Simulating models of polymer collapse

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SCS Seminar, Florida State University
April 27, 2006

Outline

- Polymers in solution:
  - Equilibrium statistical mechanics, lattice models, exponents
- Algorithm:
  - Stochastic growth & flat histogram (PERM/flatPERM)
- Simulations and results:
  - Canonical model: interacting self-avoiding walks (ISAW)
  - Site-weighted random walks (SWRW): a tale of surprises

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- Polymers in solution:
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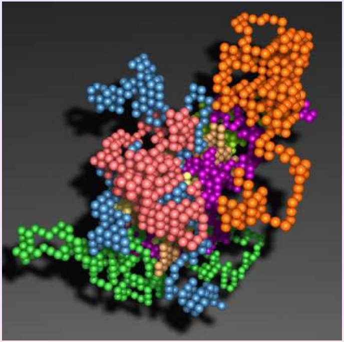
  - Stochastic growth & flat histogram (PERM/flatPERM)
- Simulations and results:
  - Canonical model: interacting self-avoiding walks (ISAW)
  - Site-weighted random walks (SWRW): a tale of surprises
- Other applications:
  - Bulk vs surface phenomena:
    - confined polymers, force-induced desorption, interplay of collapse and adsorption
  - Polymer collapse in high dimension:
    - pseudo-first-order transition (talk at FSU in 2003)

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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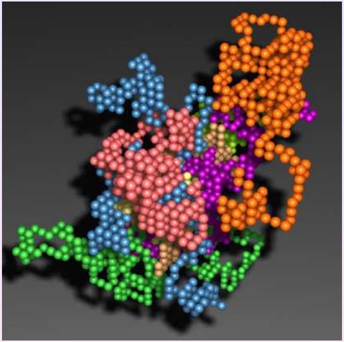
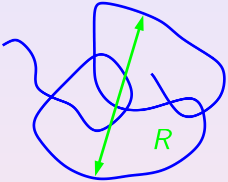


A Model of a Polymer in Solution

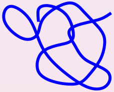
Random Walk + Excluded Volume + Short Range Attraction

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)

Critical Exponents

Length scale exponent ν: $R_N \sim N^{\nu}$

d	Coil	Θ	Globule
2	$3/4$	$4/7$	$1/2$
3	$0.587\ldots$	$1/2(\log)$	$1/3$
4	$1/2(\log)$	$1/2$	$1/4$

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Entropic exponent γ*:* $Z_N \sim \mu^N N^{\gamma-1}$

d	Coil	Θ	Globule
2	$43/32$	$8/7$	different scaling form
3	$1.15\ldots$	$1(\log)$	$Z_N \sim \mu^N {\mu_s}^{N^{\sigma}} N^{\gamma-1}$
4	$1(\log)$	1	$\sigma = (d-1)/d$ (surface)

Crossover Scaling at the Θ-Point

Crossover exponent ϕ

$$R_N \sim N^{\nu} \mathcal{R}(N^{\phi} \Delta T) \qquad Z_N \sim \mu^N N^{\gamma-1} \mathcal{Z}(N^{\phi} \Delta T)$$

Specific heat of Z_N at $T = T_c$: $C_N \sim N^{\alpha\phi}$

$$2 - \alpha = 1/\phi \qquad \text{tri-critical scaling relation}$$

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Poor man's mean field theory of the Θ-Point for $d \geq 3$

Balance between "excluded volume" and attractive interaction
$\Rightarrow$ polymer behaves like random walk: $\nu = 1/2$, $\gamma = 1$
$\Rightarrow$ weak thermodynamic phase transition $\alpha = 0$, i.e. $\phi = 1/2$

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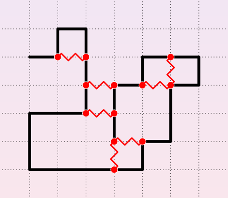
d	2	3	4
ϕ	3/7	1/2(log)	1/2

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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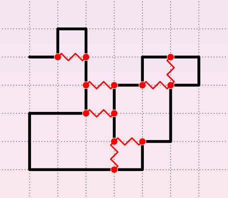
Partition function:

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



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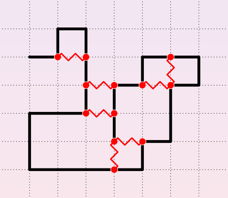

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Thermodynamic Limit for a dilute solution:

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

Theory and Models

- Theoretical results from e.g.
  - $d = 2$: Coulomb gas methods, conformal invariance, SLE, ...
  - $d \geq 3$: self-consistent mean field theory
  - field theory: $\phi^4 - \phi^6$ $O(n)$-model for $n \to 0$

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A Model of a Polymer in Solution

