

PERM and all that

a comparison of growth algorithms

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Topic Outline

1 Introduction

- A Zoology of Growth Algorithms
- Which Algorithm is Best?
- ISAW - the canonical lattice model

2 The 'Old' Algorithms

- Rosenbluth²
- PERM
- Multicanonical PERM
- FlatPERM

3 The 'New' Algorithms

- New Ideas
- GARM
- GAS

4 Conclusion

- Outlook
- Thanks

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Acronyms and Algorithms

These days there exists a zoo of growth algorithms

- 1997: PERM
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- 2009: GAS
- 201?: flatGAS

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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 . . .

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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," Phys. Rev. E 82 (2010) 031103

Putting Things into Perspective

As of April 18th,

- PERM (1997): 258 citations
- nPERM (2003): 70 citations
- Multicanonical PERM (2003): 49 citations
- flatPERM (2004): 38 citations
- GARM/flatGARM (2008): 5 citations
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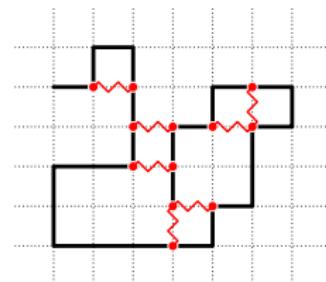
This should be compared with e.g.

- Umbrella Sampling (1977): 1090 citations
- Multicanonical Sampling (1992): 800 citations
- Wang-Landau Sampling (2001): 776 citations

ISAW - the canonical lattice model

Interacting Self-Avoiding Walk (ISAW)

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



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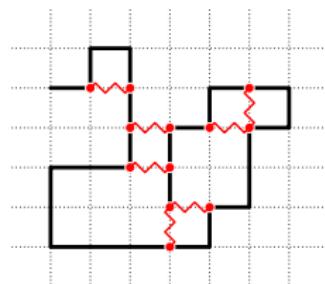
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Partition function:

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

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



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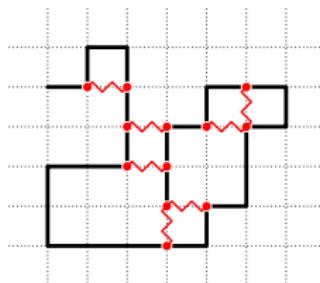
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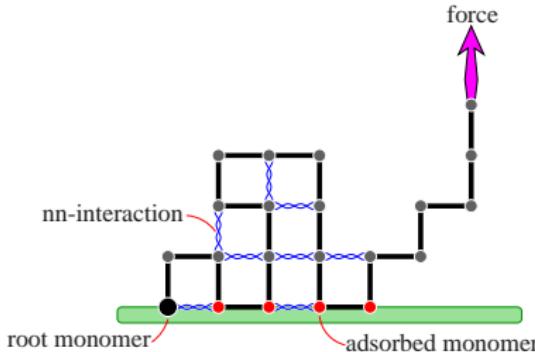


Thermodynamic Limit for a dilute solution:

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

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



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- Choose starting vertex at the origin
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(Augment with Importance Sampling for ISAW)

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- Uniform, independent samples

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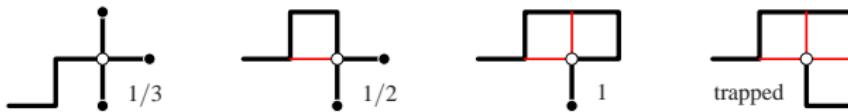
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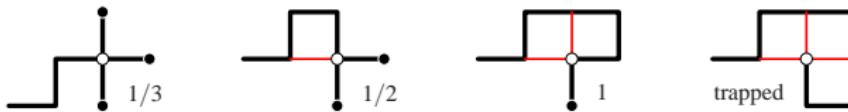
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- At step k , a_k possibilities with probability $p_k = 1/a_k$
- An N -step walk φ has weight

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

- Walks with large weights dominate ensemble

PERM: “Go with the Winners”

