PERM and all that

a comparison of growth algorithms

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Monte Carlo Algorithms in Statistical Physics
Melbourne, July 26-28

Topic Outline

Outline

1. Introduction
   - A Zoology of Growth Algorithms
   - Which Algorithm is Best?
   - ISAW - the canonical lattice model
2. The 'Old' Algorithms
   - Rosenbluth^2
   - PERM
   - Multicanonical PERM
   - FlatPERM
3. The 'New' Algorithms
   - New Ideas
   - GARM
   - GAS
4. Conclusion
   - Outlook
   - Thanks

Acronyms and Algorithms

These days there exists a zoo of growth algorithms

- 1997: PERM
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All of this is based on

- 1955: Rosenbluth & Rosenbluth

Which Algorithm is Best?

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I don't really know.

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or, perhaps slightly better,

It depends . . .

Why? It's just easiest to use your own algorithm

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- Alternative lattice models:
  - 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
  - A. L. Owczarek and T. Prellberg, "Collapse transition of self-avoiding trails on the square lattice," Physica A 373 (2007) 433-438
  - J. Doukas, A. L. Owczarek and T. Prellberg, "Identification of a polymer growth process with an equilibrium multi-critical collapse phase transition: the meeting point of swollen, collapsed and crystalline polymers," submitted to Phys. Rev. E

Putting Things into Perspective

As of July 25th,

- PERM (1997): 245 citations
- nPERM (2003): 65 citations
- Multicanonical PERM (2003): 45 citations
- flatPERM (2004): 34 citations
- GARM/flatGARM (2008): 3 citations
- GAS/flatGAS (2009): 1 citation

Putting Things into Perspective

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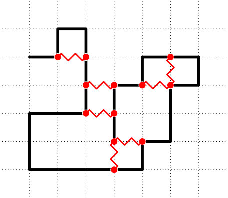
This should be compared with e.g.

- Umbrella Sampling (1977): 994 citations
- Multicanonical Sampling (1992): 751 citations
- Wang-Landau Sampling (2001): 693 citations

ISAW - the canonical lattice model

Interacting Self-Avoiding Walk (ISAW)

- Physical space $\rightarrow$ simple cubic lattice $\mathbb{Z}^3$
- Polymer $\rightarrow$ self-avoiding N-step random walk (SAW) φ
- Quality of solvent $\rightarrow$ short-range interaction ϵ, Energy $E_N(\varphi) = m(\varphi)\epsilon$



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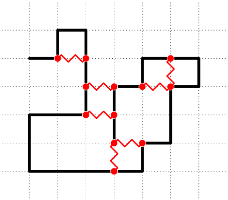
Partition function:

$$Z_N(\beta) = \sum_m C_{N,m} e^{-\beta m \epsilon}$$



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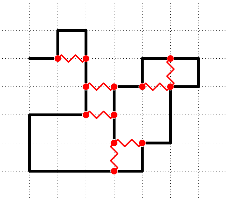

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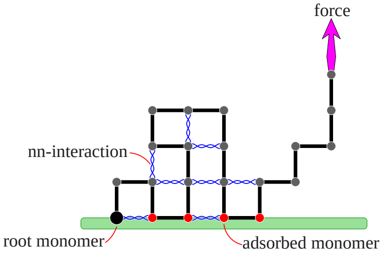
Thermodynamic Limit for a dilute solution:

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

Extensions of the Model

- In addition to
  - polymer and solvent modelling (bulk interaction)
- add
  - protein-like structure (HP interactions)
  - adsorption (surface interaction)
  - micromechanical deformations
    e.g. force on chain end (optical tweezers)



- Complete description through high-dimensional density of states: (a) bulk and (b) surface interactions, (c) positions of chain end

Outline

Rosenbluth versus Simple Sampling

Simple Sampling (for SAW)

- Choose starting vertex at the origin
- Draw one of the neighbouring sites uniformly at random
- If occupied, reject entire walk and start again
- If unoccupied, accept and repeat (up to some maximal walk length)

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(Augment with Importance Sampling for ISAW)

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- Uniform, independent samples

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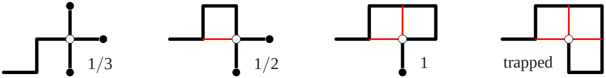

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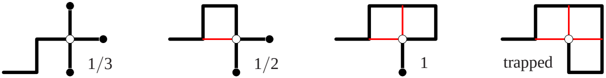

- At step k, a_k possibilities with probability $p_k = 1/a_k$
- An N-step walk φ has weight

$$W(\varphi) \propto \prod_{k<N} a_k(\varphi)$$

- Walks with large weights dominate ensemble

PERM: "Go with the Winners"

PERM = Pruned and Enriched Rosenbluth Method

P Grassberger, Phys Rev E 56 (1997) 3682

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BA Berg and T Neuhaus, Phys Lett B 267 (1991) 249

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The resulting algorithm is called multicanonical PERM

M Bachmann and W Janke, PRL 91 (2003) 208105

Revisit PERM

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$$C_N^{\mathrm{est}} = \langle W \rangle_N = \frac{1}{S} \sum_i W(\varphi_i)$$

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$$r = W(\varphi)/\langle W \rangle_N$$

1. If $r > 1$, make $c = \min(\lfloor r \rfloor, a_N)$ distinct copies and update

$$W(\varphi) \leftarrow W(\varphi)/c$$

2. If $r < 1$, prune with probability $1 - r$ and update

$$W(\varphi) \leftarrow W(\varphi)/r$$

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An important observation:

