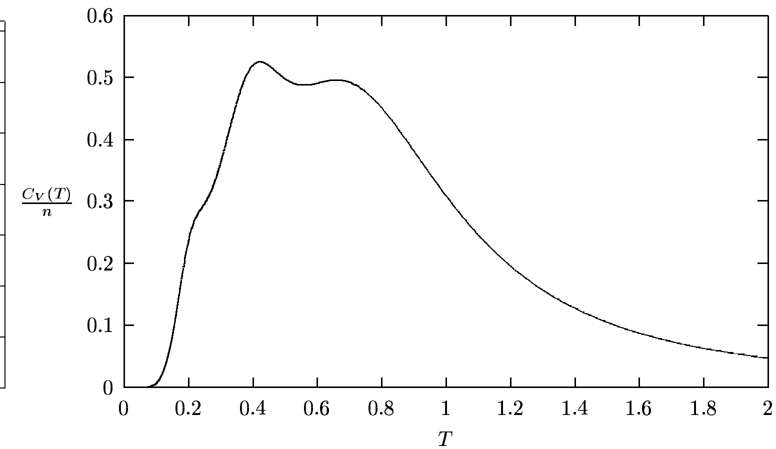


- Pedagogical example, engineered for native ground state
- Perfect agreement with exact enumeration

Simulation results: HP model

- Sequence II (85 Monomers, $d = 2$):





- Investigated several other sequences in $d = 2$ and $d = 3$
- Collapsed regime accessible
- Reproduced known ground state energies
- Obtained $C_{n,m}$ over large range