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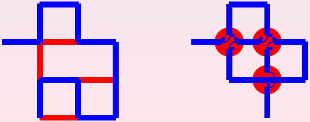
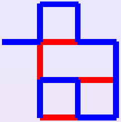
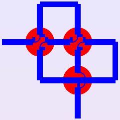
- Canonical model: interacting self-avoiding walks (ISAW)
- Alternative model: interacting self-avoiding trails (ISAT)

vertex avoidance (walks) ⇔ edge avoidance (trails)



nearest-neighbour interaction ⇔ contact interaction

ISAW versus ISAT

ISAW   ISAT

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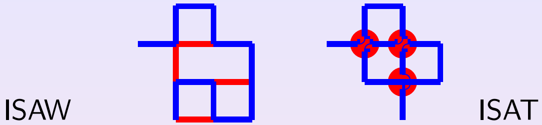

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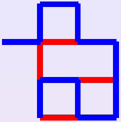
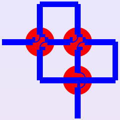
ISAW   ISAT

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Length scale exponent ν for $\mathbb{Z}^2$:

Model	Coil	Θ	Globule
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Crossover exponent ϕ for $\mathbb{Z}^2$:

Model	
ISAW	$3/7$
ISAT	$0.84(3)$

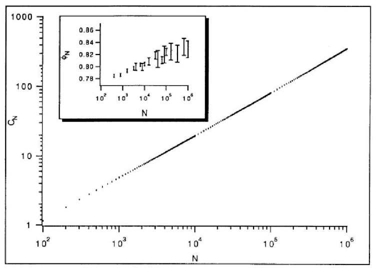
Simulations of ISAT

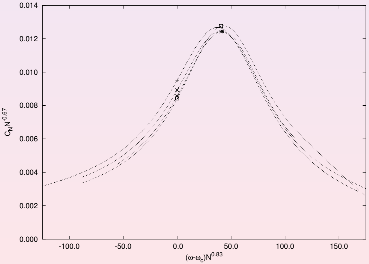
- At critical T_c, ISAT can be modelled as kinetic growth; simulations up to $N = 10^6$

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, submitted to Physica A





ISAW versus ISAT

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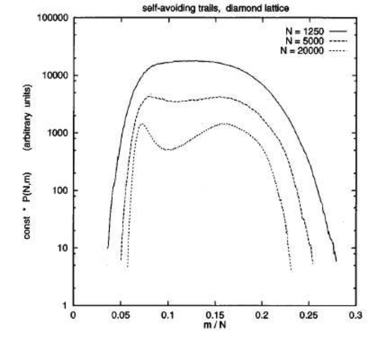

T Prellberg and AL Owczarek, Phys. Rev. E 51 (1995) 2142-214

(figure from) P Grassberger and R Hegger, J. Phys. A 29 (1996) 279-288

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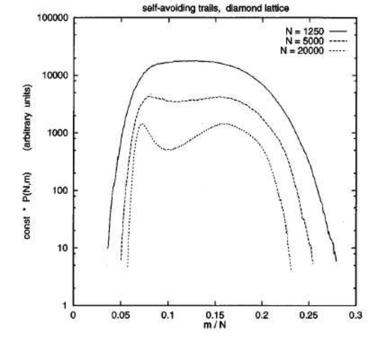

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10 years later, this is still not understood!

A Proposal of a New Model

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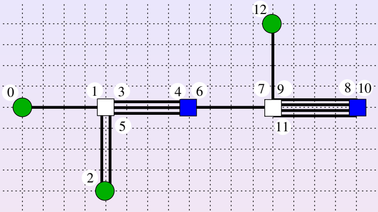
- Incorporate self-avoidance and attraction via choice of $f(t)$. For example, $f(0) = f(1) = 0$,

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

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

Site-Weighted Random Walk (ctd)



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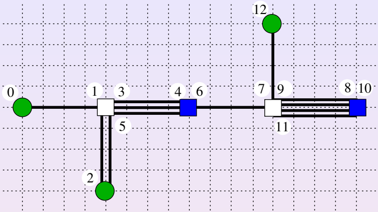
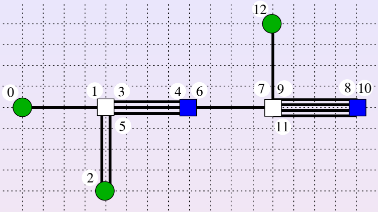


- Partition function

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

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



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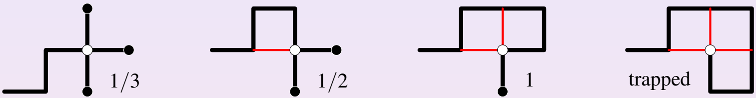
- Simulate two variants of the model on the square and simple cubic lattice
  - random walks with immediate reversal allowed (RA2, RA3)
  - random walks with immediate reversal forbidden (RF2, RF3)