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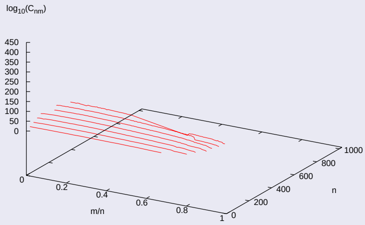
- Parameter-free implementation

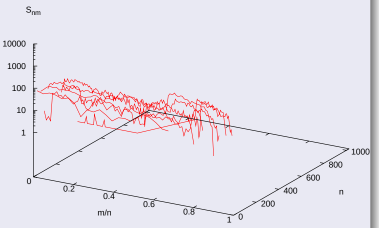
Example: 2dim ISAW simulation up to $N = 1024$

- flatPERM starts with poor estimates of the average weights $\langle W \rangle$
- To stabilise algorithm (avoid initial overflow/underflow):
  delay growth of large configurations by increasing lengths gradually

Example: 2dim ISAW simulation up to $N = 1024$

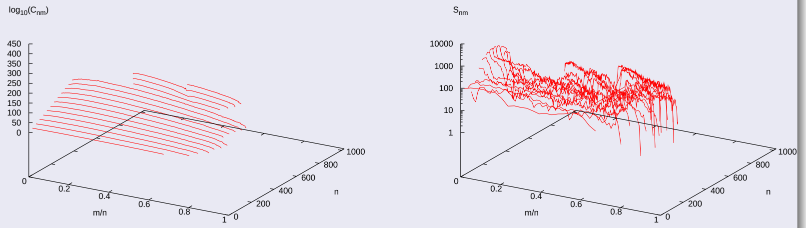
Total sample size: $1,000,000$





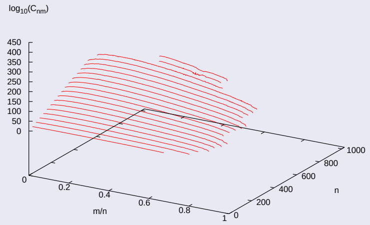
Example: 2dim ISAW simulation up to $N = 1024$

Total sample size: $10,000,000$



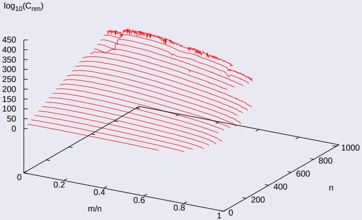
Example: 2dim ISAW simulation up to $N = 1024$

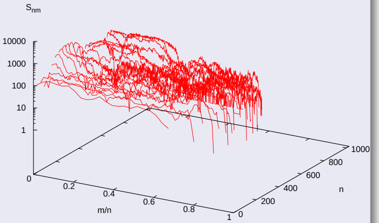
Total sample size: $20,000,000$



Example: 2dim ISAW simulation up to $N = 1024$

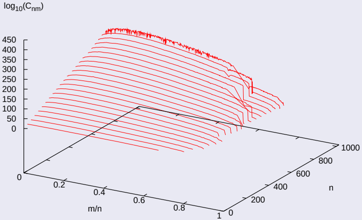
Total sample size: $30,000,000$

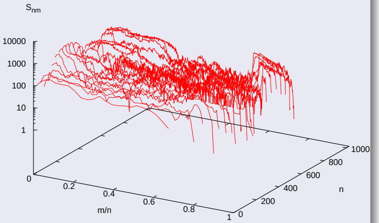




Example: 2dim ISAW simulation up to $N = 1024$

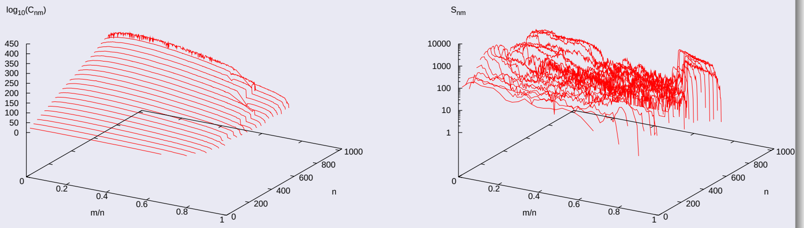
Total sample size: $40,000,000$





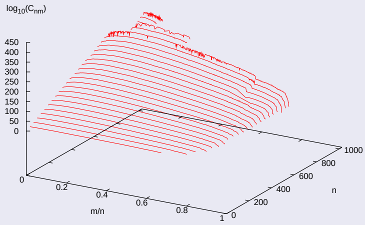
Example: 2dim ISAW simulation up to $N = 1024$