Simulation: Equilibration for 2d ISAW

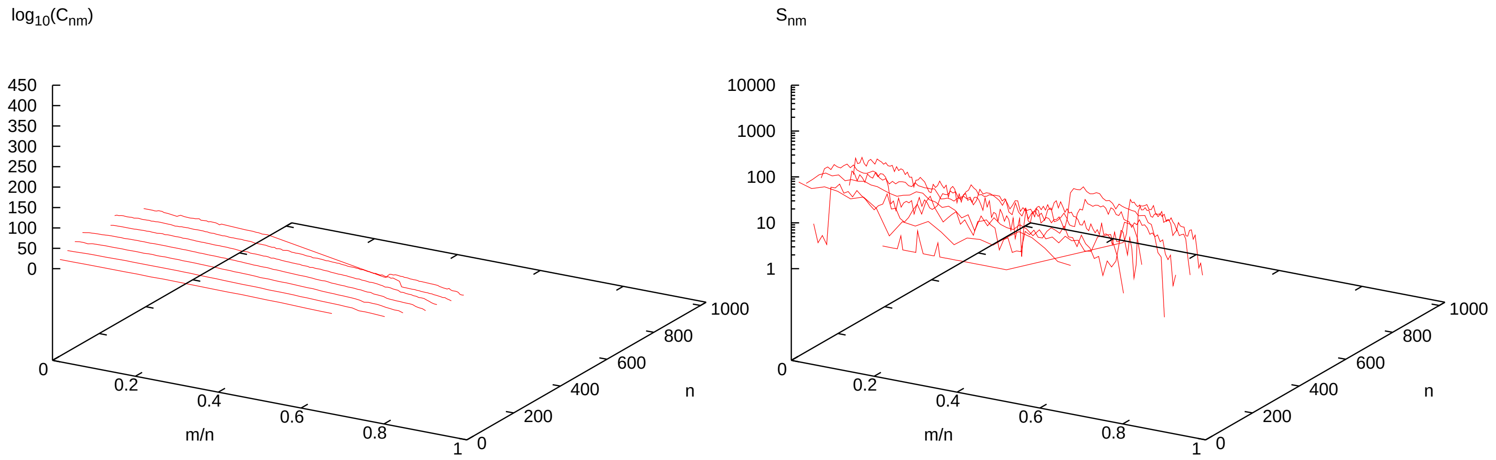
2d ISAW simulation up to $n = 1024$

- Equilibration with delay 0.1:
  after t tours growth up to length $10t$

Simulation: Equilibration for 2d ISAW

2d ISAW simulation up to $n = 1024$

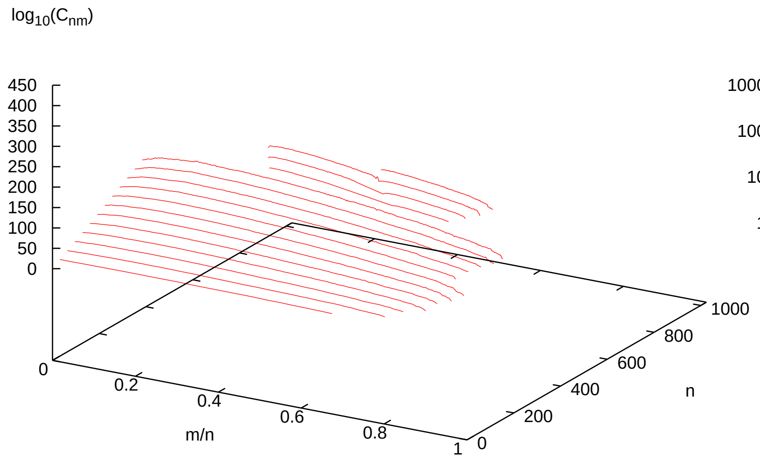
- Total sample size: $1,000,000$

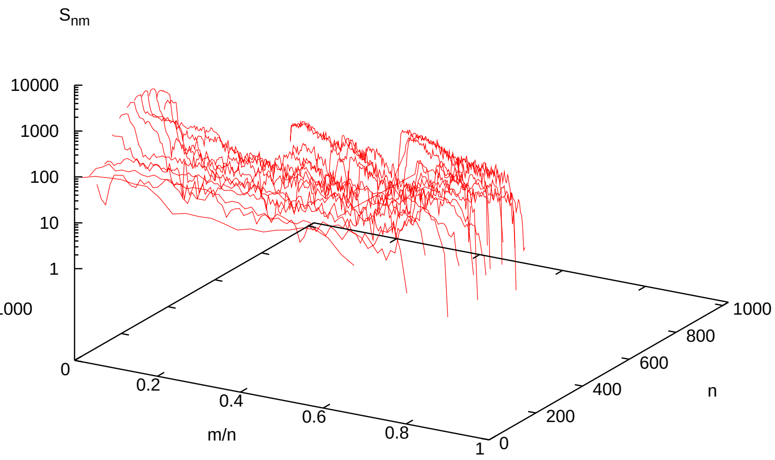


Simulation: Equilibration for 2d ISAW

2d ISAW simulation up to $n = 1024$

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

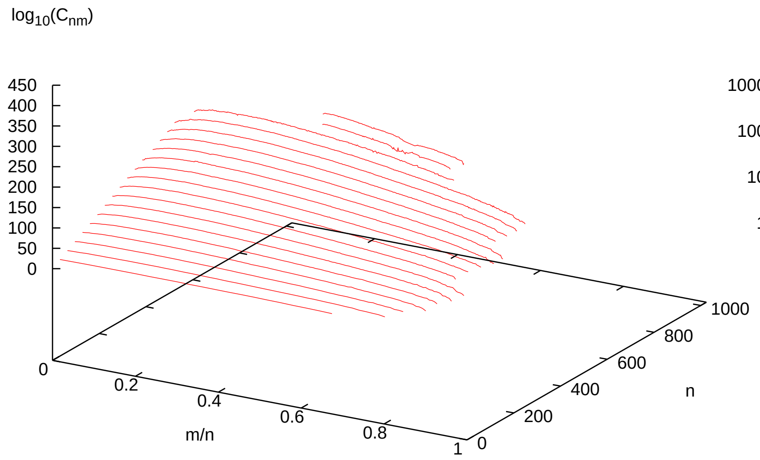


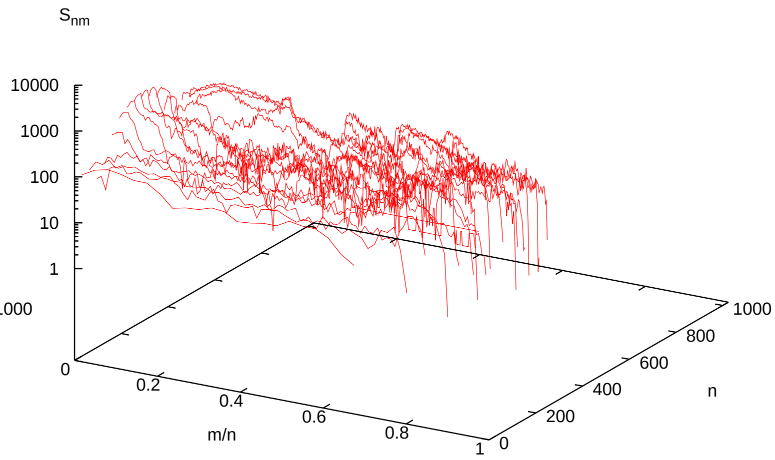


Simulation: Equilibration for 2d ISAW

2d ISAW simulation up to $n = 1024$

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

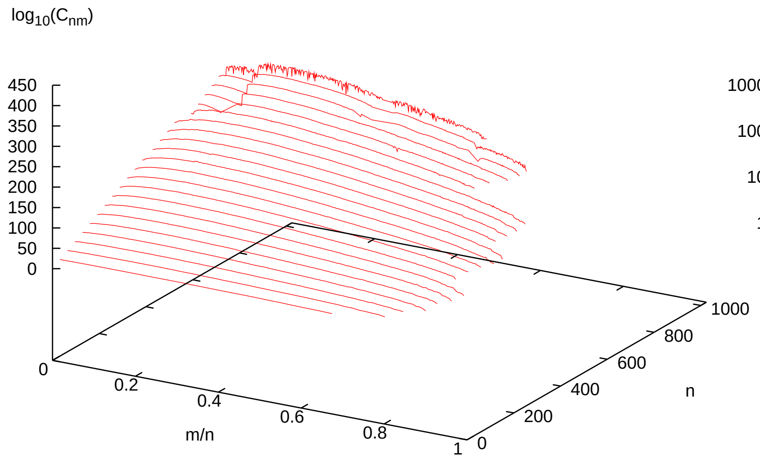


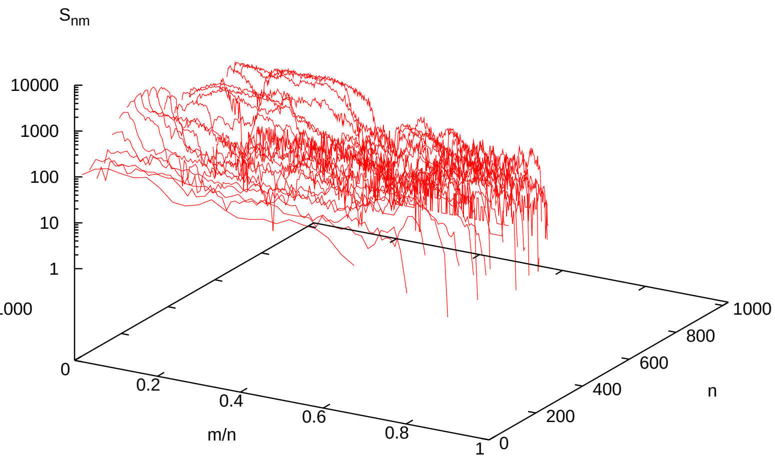


Simulation: Equilibration for 2d ISAW

2d ISAW simulation up to $n = 1024$