PERM = Pruned and Enriched Rosenbluth Method

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

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

Revisit PERM

- Exact enumeration: choose all **a** continuations with weight **1**

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

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

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

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

- ➋ 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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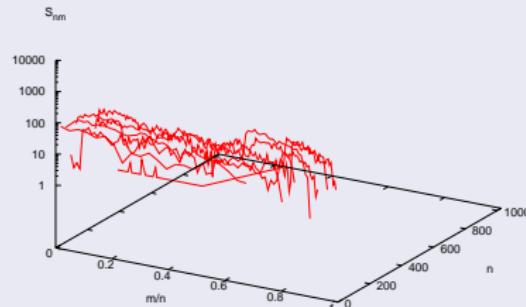
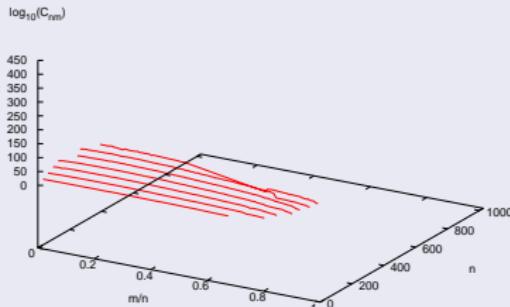
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- Parameter-free implementation

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

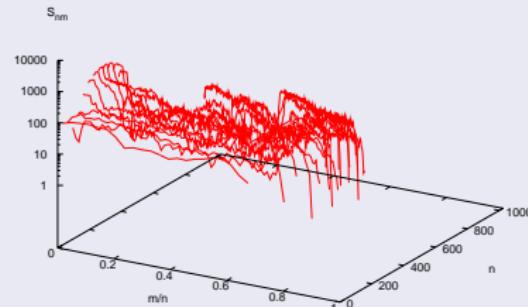
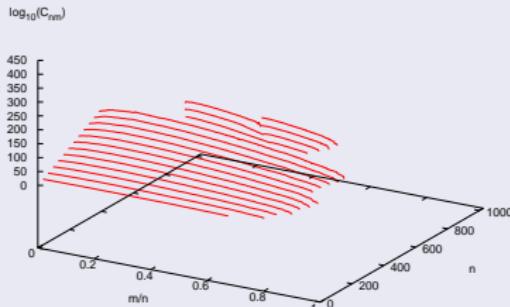
Example: 2dim ISAW simulation up to $N = 1024$

Total sample size: 1,000,000



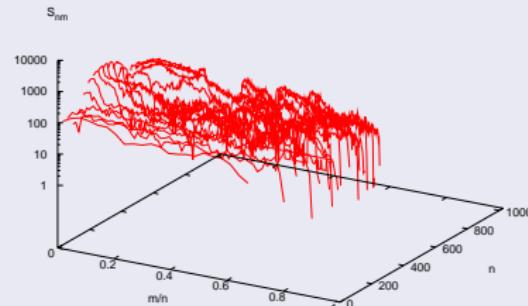
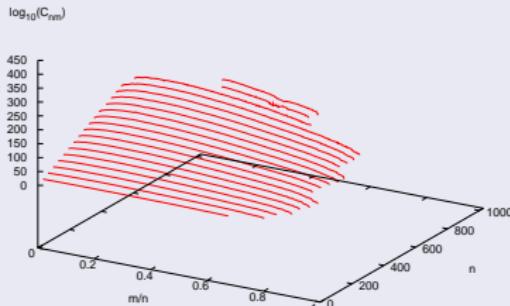
Example: 2dim ISAW simulation up to $N = 1024$

Total sample size: 10,000,000



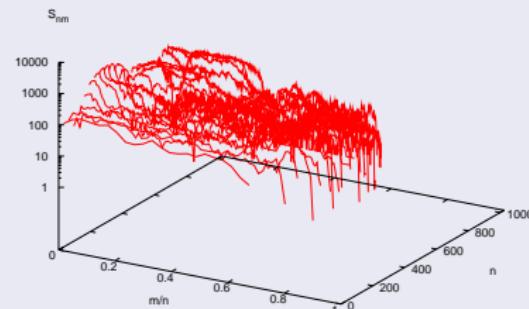
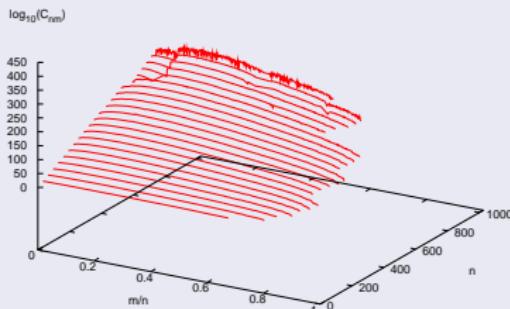
Example: 2dim ISAW simulation up to $N = 1024$