The Algorithm

PERM = Pruned and Enriched Rosenbluth Method

Grassberger, Phys Rev E 56 (1997) 3682

- Rosenbluth Method: kinetic growth



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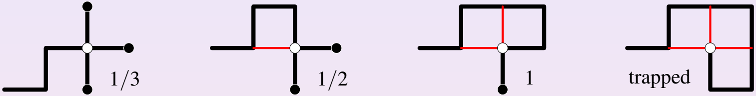

- Enrichment: weight too large → make copies of configuration
- Pruning: weight too small → remove configuration occasionally

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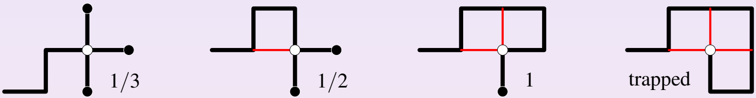

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Current work: flatPERM = flat histogram PERM

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 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 $Z_N(\beta)$
    - $Z_N^{est}(\beta) = \langle W \exp(-\beta E) \rangle_N$
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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 $C_{N,\vec{m}}$
    - $C_{N,\vec{m}}^{est} = \langle W \rangle_{N,\vec{m}}$
    - $r = W_{N,\vec{m}}^{(i)} / C_{N,\vec{m}}^{est}$

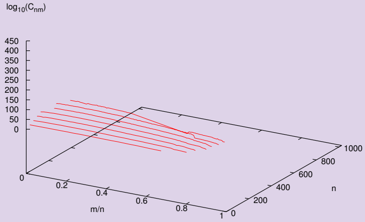
Simulations and Results

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: $1,000,000$



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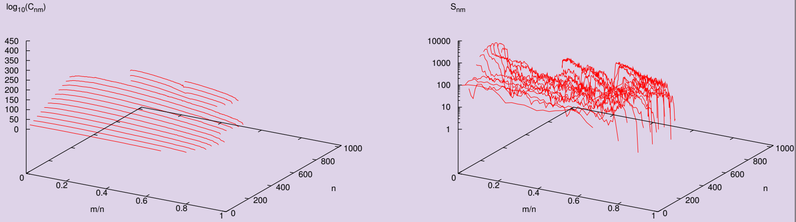
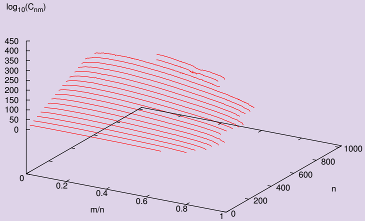
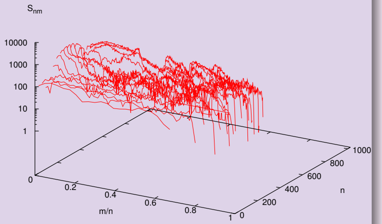