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

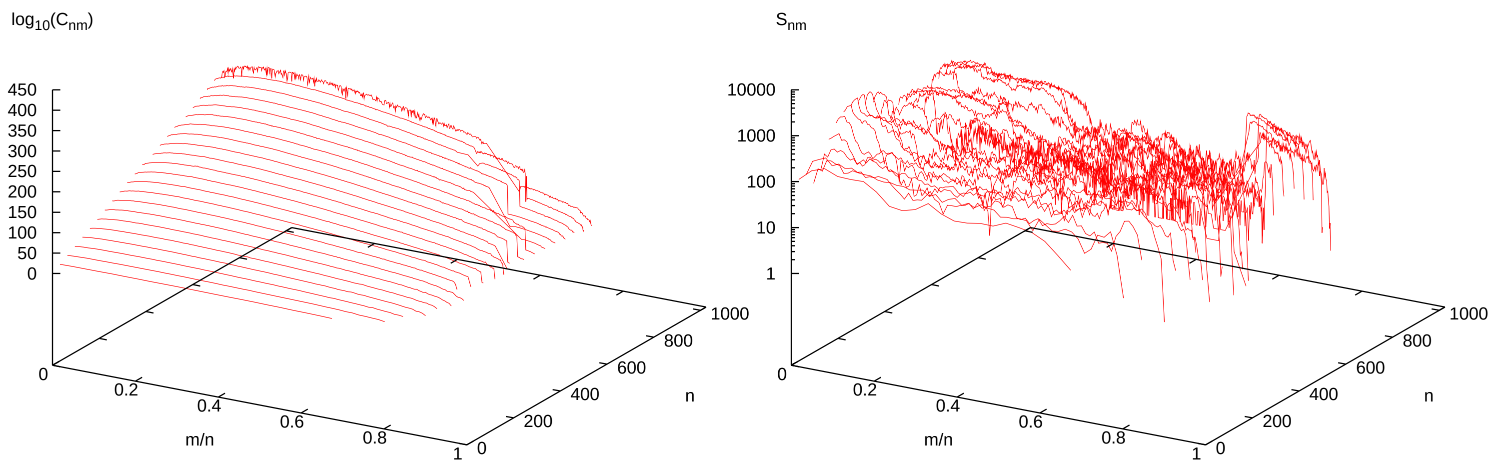




Simulation: Equilibration for 2d ISAW

2d ISAW simulation up to $n = 1024$

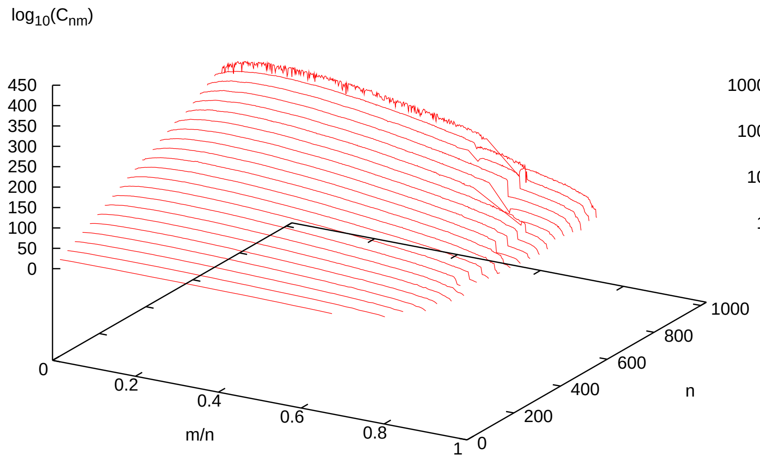
- Total sample size: $40,000,000$

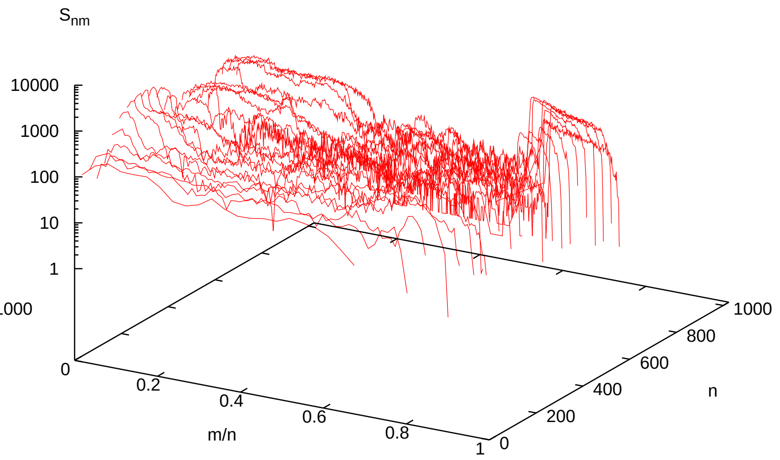


Simulation: Equilibration for 2d ISAW

2d ISAW simulation up to $n = 1024$

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

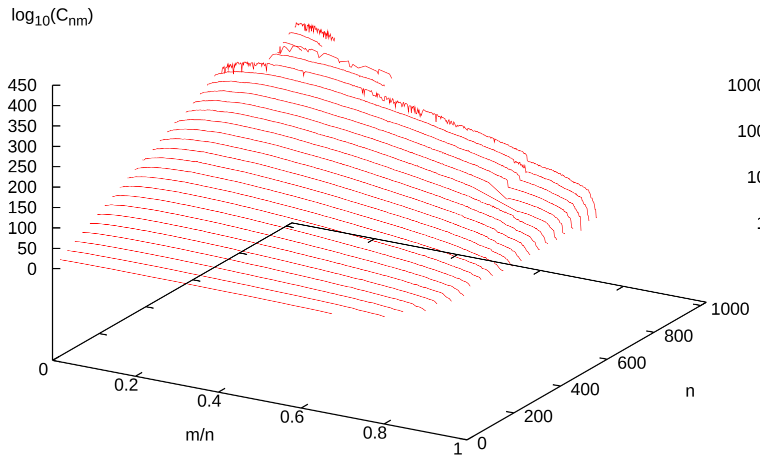


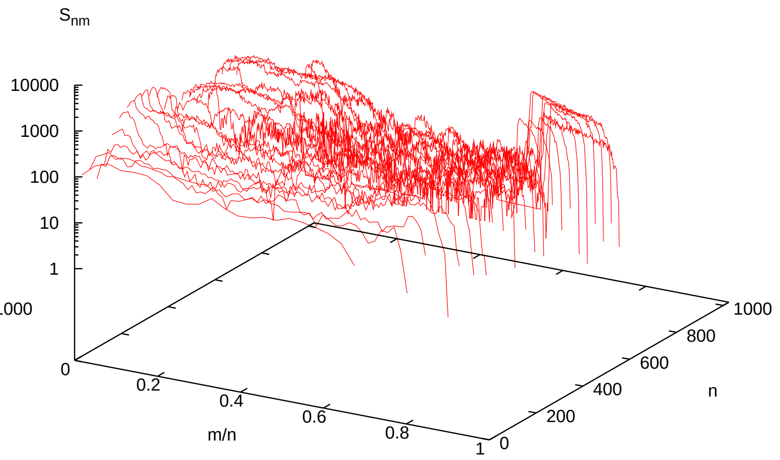


Simulation: Equilibration for 2d ISAW

2d ISAW simulation up to $n = 1024$

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

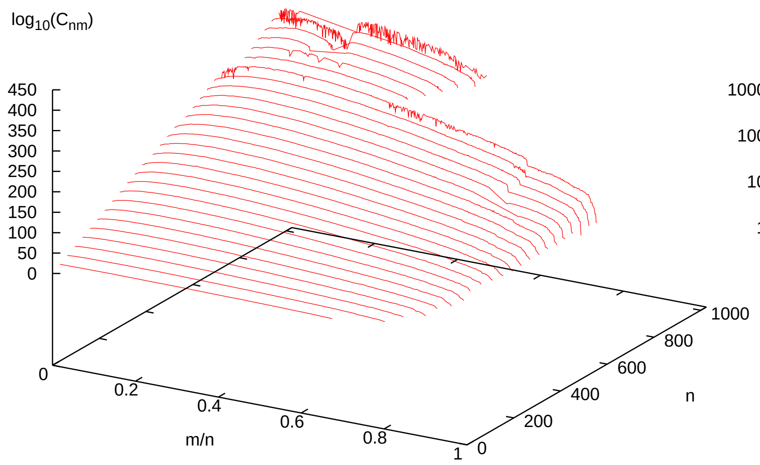


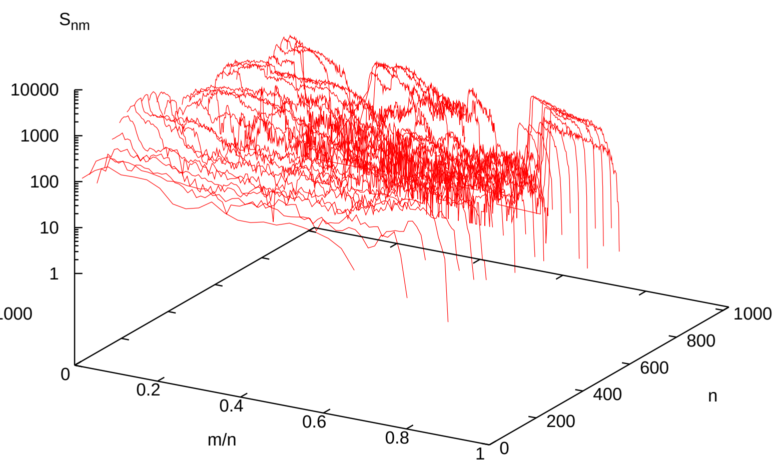


Simulation: Equilibration for 2d ISAW

2d ISAW simulation up to $n = 1024$

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

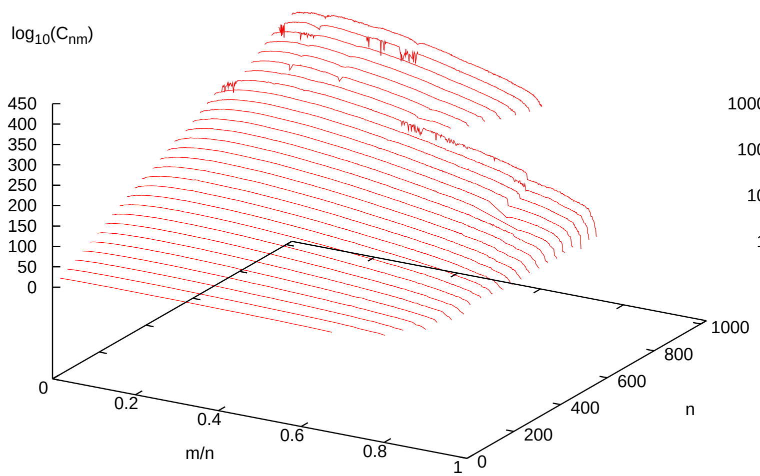