Total sample size: 20,000,000



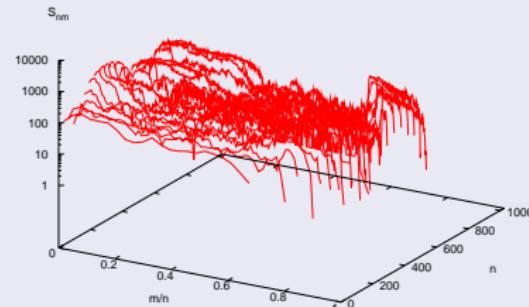
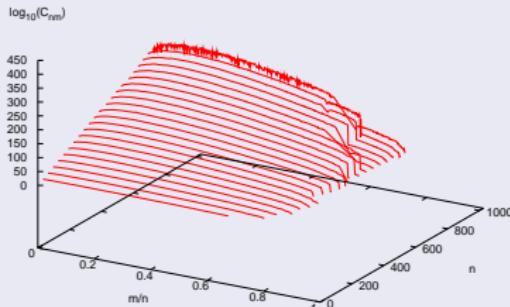
Example: 2dim ISAW simulation up to $N = 1024$

Total sample size: 30,000,000



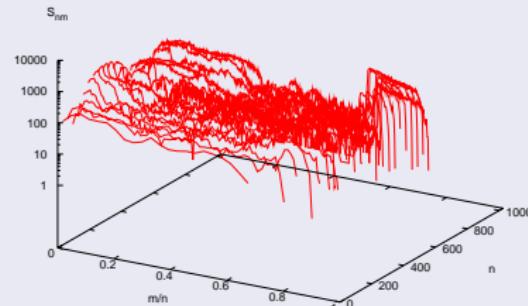
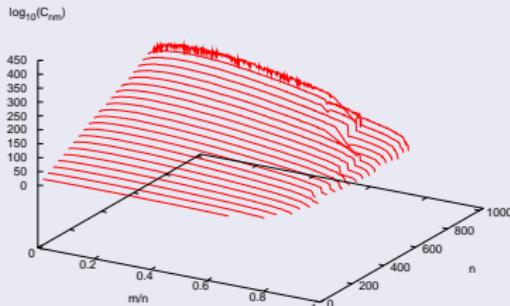
Example: 2dim ISAW simulation up to $N = 1024$

Total sample size: 40,000,000



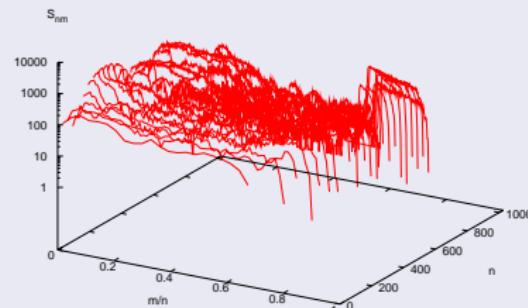
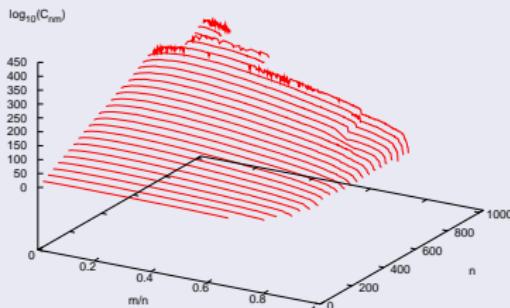
Example: 2dim ISAW simulation up to $N = 1024$

Total sample size: 50,000,000



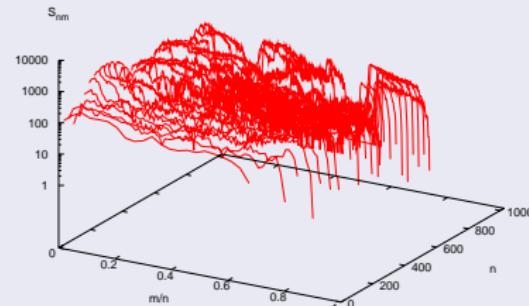
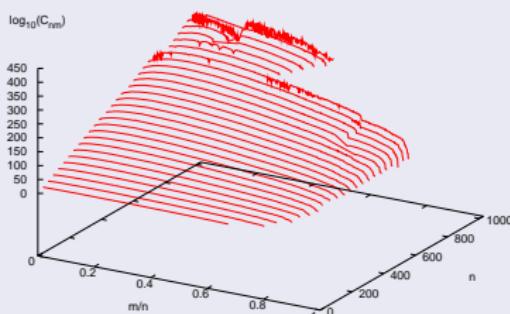
Example: 2dim ISAW simulation up to $N = 1024$