2d ISAW simulation up to $N = 1024$

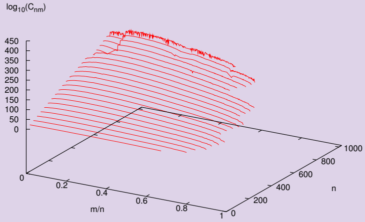
Total sample size: $20,000,000$





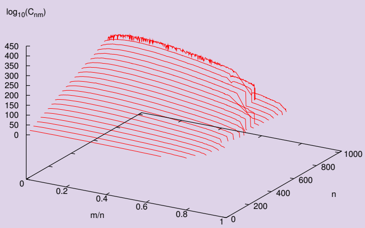
2d ISAW simulation up to $N = 1024$

Total sample size: $30,000,000$



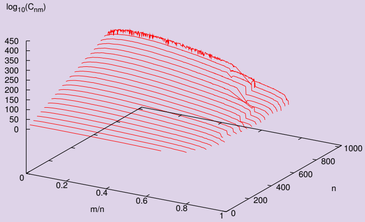
2d ISAW simulation up to $N = 1024$

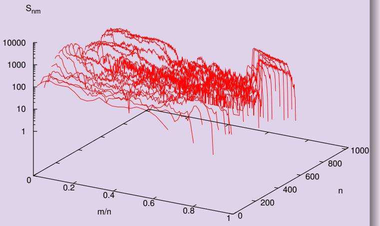
Total sample size: $40,000,000$



2d ISAW simulation up to $N = 1024$

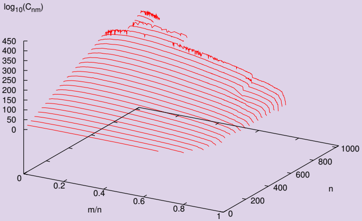
Total sample size: $50,000,000$

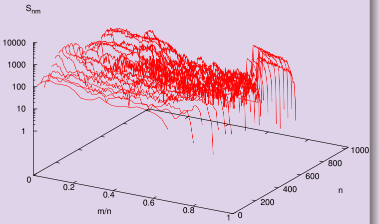




2d ISAW simulation up to $N = 1024$

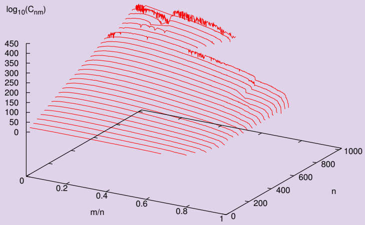
Total sample size: $60,000,000$

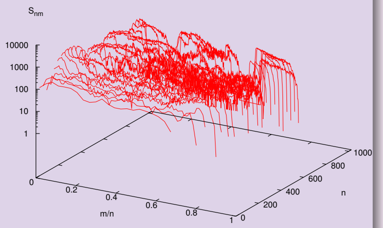




2d ISAW simulation up to $N = 1024$

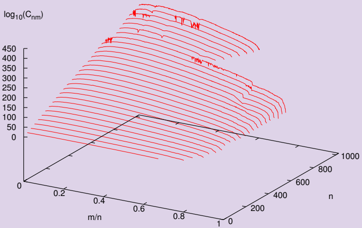
Total sample size: $70,000,000$

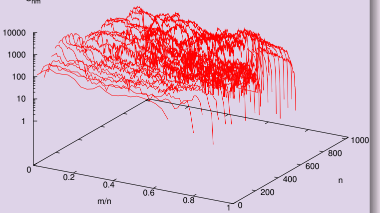




2d ISAW simulation up to $N = 1024$

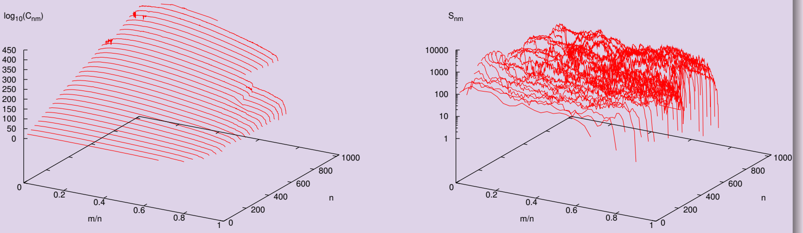
Total sample size: $80,000,000$





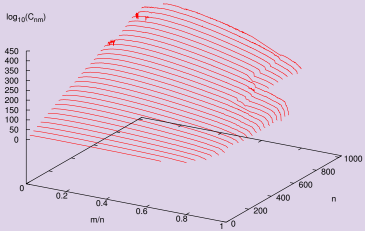
2d ISAW simulation up to $N = 1024$

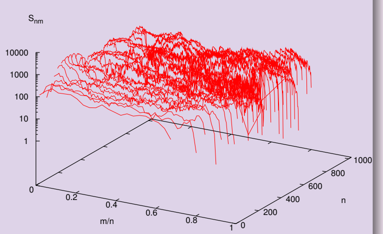
Total sample size: $90,000,000$