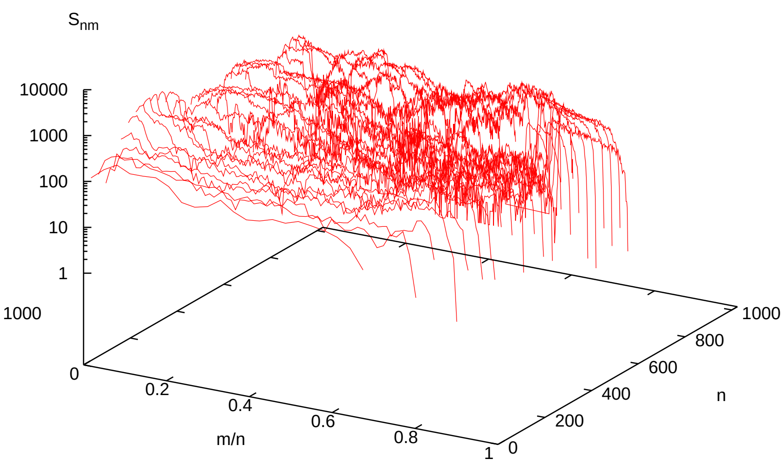


Simulation: Equilibration for 2d ISAW

2d ISAW simulation up to $n = 1024$

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

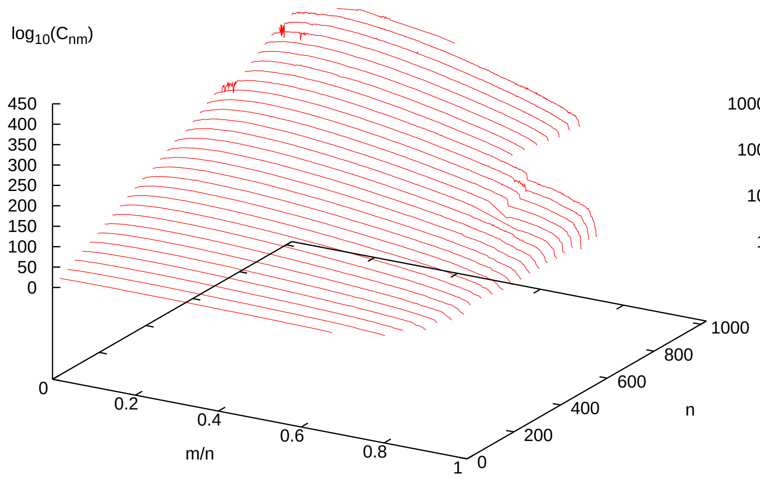


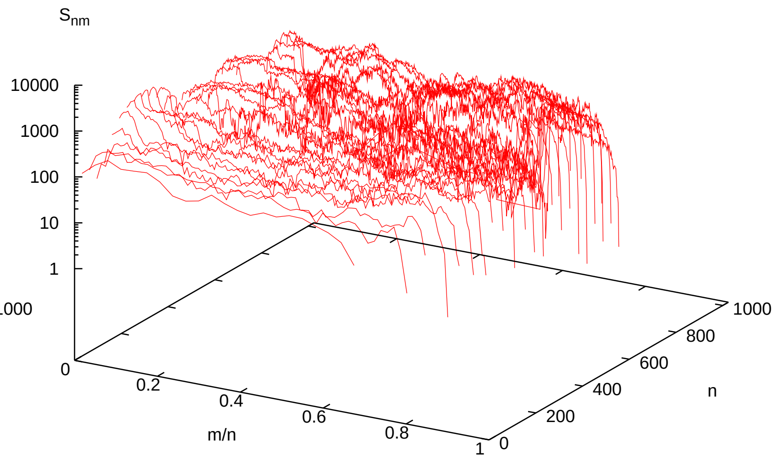


Simulation: Equilibration for 2d ISAW

2d ISAW simulation up to $n = 1024$

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

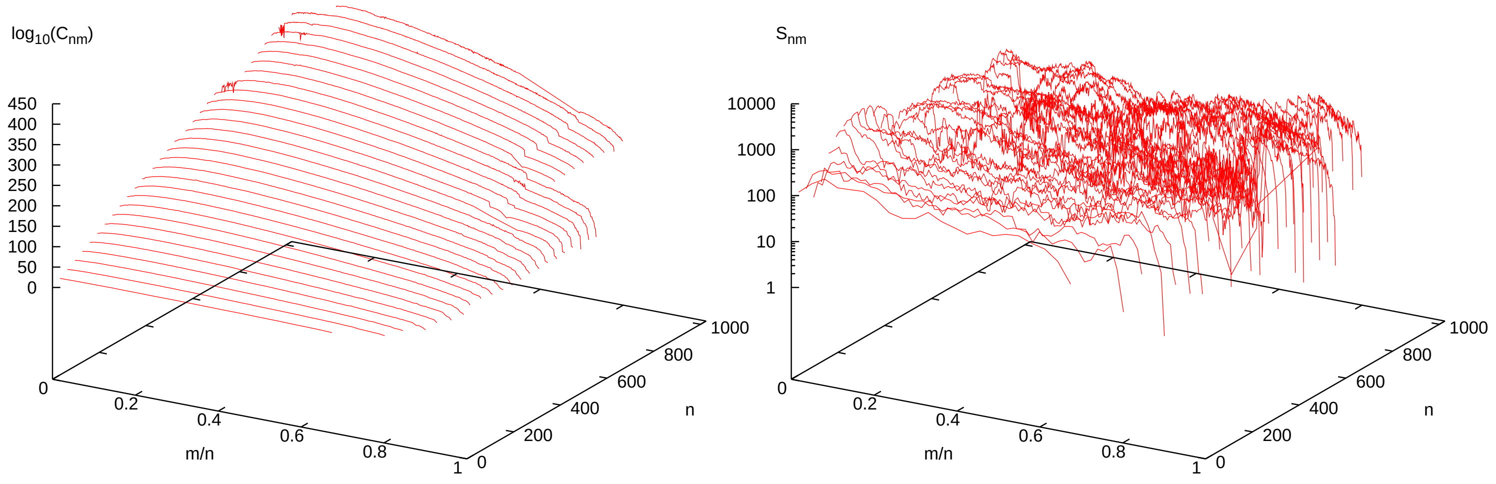




Simulation: Equilibration for 2d ISAW

2d ISAW simulation up to $n = 1024$

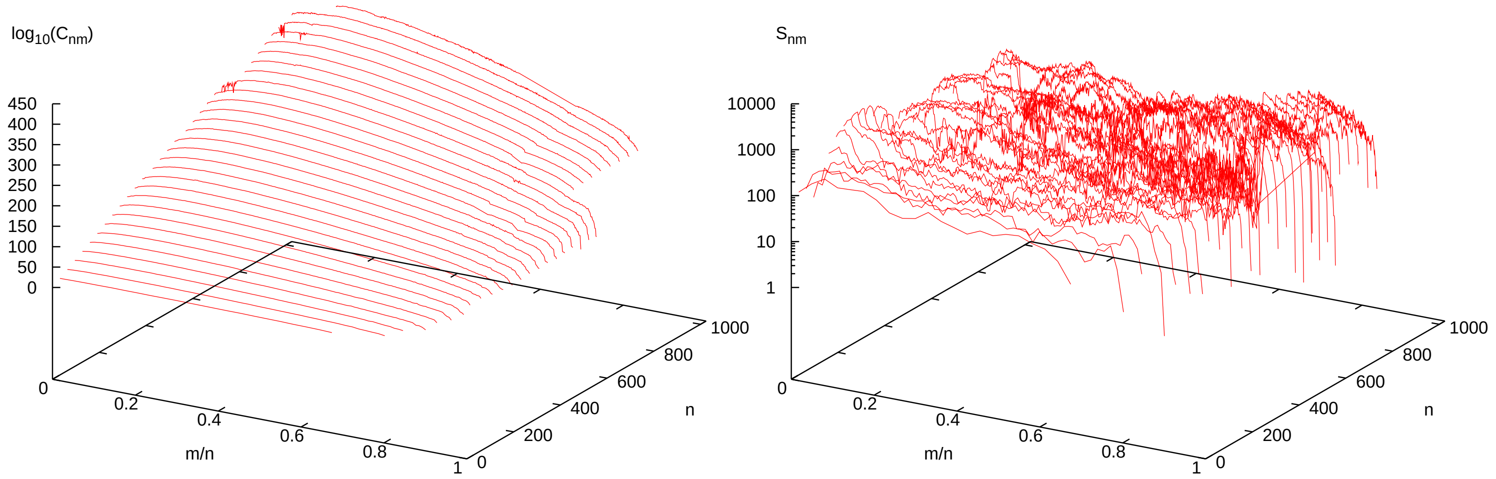
- Total sample size: $100,000,000$



Simulation: Equilibration for 2d ISAW

2d ISAW simulation up to $n = 1024$

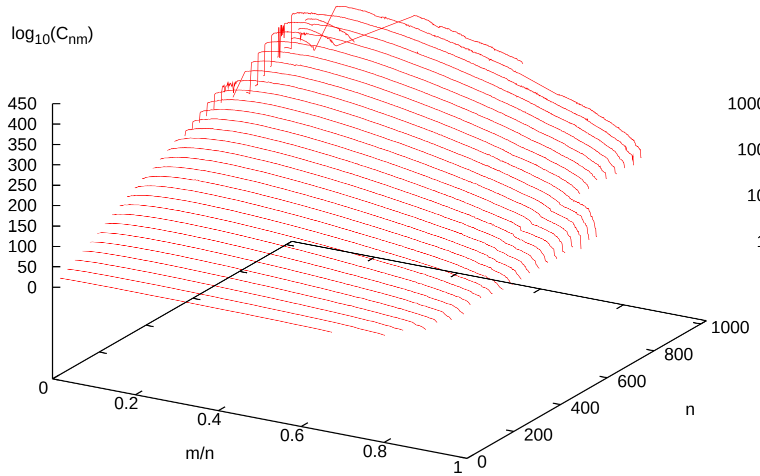
- Total sample size: $110,000,000$

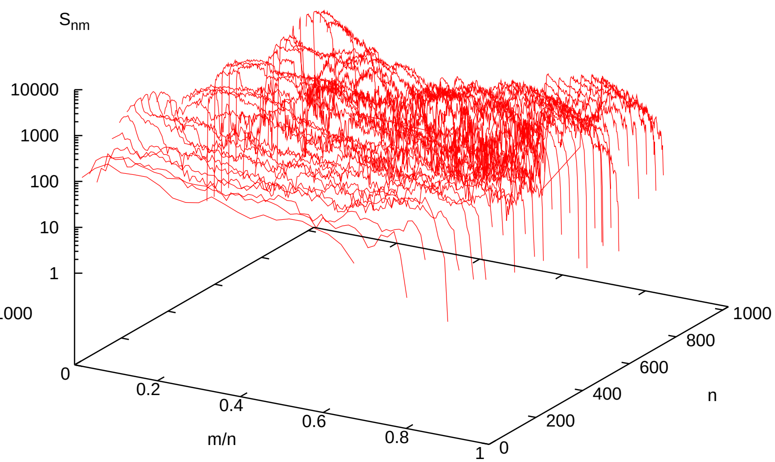


Simulation: Equilibration for 2d ISAW

2d ISAW simulation up to $n = 1024$

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