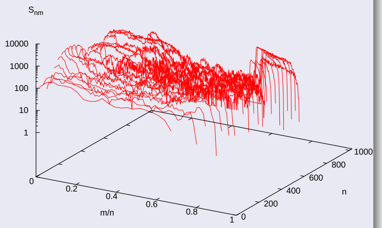
Total sample size: $50,000,000$



Example: 2dim ISAW simulation up to $N = 1024$

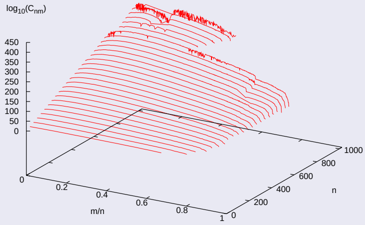
Total sample size: $60,000,000$

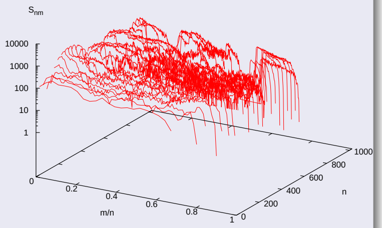




Example: 2dim ISAW simulation up to $N = 1024$

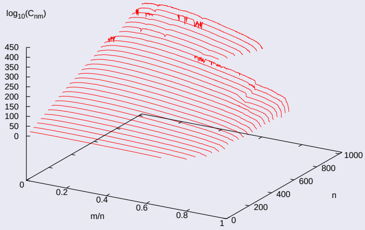
Total sample size: $70,000,000$

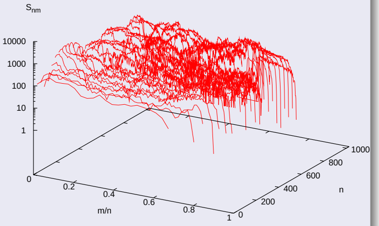




Example: 2dim ISAW simulation up to $N = 1024$

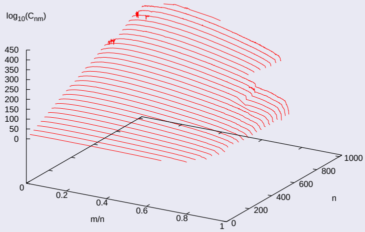
Total sample size: $80,000,000$

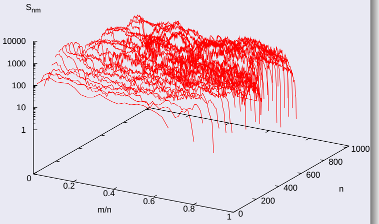




Example: 2dim ISAW simulation up to $N = 1024$

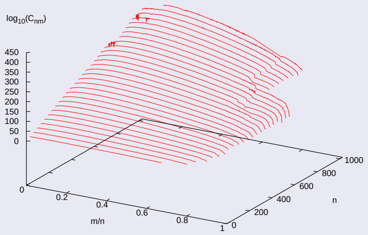
Total sample size: $90, 000, 000$

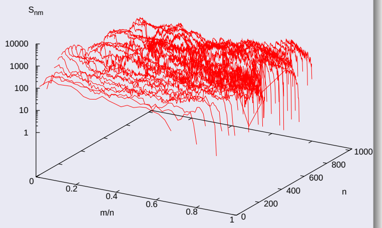




Example: 2dim ISAW simulation up to $N = 1024$

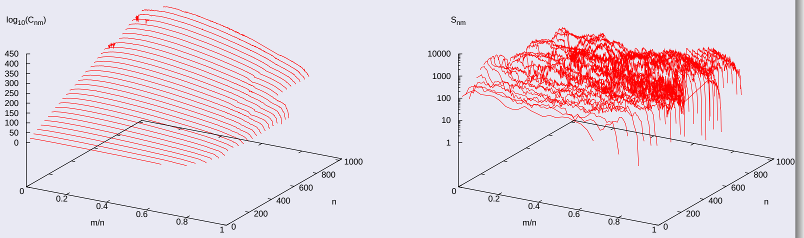
Total sample size: $100,000,000$





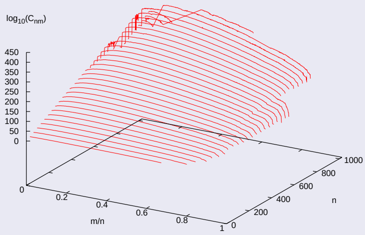
Example: 2dim ISAW simulation up to $N = 1024$

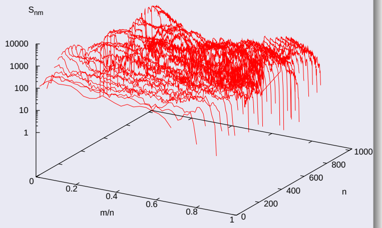
Total sample size: $110,000,000$



Example: 2dim ISAW simulation up to $N = 1024$

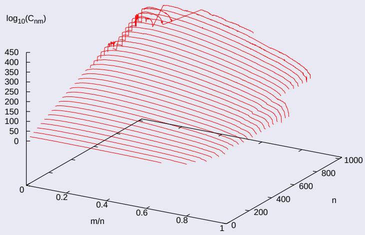
Total sample size: $120,000,000$

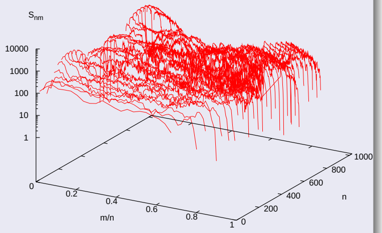




Example: 2dim ISAW simulation up to $N = 1024$

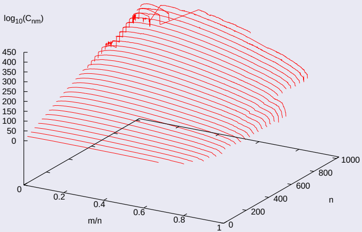
Total sample size: $130,000,000$

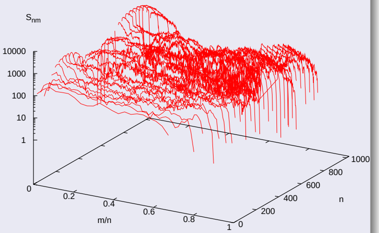




Example: 2dim ISAW simulation up to $N = 1024$

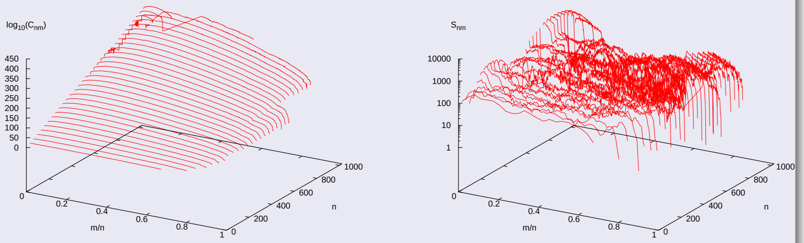
Total sample size: $140,000,000$





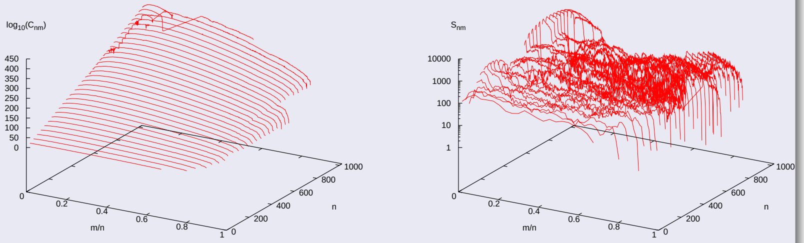
Example: 2dim ISAW simulation up to $N = 1024$