2d ISAW simulation up to $N = 1024$

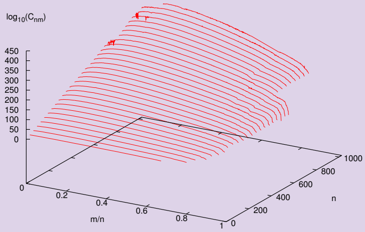
Total sample size: $100,000,000$

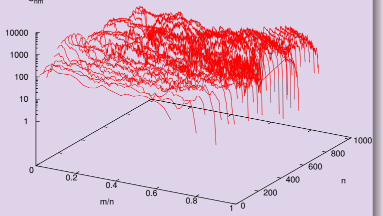




2d ISAW simulation up to $N = 1024$

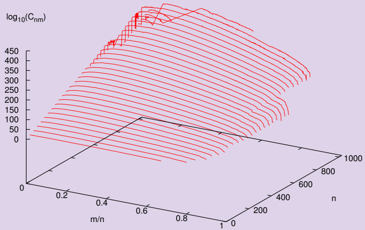
Total sample size: $110,000,000$

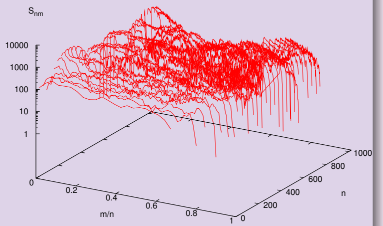




2d ISAW simulation up to $N = 1024$

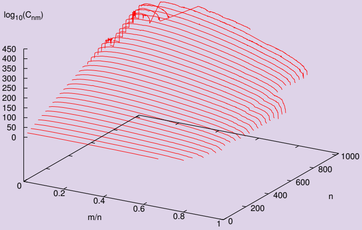
Total sample size: $120,000,000$

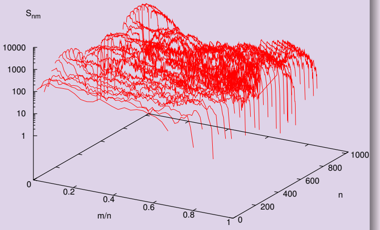




2d ISAW simulation up to $N = 1024$

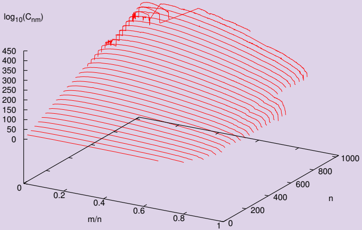
Total sample size: $130,000,000$

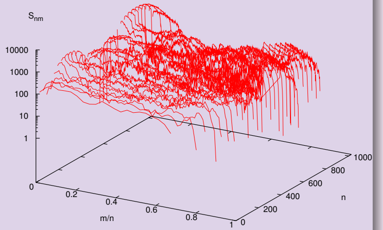




2d ISAW simulation up to $N = 1024$

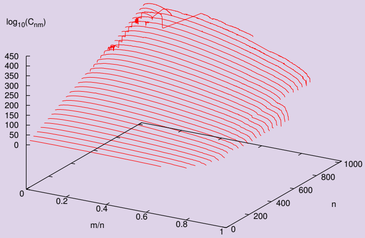
Total sample size: $140,000,000$

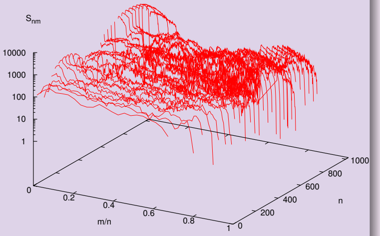




2d ISAW simulation up to $N = 1024$

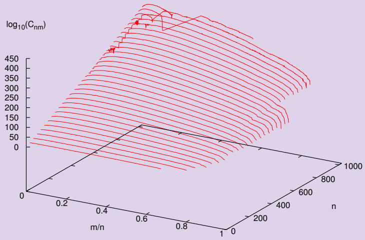
Total sample size: $150,000,000$





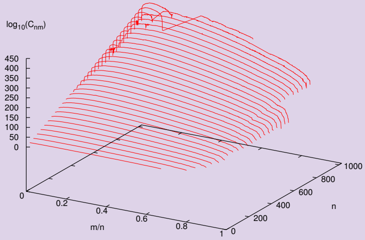
2d ISAW simulation up to $N = 1024$

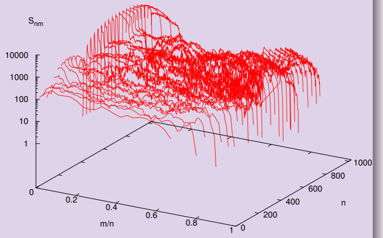
Total sample size: $160,000,000$



2d ISAW simulation up to $N = 1024$