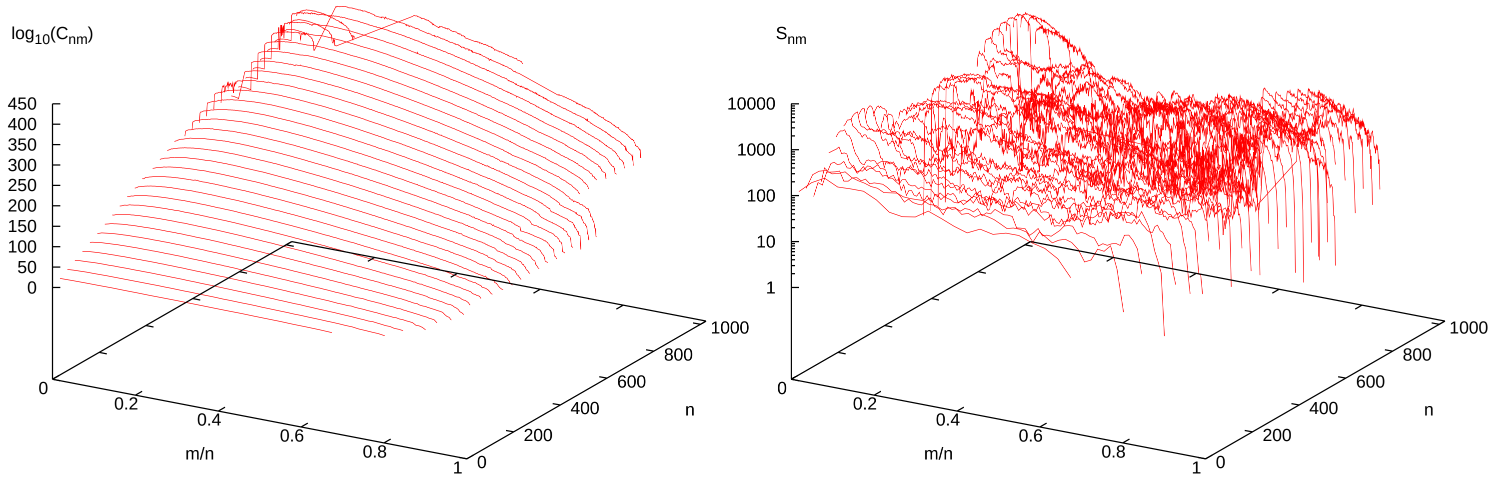




Simulation: Equilibration for 2d ISAW

2d ISAW simulation up to $n = 1024$

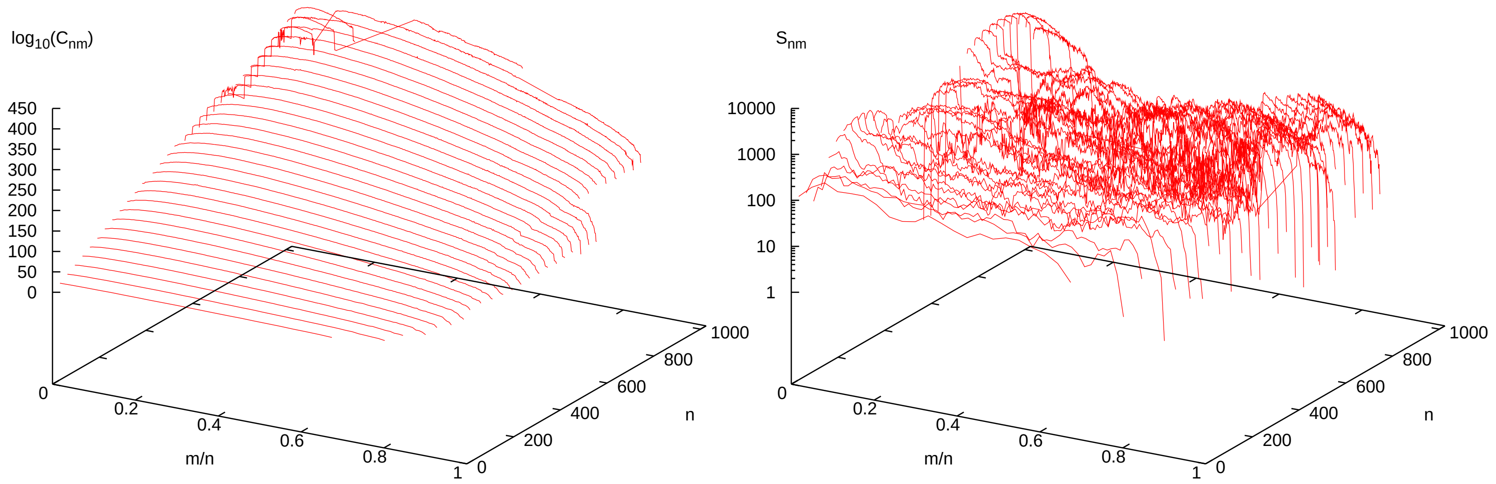
- Total sample size: $130,000,000$



Simulation: Equilibration for 2d ISAW

2d ISAW simulation up to $n = 1024$

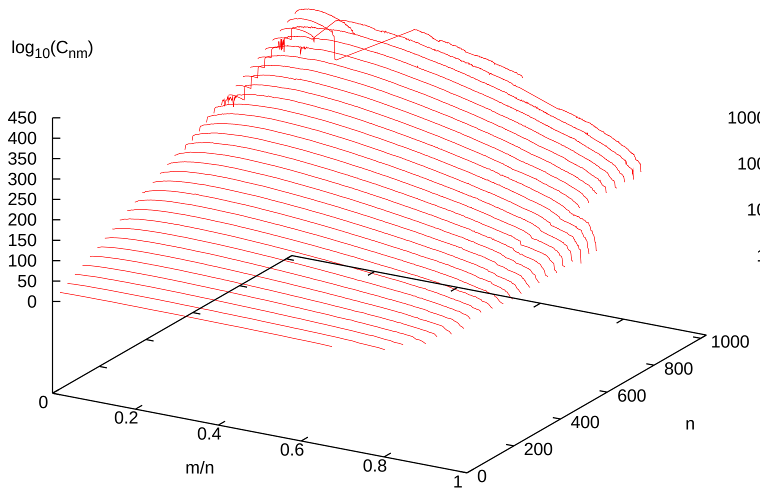
- Total sample size: $140, 000, 000$

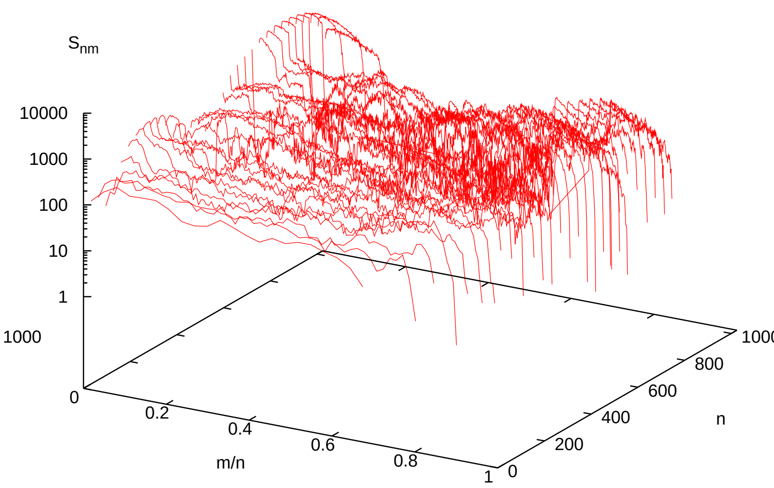


Simulation: Equilibration for 2d ISAW

2d ISAW simulation up to $n = 1024$

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

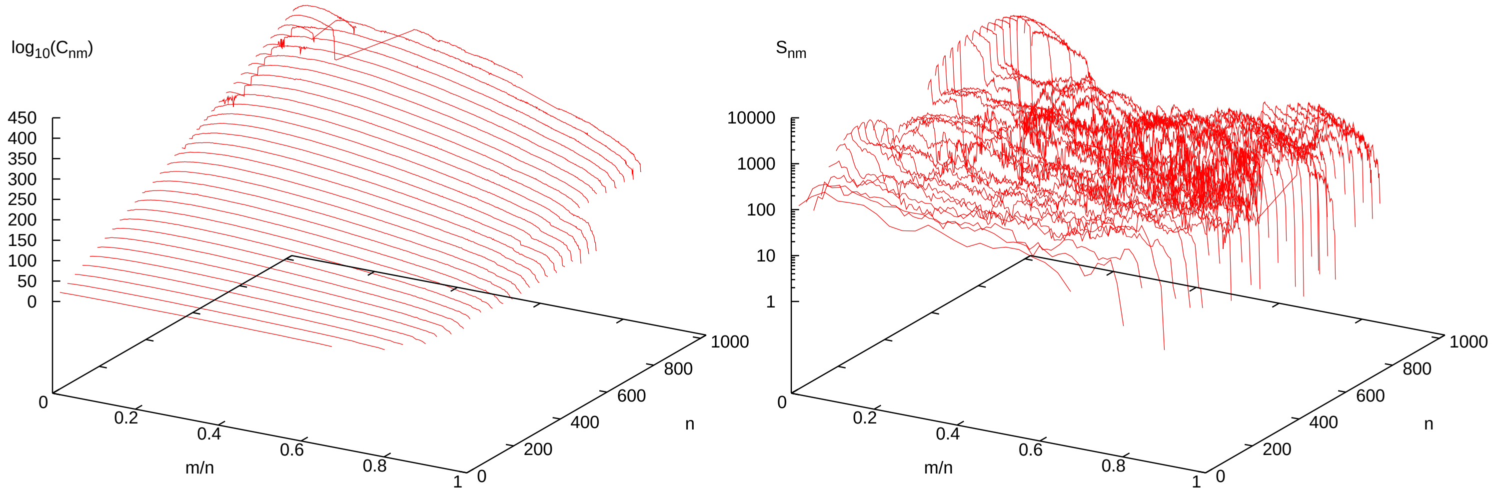




Simulation: Equilibration for 2d ISAW

2d ISAW simulation up to $n = 1024$

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



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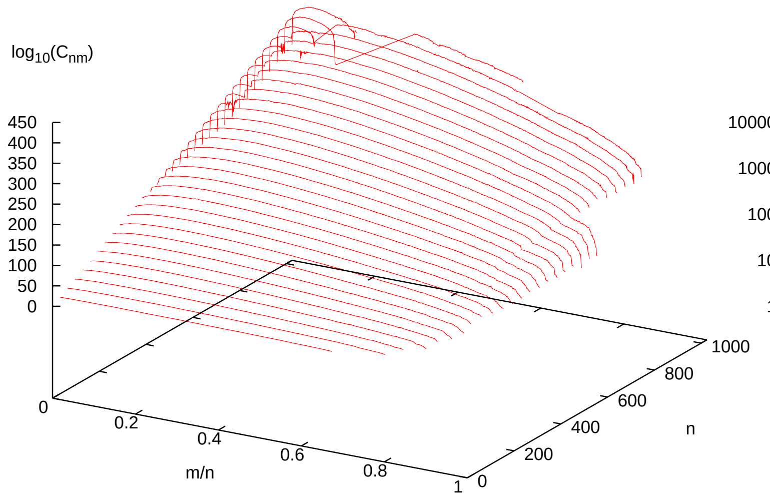
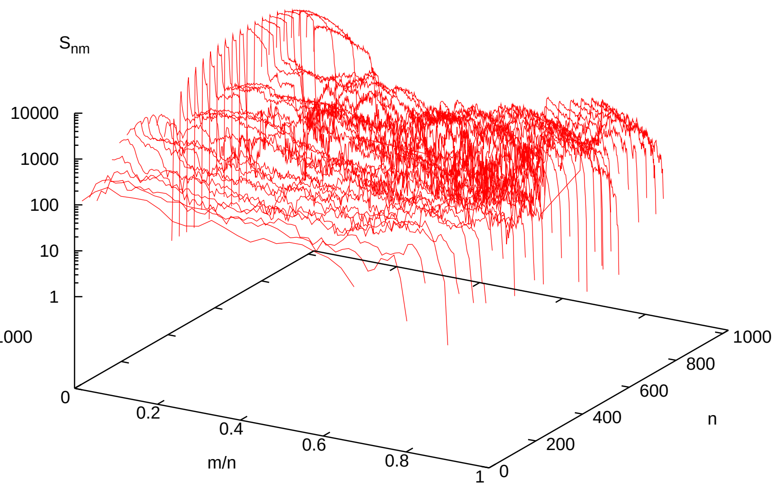
2d ISAW simulation up to $n = 1024$