Total sample size: $150,000,000$



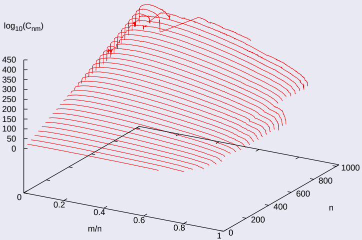
Example: 2dim ISAW simulation up to $N = 1024$

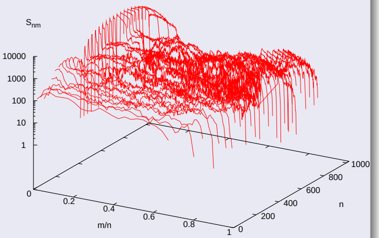
Total sample size: $160,000,000$



Example: 2dim ISAW simulation up to $N = 1024$

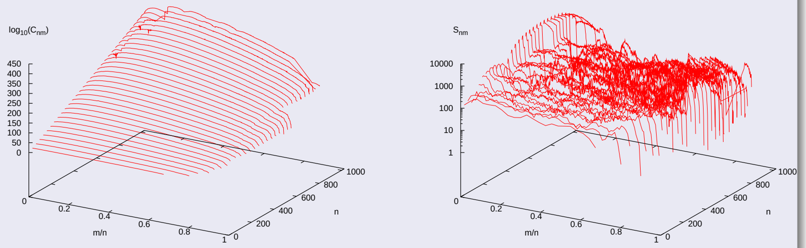
Total sample size: $170,000,000$





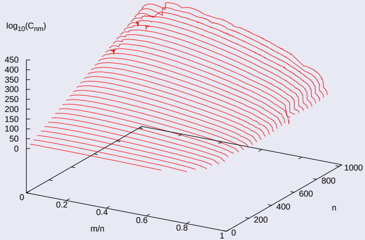
Example: 2dim ISAW simulation up to $N = 1024$

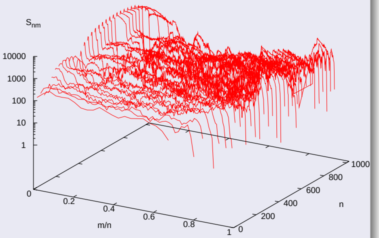
Total sample size: $180,000,000$



Example: 2dim ISAW simulation up to $N = 1024$

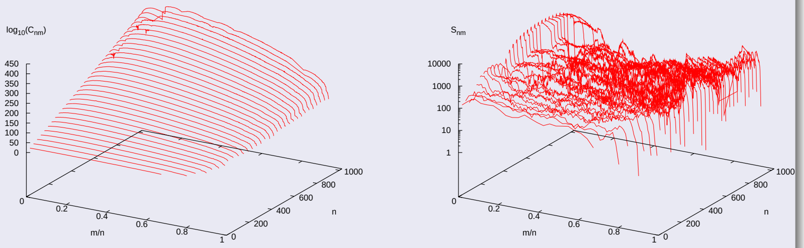
Total sample size: $190,000,000$





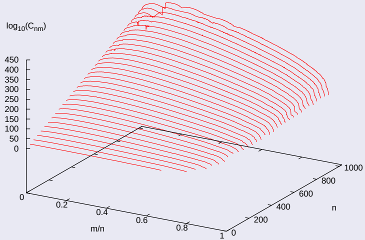
Example: 2dim ISAW simulation up to $N = 1024$