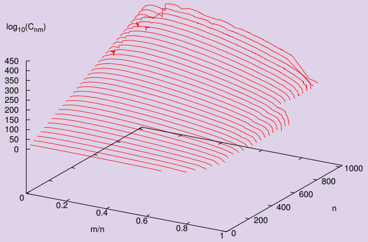
Total sample size: $170,000,000$





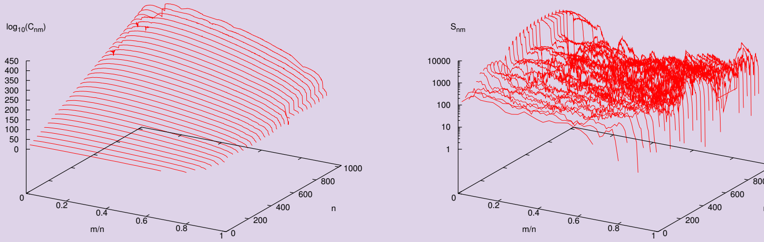
2d ISAW simulation up to $N = 1024$

Total sample size: $180,000,000$



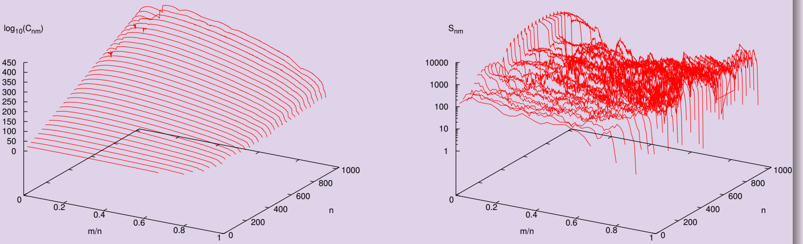
2d ISAW simulation up to $N = 1024$

Total sample size: $190,000,000$



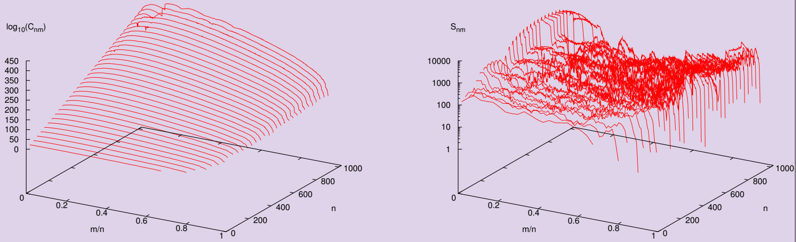
2d ISAW simulation up to $N = 1024$

Total sample size: $200,000,000$



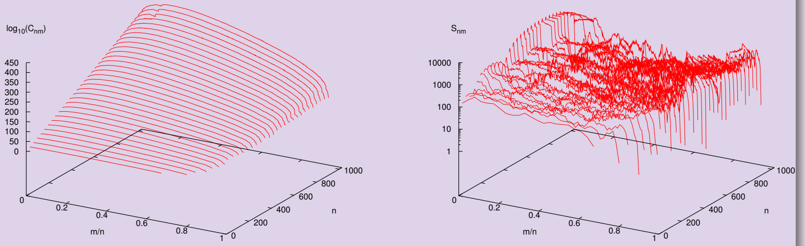
2d ISAW simulation up to $N = 1024$

Total sample size: $210,000,000$



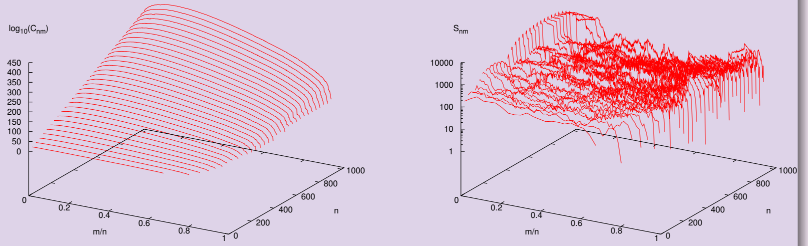
2d ISAW simulation up to $N = 1024$

Total sample size: $220,000,000$



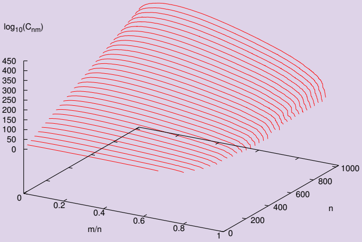
2d ISAW simulation up to $N = 1024$

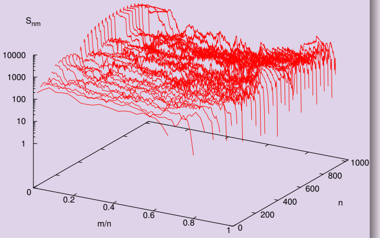
Total sample size: $230,000,000$



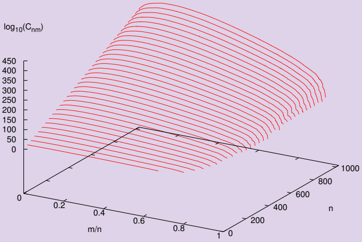
2d ISAW simulation up to $N = 1024$

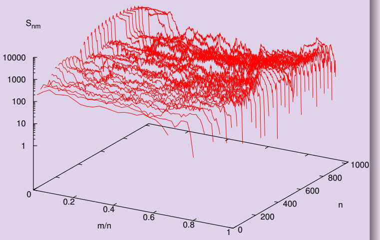
Total sample size: $240,000,000$



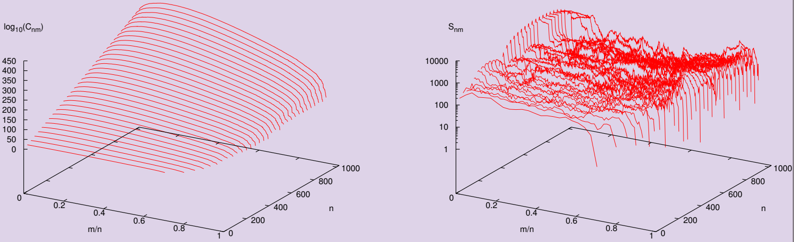


Total sample size: $250,000,000$



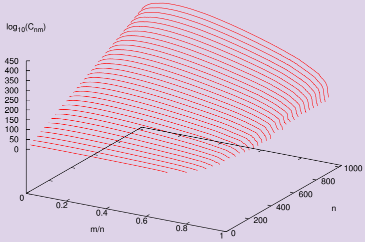


Total sample size: $260,000,000$