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

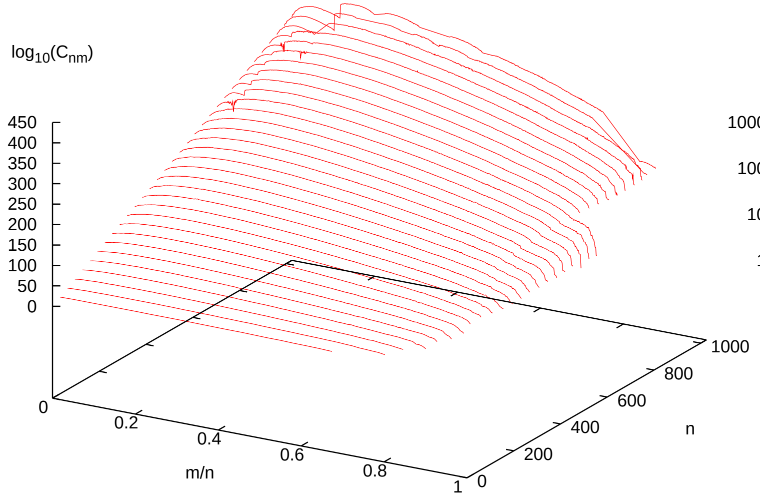


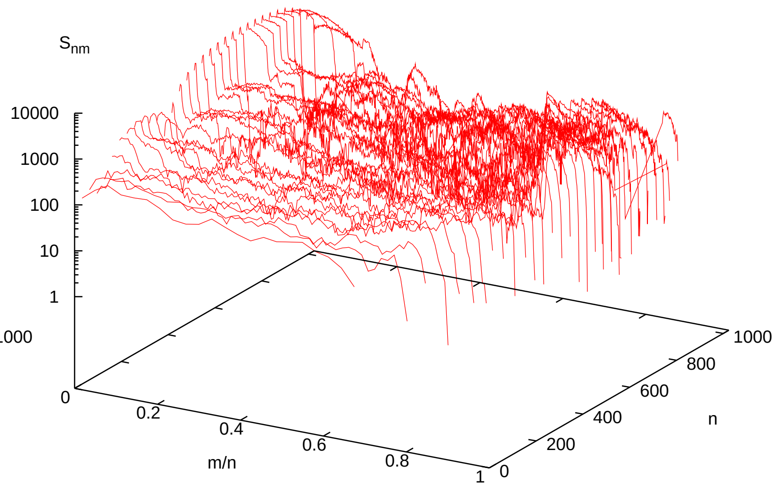


Simulation: Equilibration for 2d ISAW

2d ISAW simulation up to $n = 1024$

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

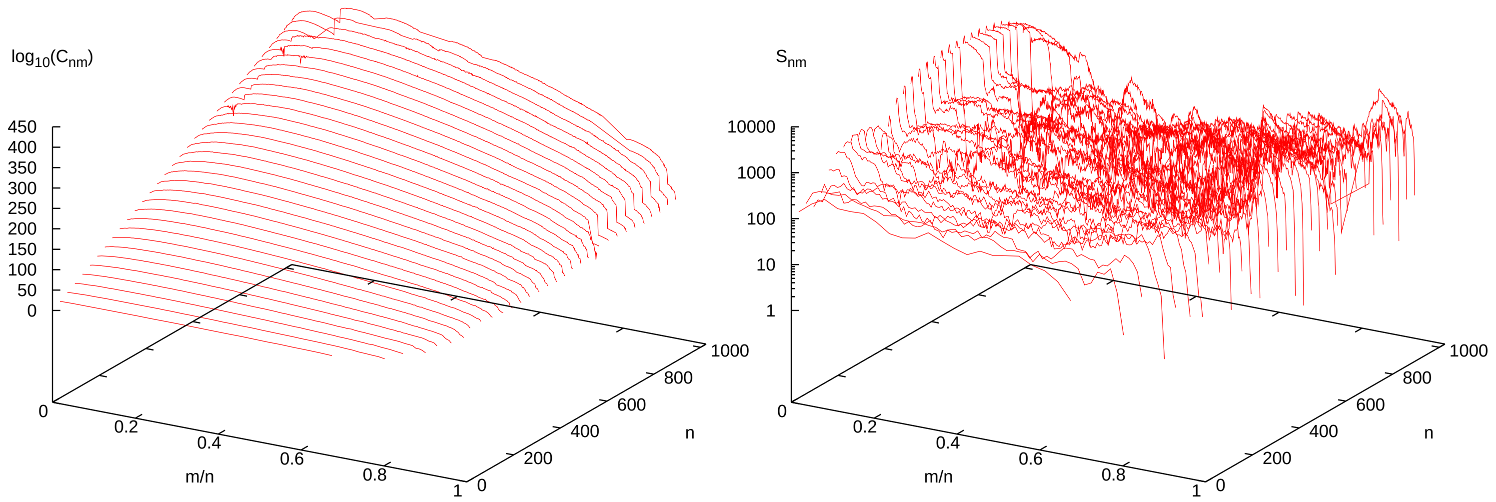




Simulation: Equilibration for 2d ISAW

2d ISAW simulation up to $n = 1024$

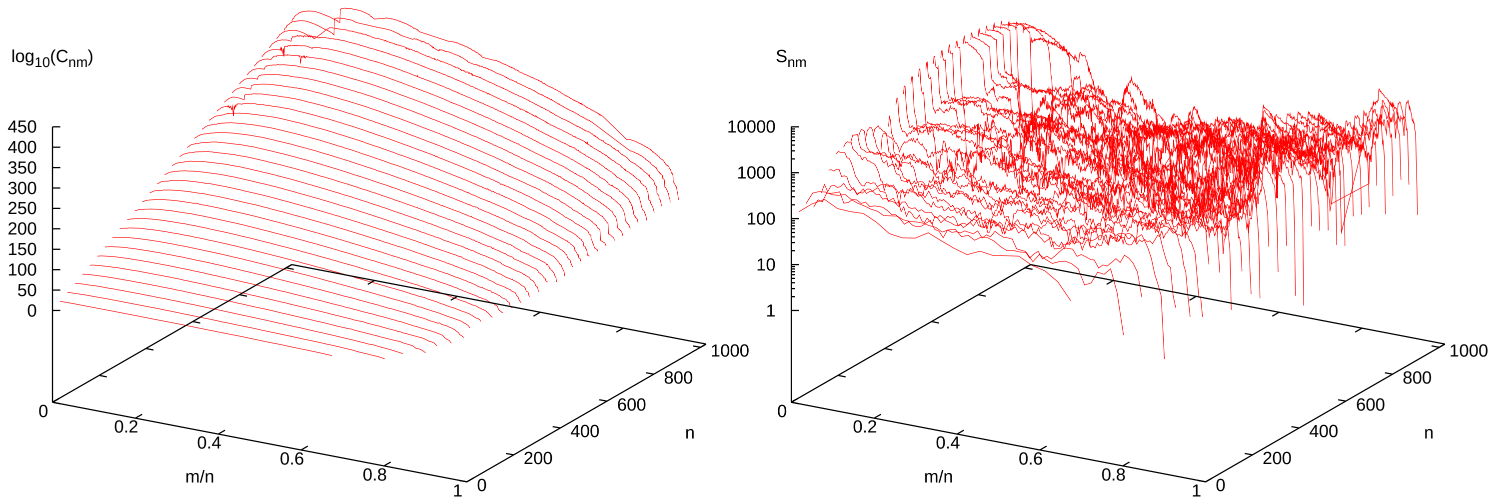
- Total sample size: $190,000,000$



Simulation: Equilibration for 2d ISAW

2d ISAW simulation up to $n = 1024$

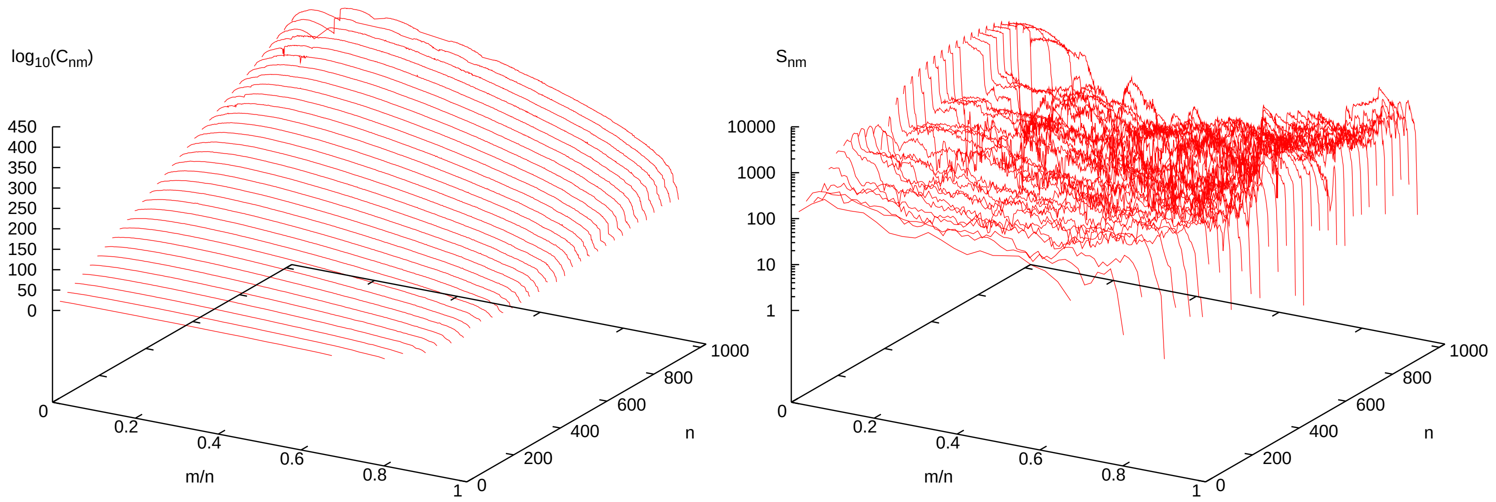
- Total sample size: $200,000,000$



Simulation: Equilibration for 2d ISAW

2d ISAW simulation up to $n = 1024$

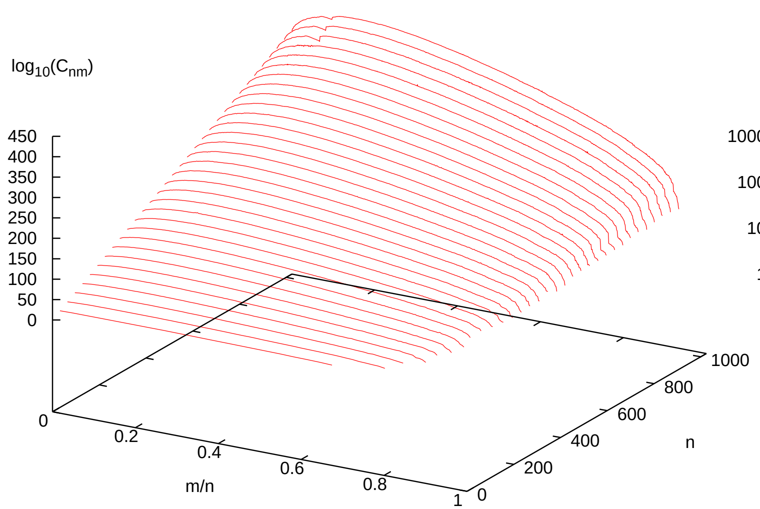
- Total sample size: $210,000,000$

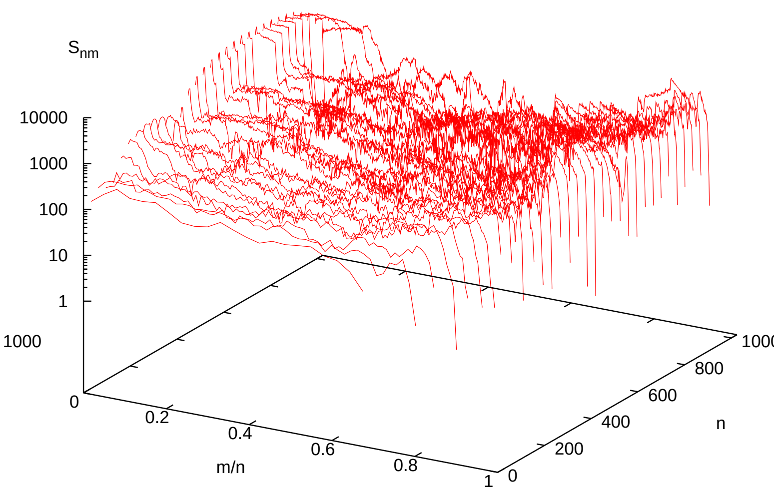


Simulation: Equilibration for 2d ISAW

2d ISAW simulation up to $n = 1024$

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

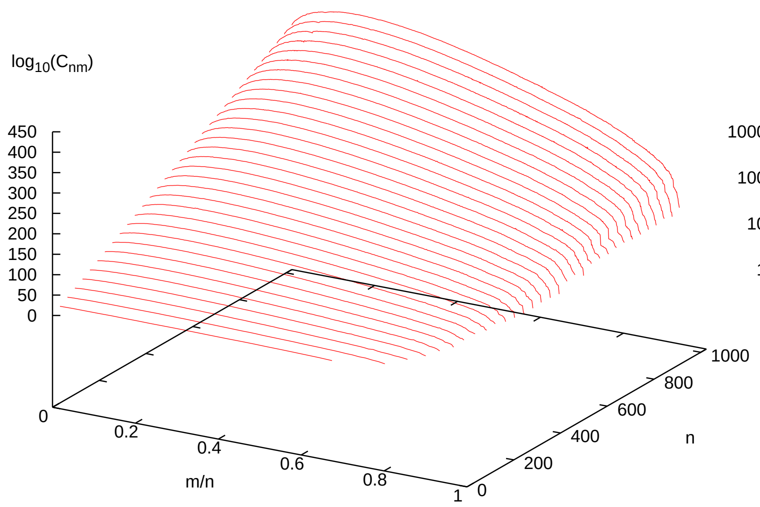


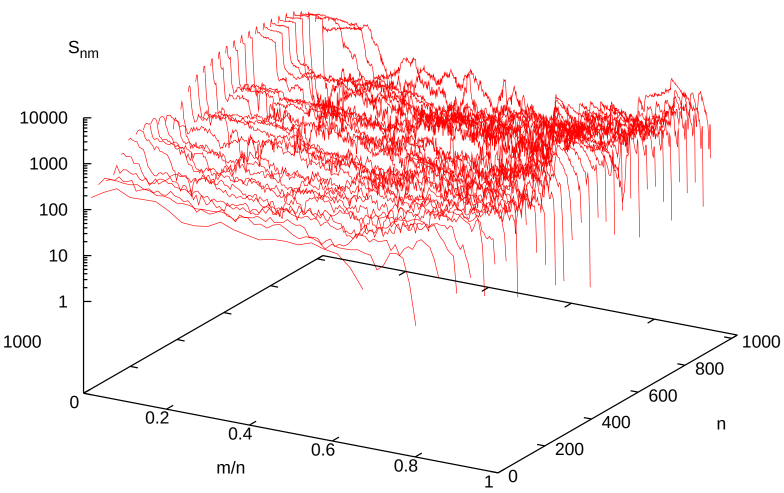


Simulation: Equilibration for 2d ISAW

2d ISAW simulation up to $n = 1024$

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

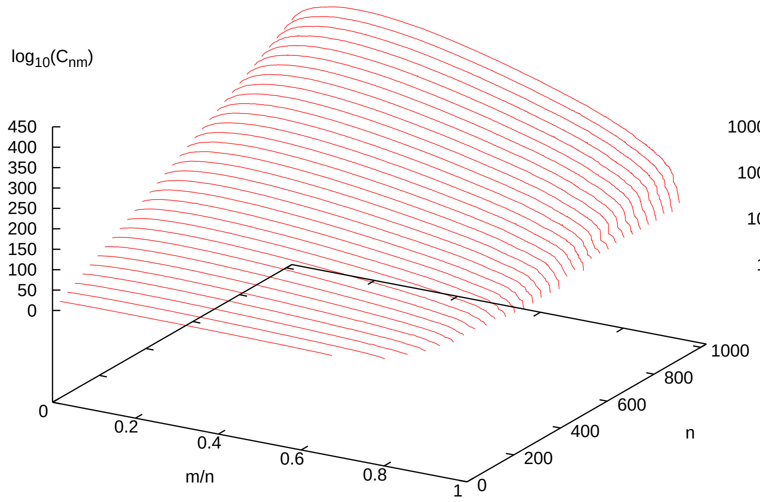


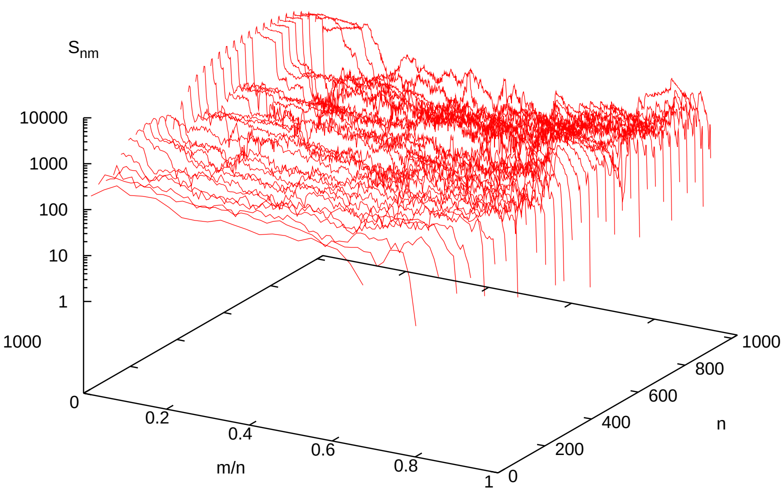


Simulation: Equilibration for 2d ISAW