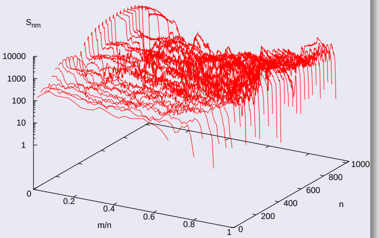
Total sample size: $200,000,000$



Example: 2dim ISAW simulation up to $N = 1024$

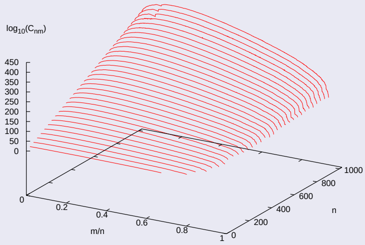
Total sample size: $210,000,000$

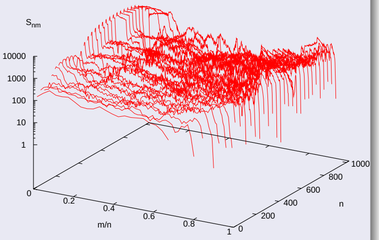




Example: 2dim ISAW simulation up to $N = 1024$

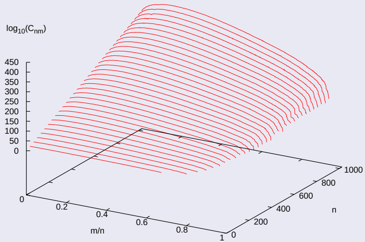
Total sample size: $220,000,000$

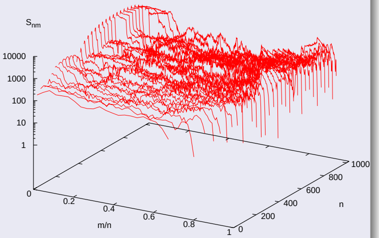




Example: 2dim ISAW simulation up to $N = 1024$

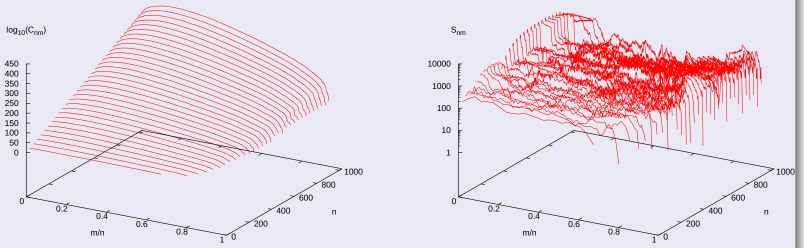
Total sample size: $230,000,000$





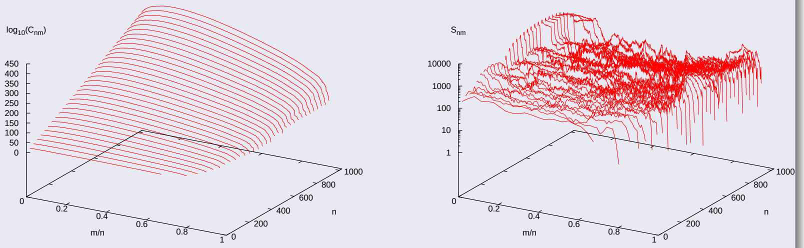
Example: 2dim ISAW simulation up to $N = 1024$

Total sample size: $240,000,000$



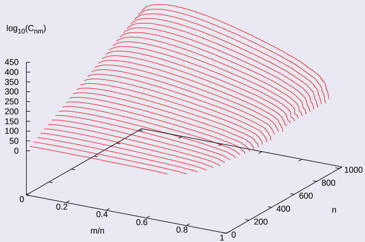
Example: 2dim ISAW simulation up to $N = 1024$

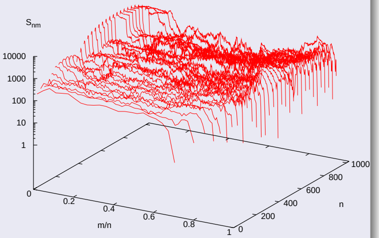
Total sample size: $250,000,000$



Example: 2dim ISAW simulation up to $N = 1024$

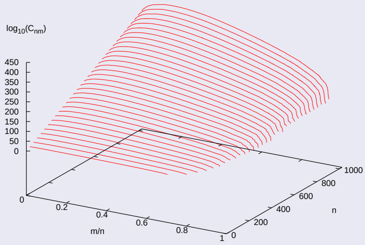
Total sample size: $260,000,000$

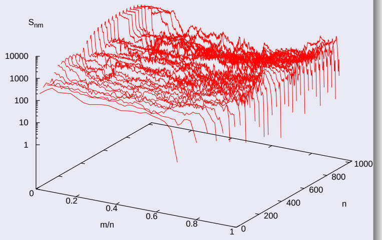




Example: 2dim ISAW simulation up to $N = 1024$

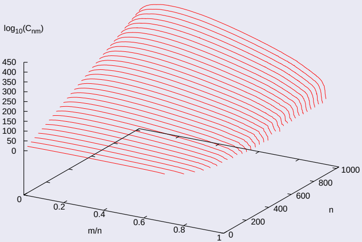
Total sample size: $270,000,000$

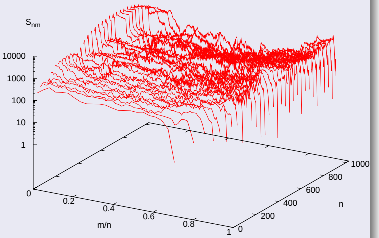




Example: 2dim ISAW simulation up to $N = 1024$

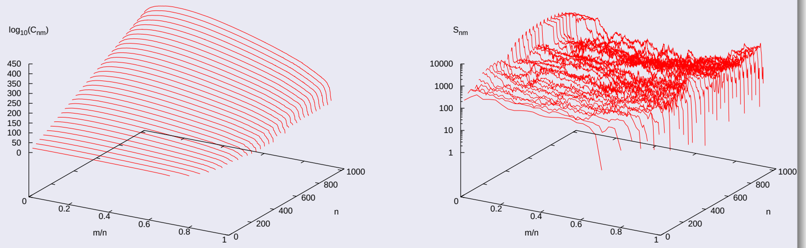
Total sample size: $280,000,000$





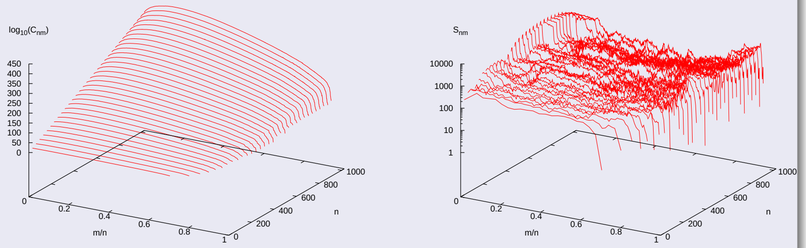
Example: 2dim ISAW simulation up to $N = 1024$