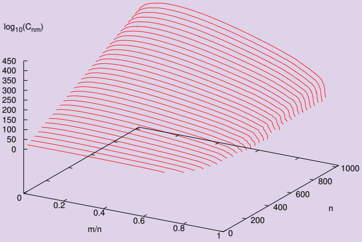
2d ISAW simulation up to $N = 1024$

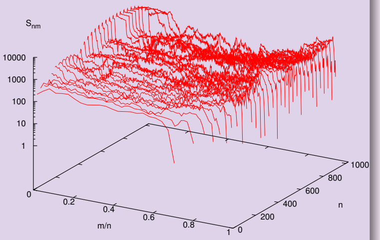
Total sample size: $270,000,000$



2d ISAW simulation up to $N = 1024$

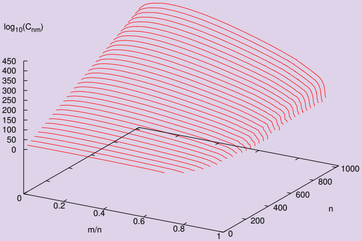
Total sample size: $280,000,000$

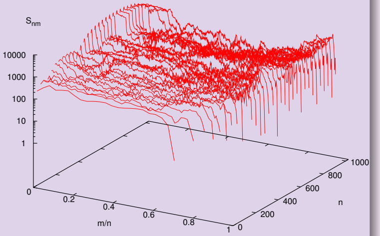




2d ISAW simulation up to $N = 1024$

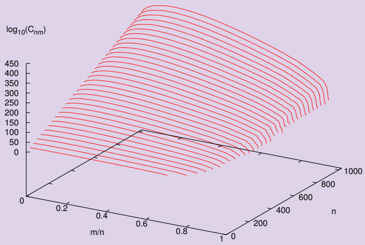
Total sample size: $290,000,000$

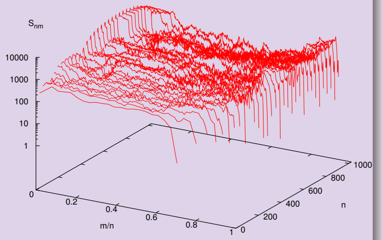




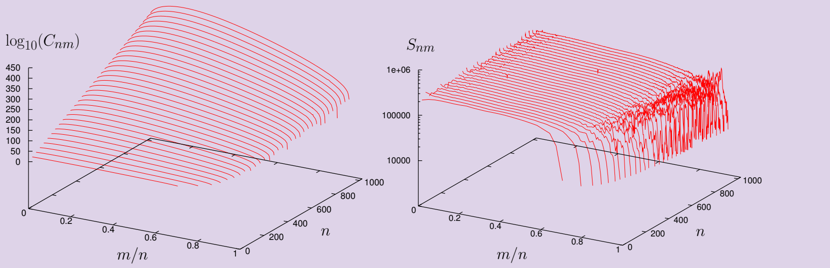
2d ISAW simulation up to $N = 1024$

Total sample size: $300,000,000$



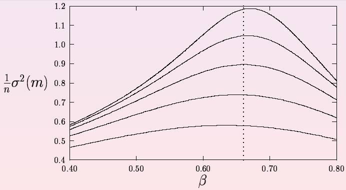


ISAW simulations

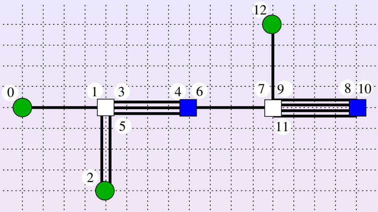


- 2d ISAW up to $n = 1024$
- One simulation suffices
- 400 orders of magnitude

(only 2d shown, 3d similar)

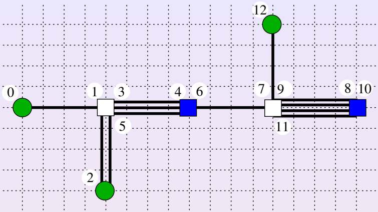


SWRW simulations



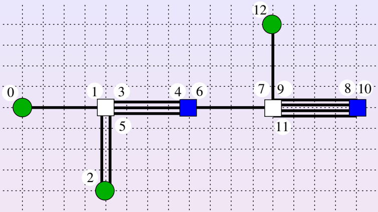
- Four simulations: reversal allowed/forbidden, 2d/3d

SWRW simulations



- Four simulations: reversal allowed/forbidden, 2d/3d
- Density of states C_{N,m_1,m_2} accessible up to $N = 256$