2d ISAW simulation up to $n = 1024$

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

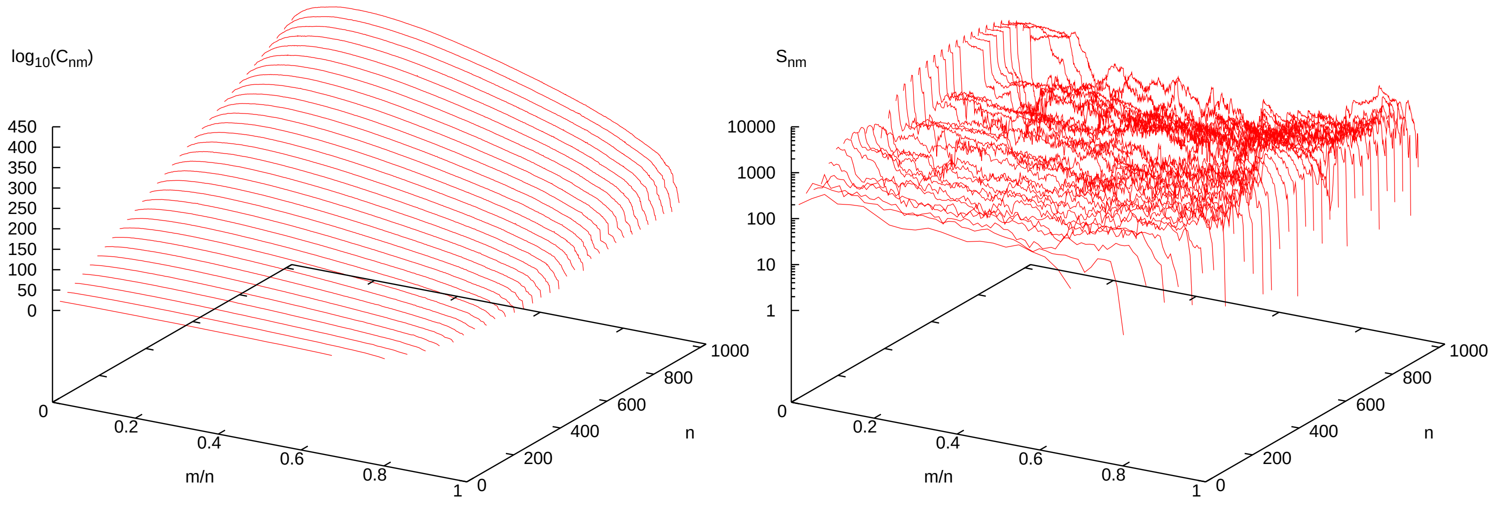




Simulation: Equilibration for 2d ISAW

2d ISAW simulation up to $n = 1024$

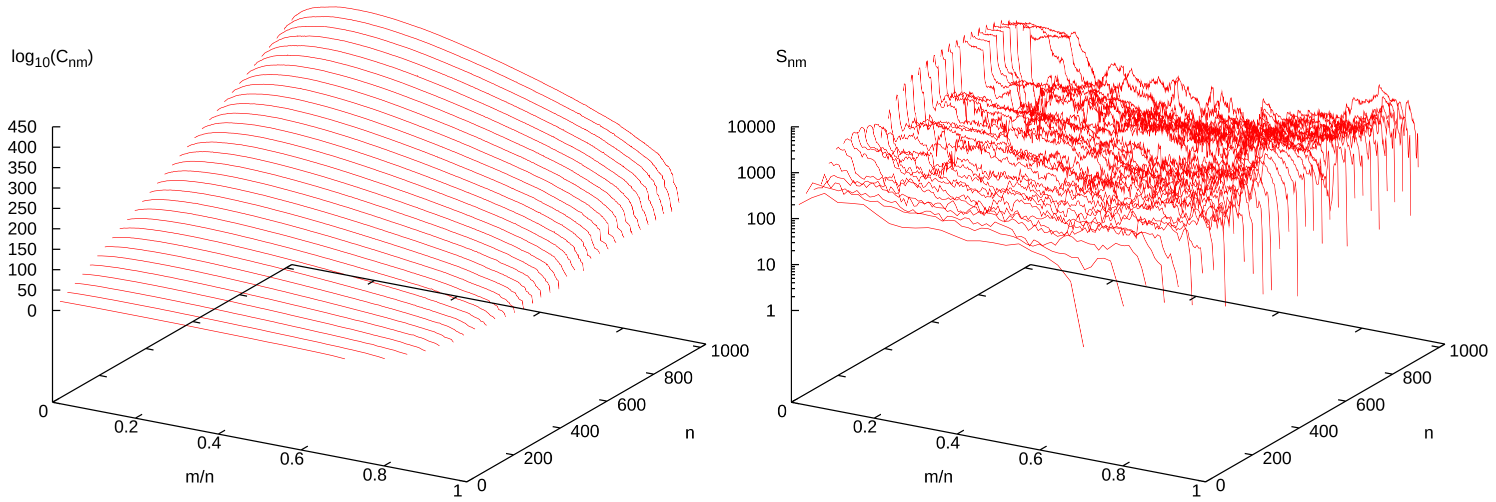
- Total sample size: $250,000,000$



Simulation: Equilibration for 2d ISAW

2d ISAW simulation up to $n = 1024$

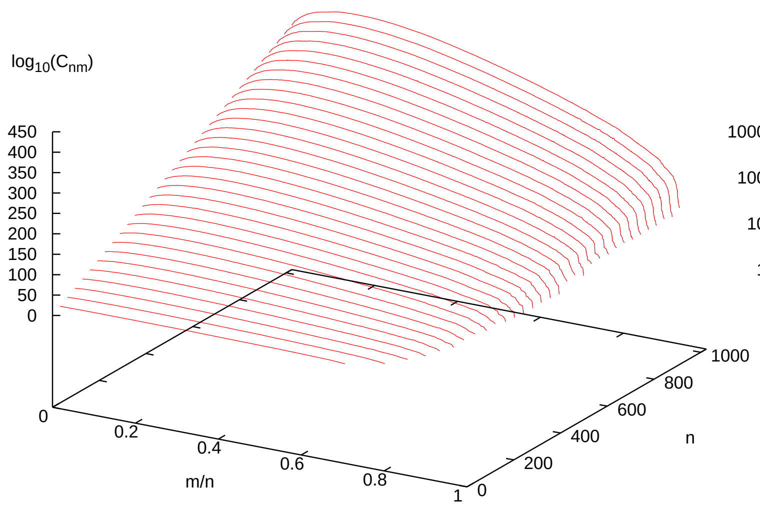
- Total sample size: $260,000,000$

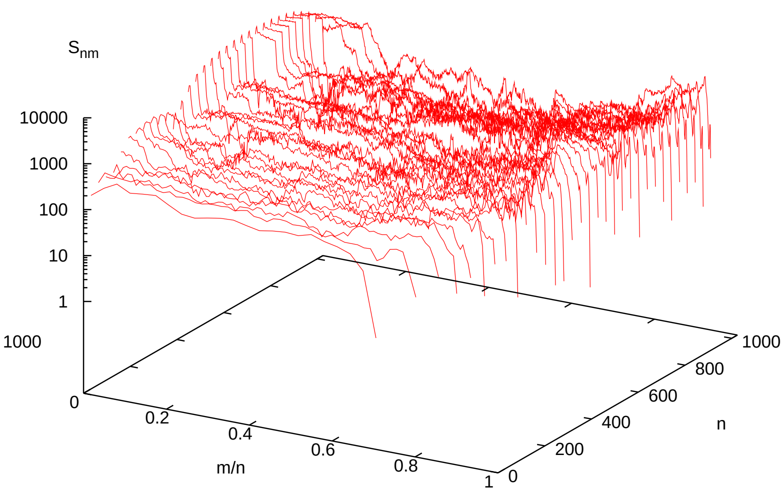


Simulation: Equilibration for 2d ISAW

2d ISAW simulation up to $n = 1024$

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

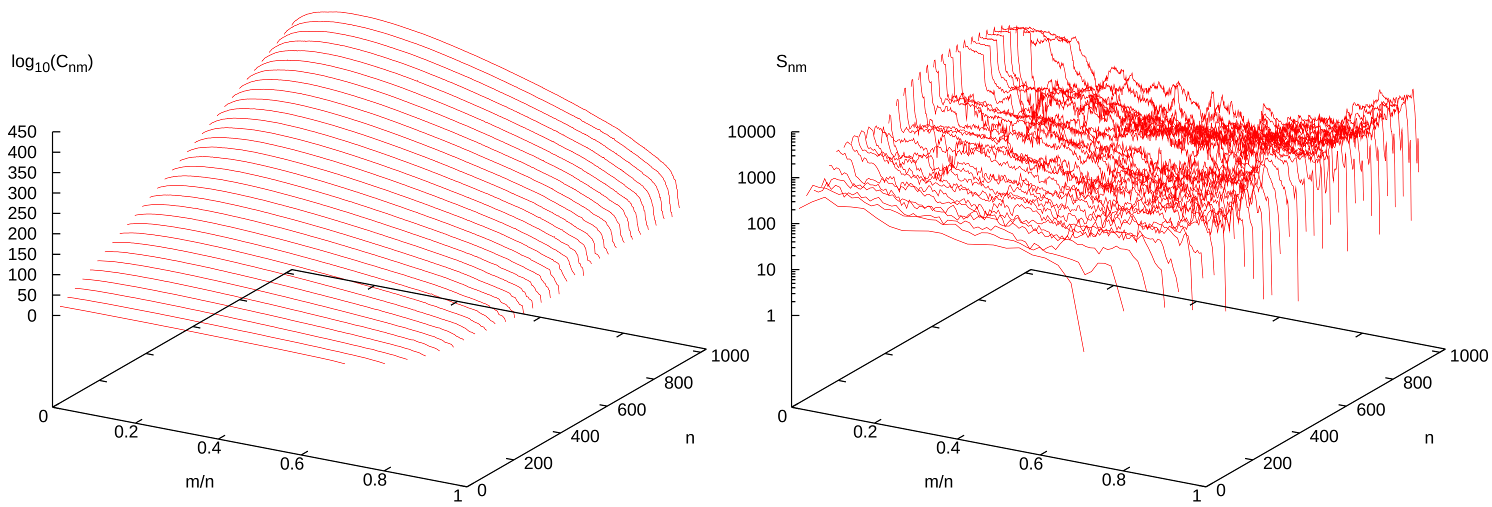




Simulation: Equilibration for 2d ISAW

2d ISAW simulation up to $n = 1024$

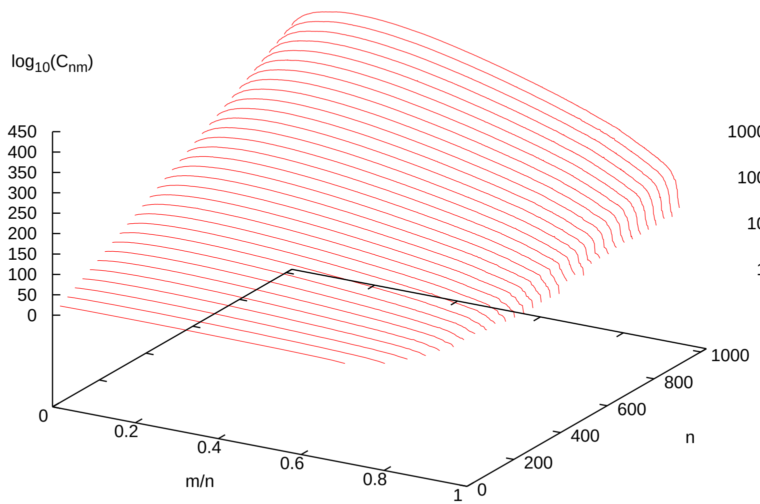
- Total sample size: $280,000,000$

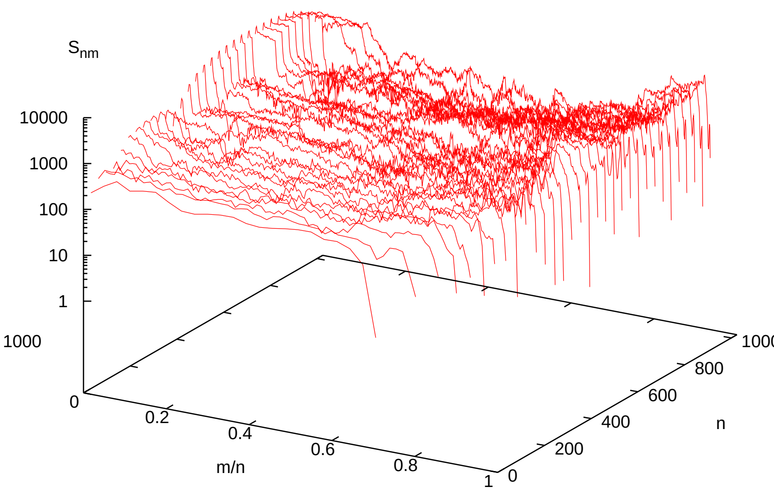


Simulation: Equilibration for 2d ISAW

2d ISAW simulation up to $n = 1024$

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

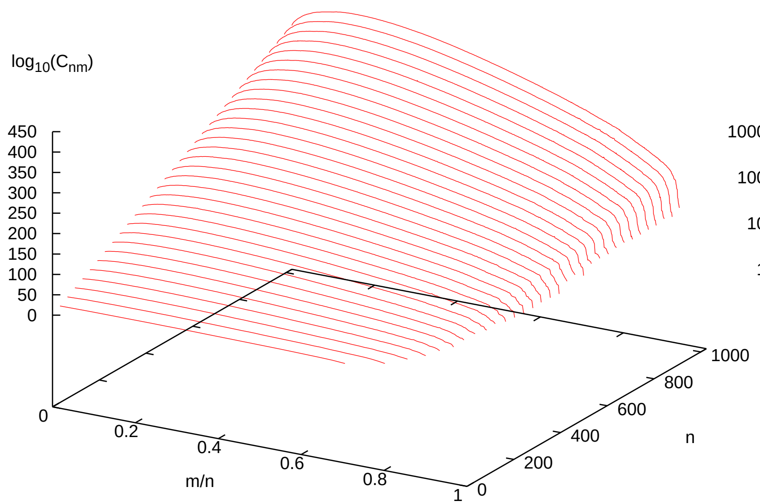


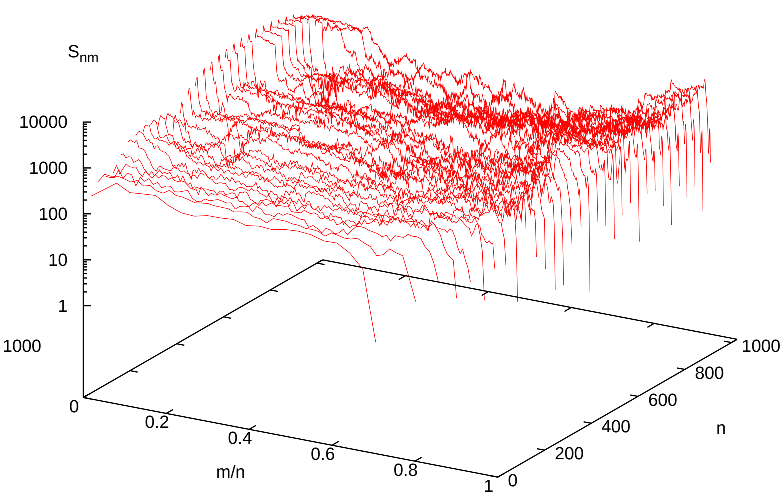


Simulation: Equilibration for 2d ISAW

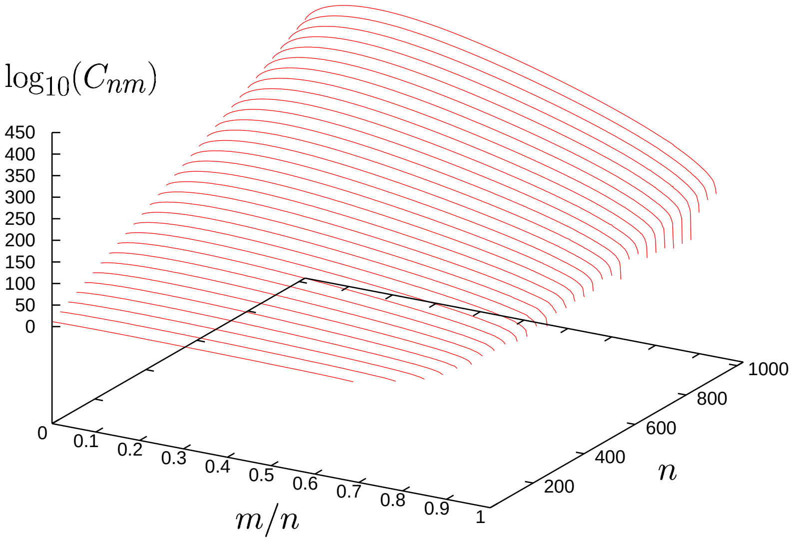
2d ISAW simulation up to $n = 1024$

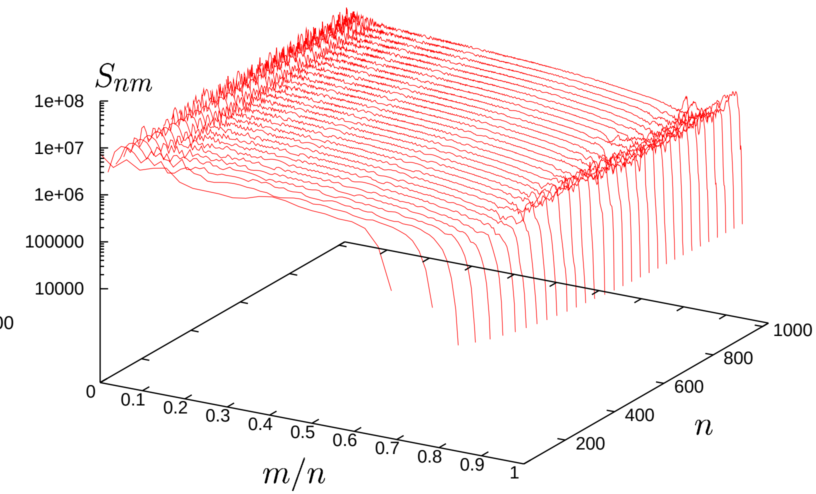
- Total sample size: $300,000,000$