Total sample size: $290,000,000$



Example: 2dim ISAW simulation up to $N = 1024$

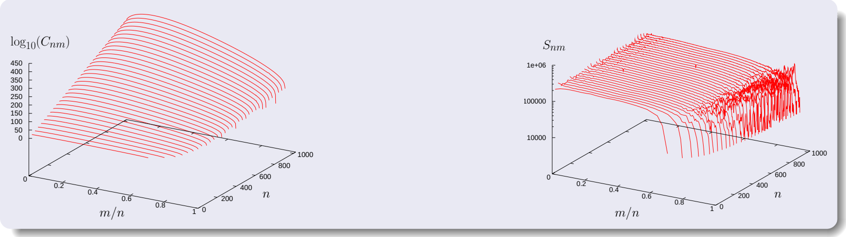
Total sample size: $300,000,000$



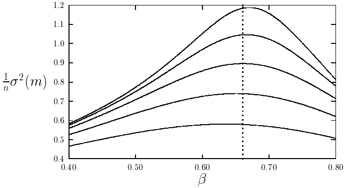
ISAW simulations

2dim ISAW density of states

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



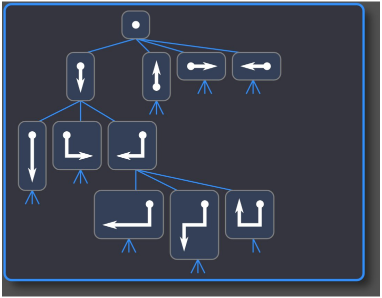
- 2d ISAW up to $n = 1024$
- One simulation suffices
- 400 orders of magnitude



Outline

Revisit Rosenbluth Sampling

- Each configuration grown uniquely by appending edges to endpoint



Revisit Rosenbluth Sampling

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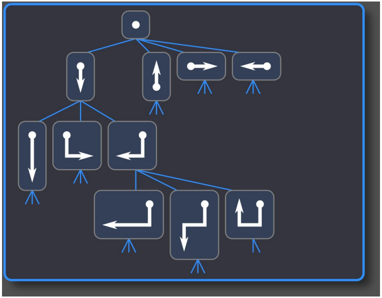

- Generating tree
  - Each node of tree is a configuration

Revisit Rosenbluth Sampling

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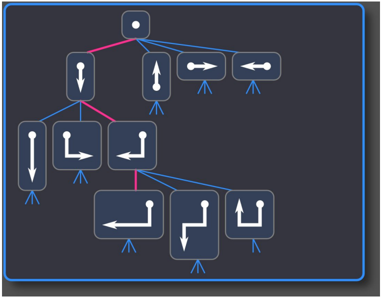

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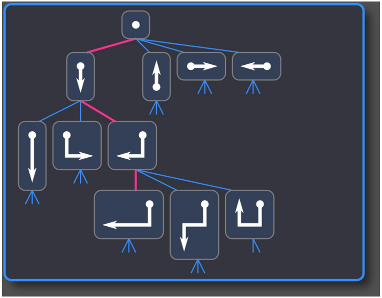

- Generating tree
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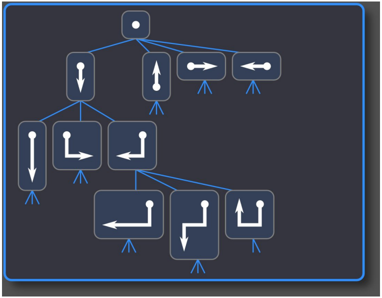
  - The weight of sample path is $W(\varphi) = \prod_{k<N} a_k(\varphi)$

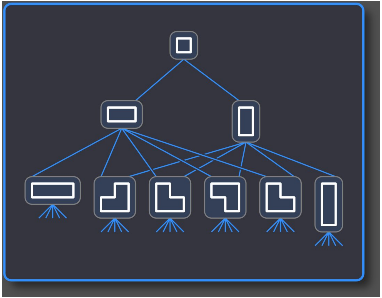
From Generating Trees to Generating Graphs

- Unique way to construct walks



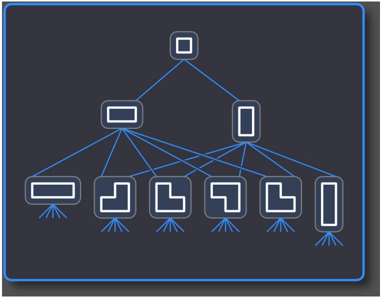
From Generating Trees to Generating Graphs

- Unique way to construct walks
- No obvious unique way to construct polygons



From Generating Trees to Generating Graphs

- Unique way to construct walks
- No obvious unique way to construct polygons
- Can we generalize from generating trees?



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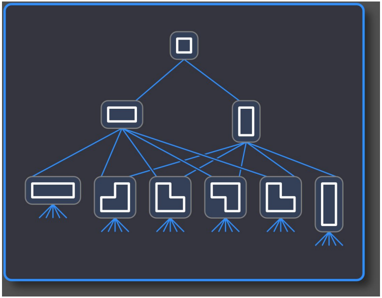

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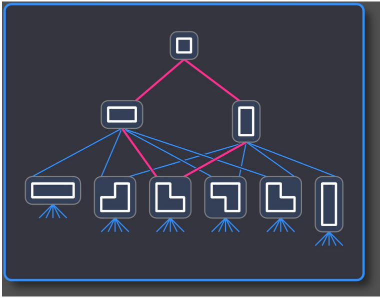

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  - Each node of graph is a configuration
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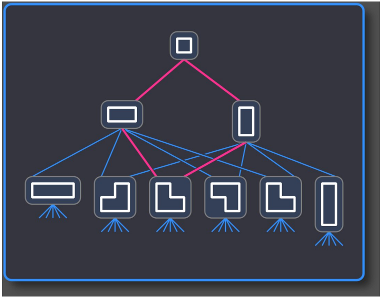