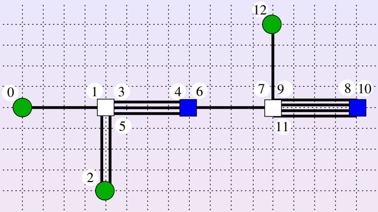
SWRW simulations



- Four simulations: reversal allowed/forbidden, 2d/3d
- Density of states C_{N,m_1,m_2} accessible up to $N = 256$
- Perform partial summation, e.g. over m_2

$$\bar{C}_{N,m_1}(\beta_2) = \sum_{m_2} C_{N,m_1,m_2} e^{\beta_2 m_2}$$

SWRW simulations

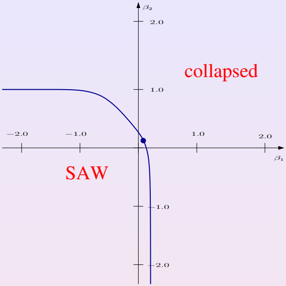


- Four simulations: reversal allowed/forbidden, 2d/3d
- Density of states C_{N,m_1,m_2} accessible up to $N = 256$
- Perform partial summation, e.g. over m_2

$$\bar{C}_{N,m_1}(\beta_2) = \sum_{m_2} C_{N,m_1,m_2} e^{\beta_2 m_2}$$

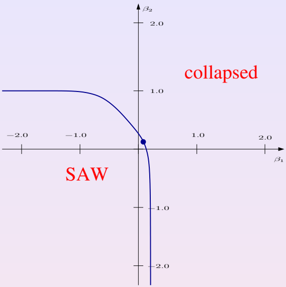
- Density of states $\bar{C}_{N,m_1}(\beta_2)$ accessible up to $N = 1024$ (for β_2 fixed)

SWRW in 3d, reversal forbidden (RF3)



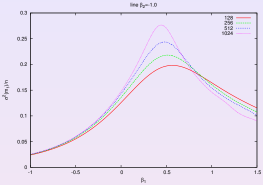
Phase diagram

SWRW in 3d, reversal forbidden (RF3)



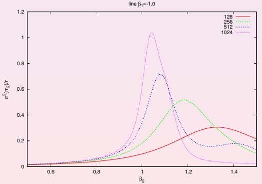
Phase diagram

$\beta_2 = -1.0$:



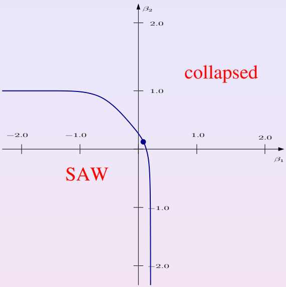
2nd order transition

$\beta_1 = -1.0$:

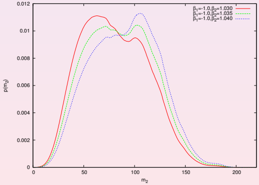


1st order transition

SWRW in 3d, reversal forbidden (RF3)

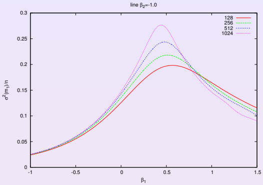


Phase diagram



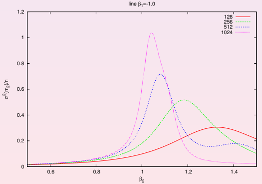
bimodal distribution

$\beta_2 = -1.0$:



2nd order transition

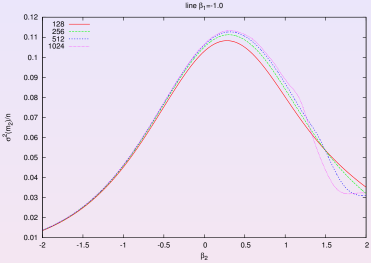
$\beta_1 = -1.0$:

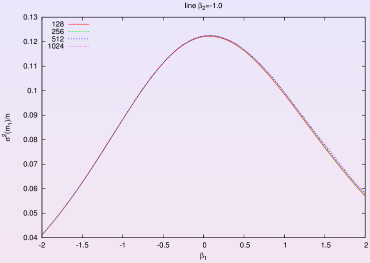


1st order transition

SWRW in 2d, reversal allowed (RA2)

We find a smooth crossover:

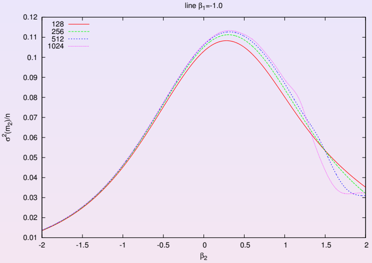


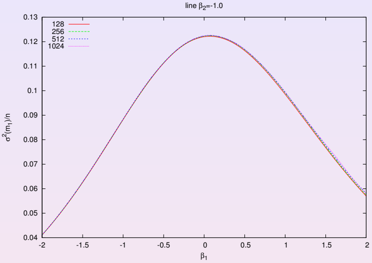


Both 1st order and 2nd order transitions have disappeared!

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
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

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 ...

Summary

- Polymers in solution:
  - Random Walk + Excluded Volume + Attraction?

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An unfinished story!

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- Things to come:
  - J. Krawczyk, A. L. Owczarek, T. Prellberg, and A. Rechnitzer, "Simulation of Lattice Polymers with Hydrogen-Like Bonding," preprint

The End