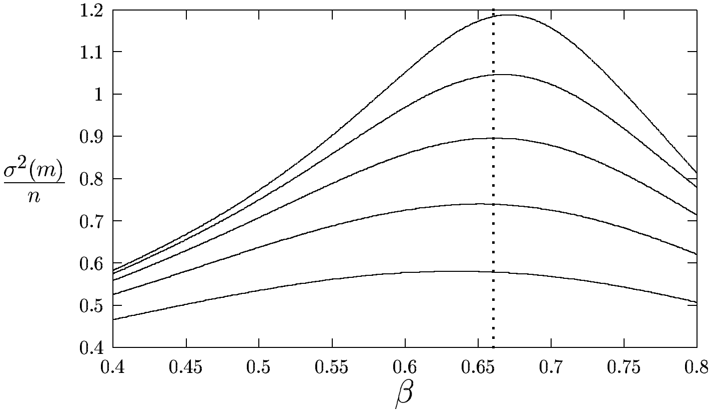


Simulation results: 2d ISAW

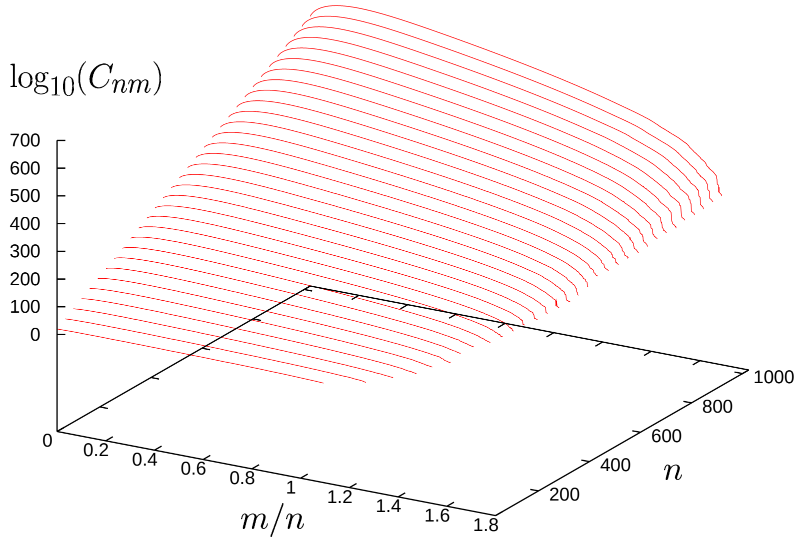


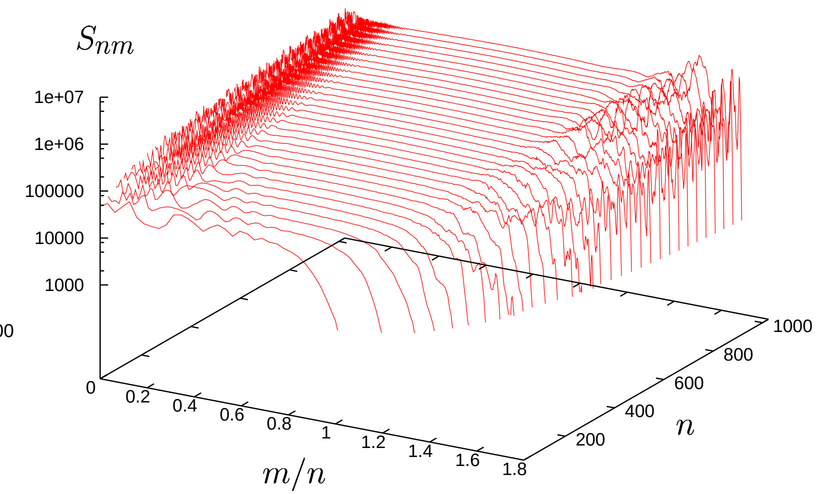


- 2d ISAW up to $n = 1024$
- One simulation suffices
- 300 orders of magnitude

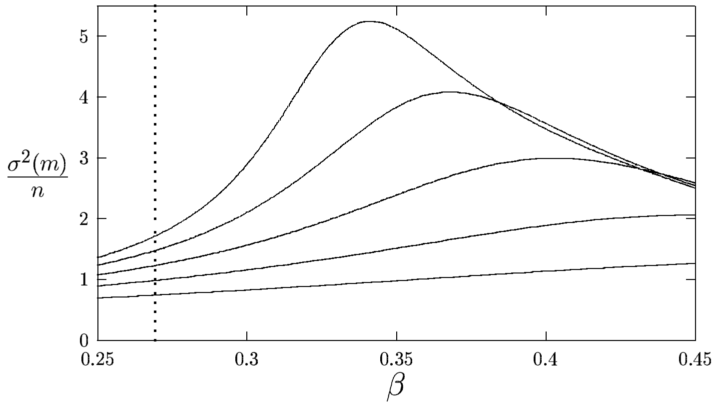


Simulation results: 3d ISAW





- 3d ISAW up to $n = 1024$
- One simulation suffices
- 400 orders of magnitude



Summary

Conclusion: A Promising New Algorithm

- Reviewed Stochastic Growth Algorithms for Polymers
- Presented “flat histogram” version of PERM
  - *One* simulation for complete density of states!
    (the range can also be selectively restricted)
- Applications: HP model, ISAW

Conclusion: A Promising New Algorithm

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  - *One* simulation for complete density of states!
    (the range can also be selectively restricted)
- Applications: HP model, ISAW

Outlook: applications to further models, e.g.

- Square lattice trees / branched polymers: with A. Rechnitzer
  - Connective constant estimate $5.1435(5)$
    (compare to $5.1434(7)$ with Pivot algorithm)
- Two-dimensional density of states with *one* simulation
  - Absorbing collapsing polymers: with A. Owczarek
  - Extended Domb-Joyce model: with J. Krawczyk

The End