- Generating graph
  - Each node of graph is a configuration
  - Sample by growing non-unique path down the graph
  - The weight of the sample path is $W(\varphi) \neq \prod_{k<N} a_k(\varphi)$

Atmospheres

- Positive and negative atmospheres of the configuration
  - Let a^{+} be the number of ways a configuration can grow
  - Let a^{-} be the number of ways a configuration can shrink

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  - The weight $W(\varphi)$ and probability $\Pr(\varphi)$ of a sample path φ are

$$W(\varphi) = \prod_{k<N} a_k^+(\varphi) \qquad \Pr(\varphi) = 1/W(\varphi)$$

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$$W(\varphi) = \prod_{k<N} a_k^+(\varphi) \qquad \Pr(\varphi) = 1/W(\varphi)$$

  - This implies

$$\sum_{\varphi} W(\varphi) \Pr(\varphi) = \sum_{\varphi} 1 = C_N$$

From Rosenbluth Sampling to GARM

- Generating tree: bijection between sample paths and configurations

$$W(\varphi) = \prod_{k<N} a_k^+(\varphi) \qquad\qquad \sum_{\varphi} W(\varphi)\,\Pr(\varphi) = C_N$$

From Rosenbluth Sampling to GARM

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EJJ van Rensburg and A Rechnitzer, J Phys A 41 (2008) 442002

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Important Extension

- Can include conventional canonical Monte Carlo moves
- Need to know a^0, the atmosphere of neutral moves

Good ideas are welcome!

Grow and Shrink

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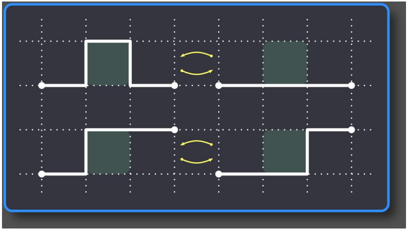

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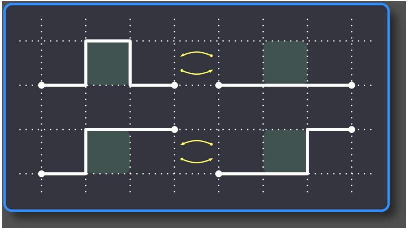

- Moves from the BFACF algorithm

B Berg and D Foester, Phys Lett B 106 (1981) 323

C Aragão de Carvalho, S Caracciolo and J Fröhlich, Nucl Phys B 215 (1983) 209

- Ergodic on each knot-type

EJJ van Rensburg, J Phys A 25 (1992) 1031

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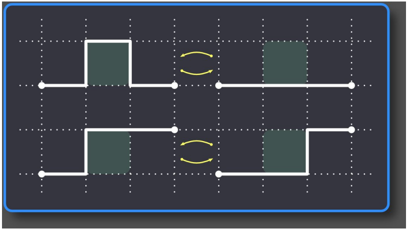
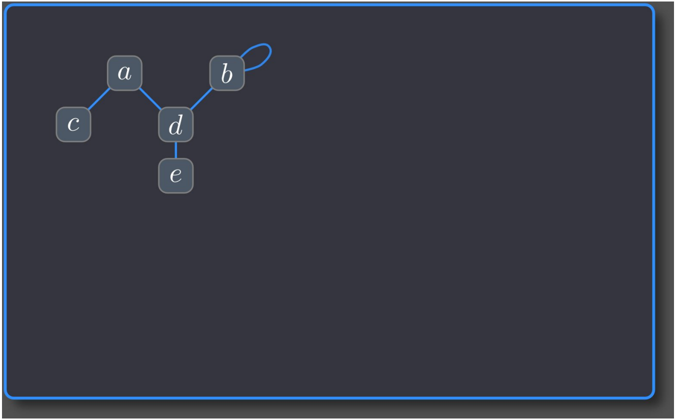


- Generating graph still exists, but now sample paths are not directed
- Need to "redirect" the graph