Total sample size: 60,000,000



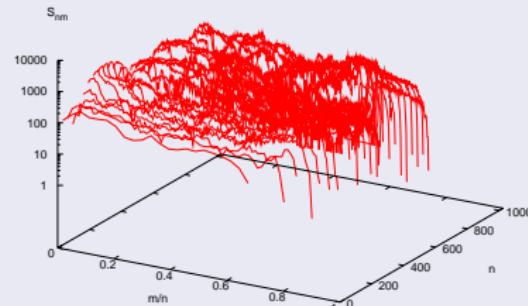
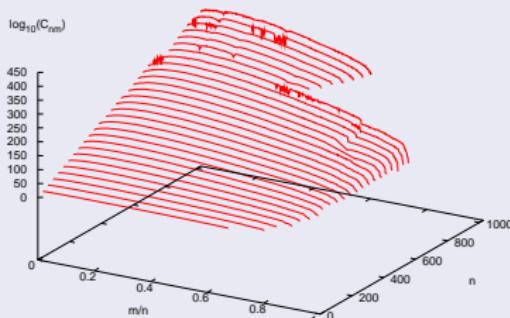
Example: 2dim ISAW simulation up to $N = 1024$

Total sample size: 70,000,000



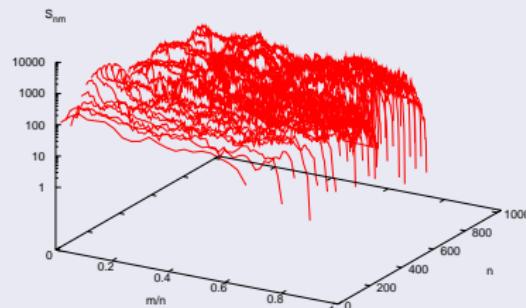
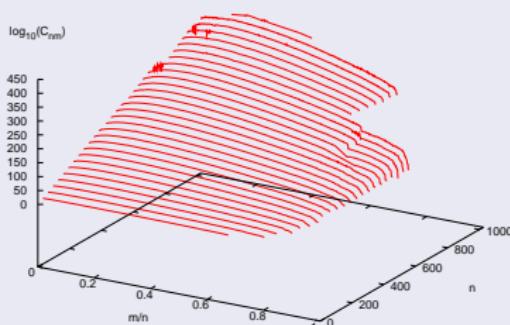
Example: 2dim ISAW simulation up to $N = 1024$

Total sample size: 80,000,000



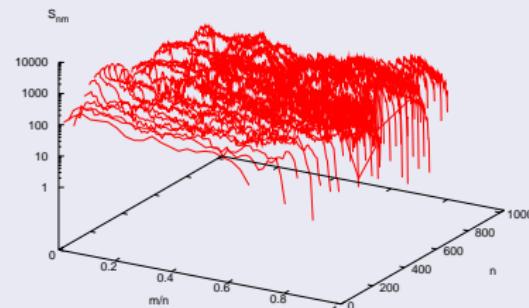
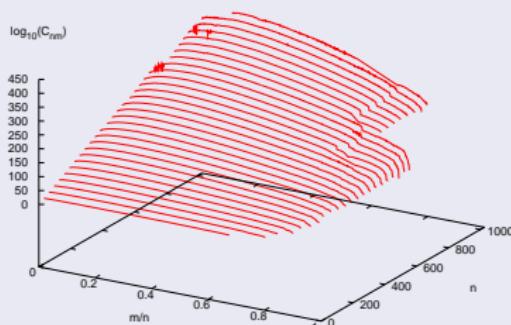
Example: 2dim ISAW simulation up to $N = 1024$

Total sample size: 90,000,000



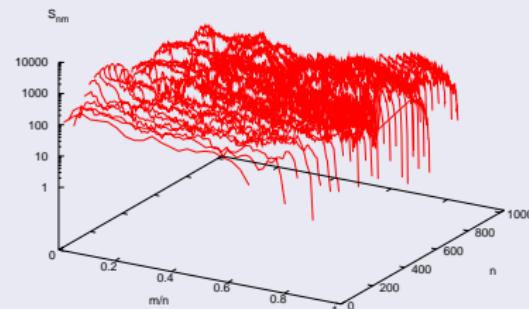
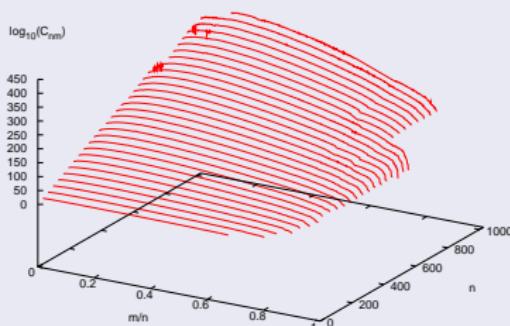
Example: 2dim ISAW simulation up to $N = 1024$