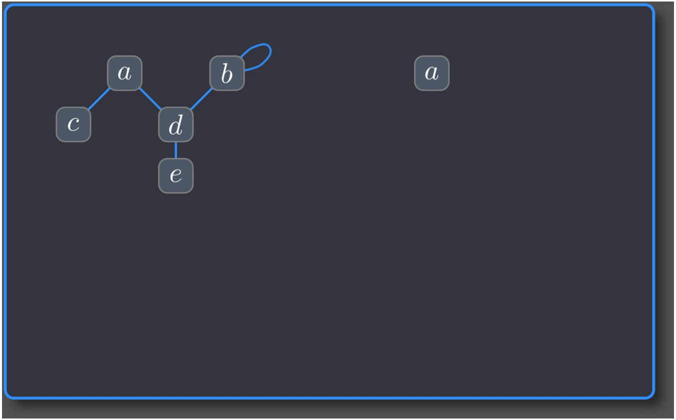
Derivative graph

- Take an arbitrary generating graph



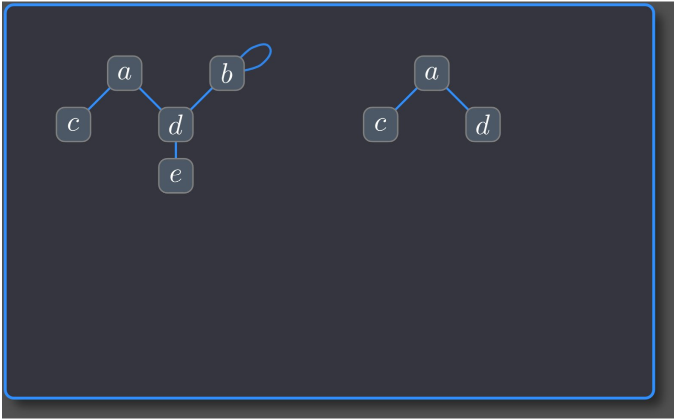
Derivative graph

- Copy the initial vertex



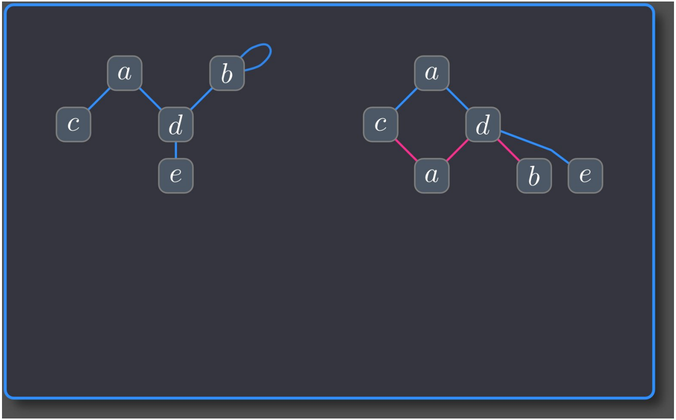
Derivative graph

- What vertices does it see? — add them to the next row



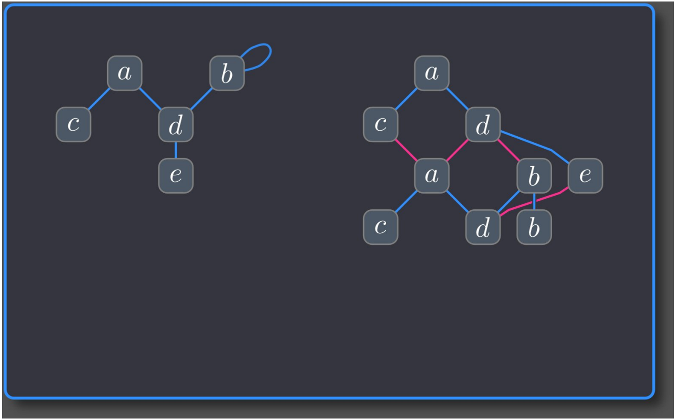
Derivative graph

- What vertices do these see? — both up and down



Derivative graph

- Keep adding new rows in this way



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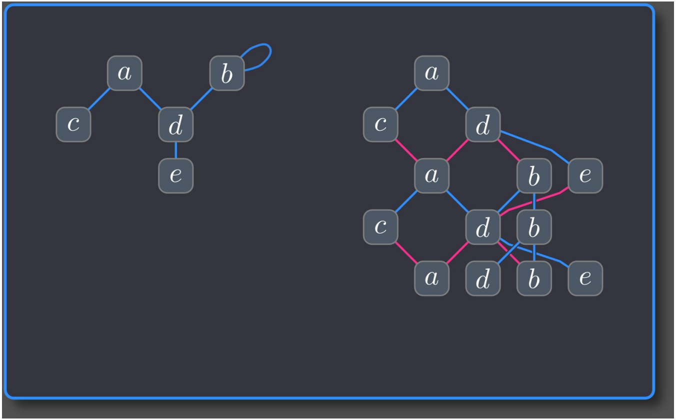
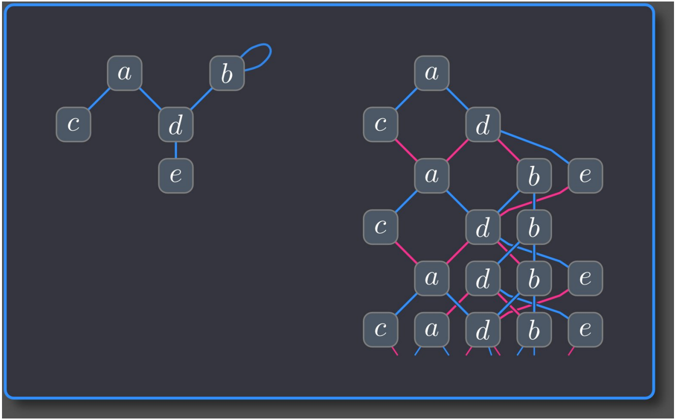


Derivative graph

- This gives the "derivative graph"



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GAS = Generalized Atmospheric Sampling = Grow And Shrink

EJJ van Rensburg and A Rechnitzer, J Phys A 42 (2009) 335001

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- Generalizes to Thermal GAS and Pruned Enriched GAS
- Multicanonical and Flat Histogram GAS seems harder

Under development

A Rechnitzer, private communication

GAS Application: Minimal Polygons

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- This can now be used to estimate e.g. the number of figure eight knots

$$\frac{C_N(4_1)}{C_{30}(4_1)} = \frac{\langle W(\varphi)\rangle_N}{\langle W(\varphi)\rangle_{30}}$$

Outline

Comparing the Algorithms?

- Testing flatPERM using 1-dim random walk

JD Jiang and YN Huang, Comp Phys Commun 180 (2009) 177

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Many more applications for GARM/GAS?

Thanks

Monte Carlo Collaborators

- Jason Doukas (Kyoto)
- Jarek Krawczyk (Dortmund)
- Aleks Owzcarek (Melbourne)
- Andrew Rechnitzer (Vancouver)

- Buks van Rensburg (Toronto)
  Monte Carlo methods for the self-avoiding walk, J Phys A 42 (2009) 323001

$$$

- Deutsche Forschungsgemeinschaft (DFG)
- MASCOS
- Royal Society

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