Total sample size: 100,000,000



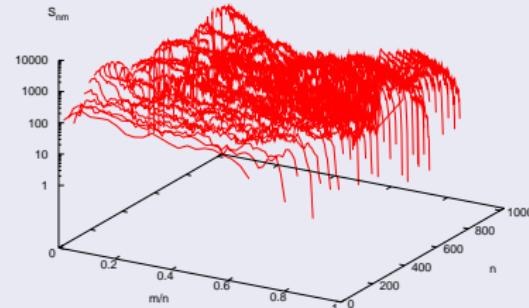
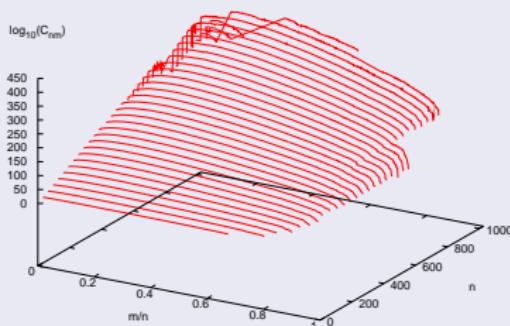
Example: 2dim ISAW simulation up to $N = 1024$

Total sample size: 110,000,000



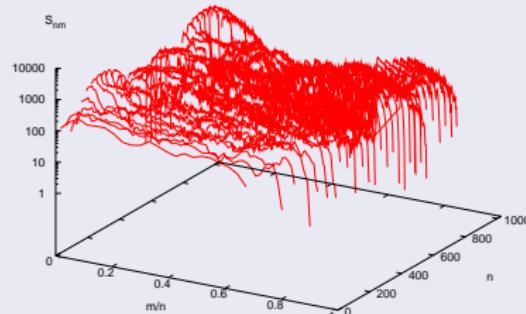
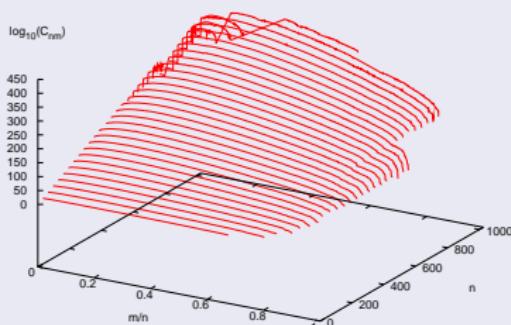
Example: 2dim ISAW simulation up to $N = 1024$

Total sample size: 120,000,000



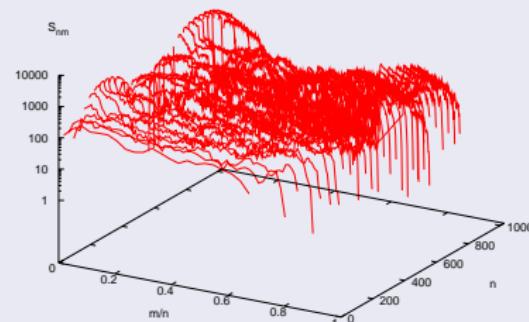
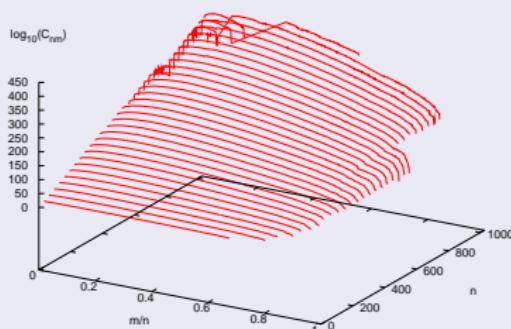
Example: 2dim ISAW simulation up to $N = 1024$

Total sample size: 130,000,000



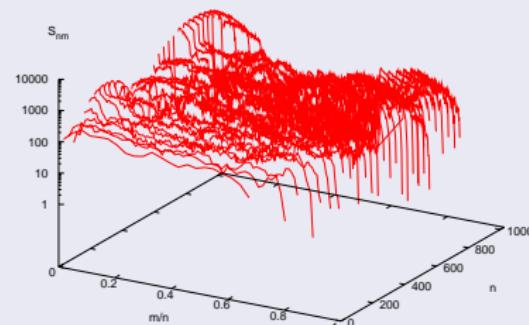
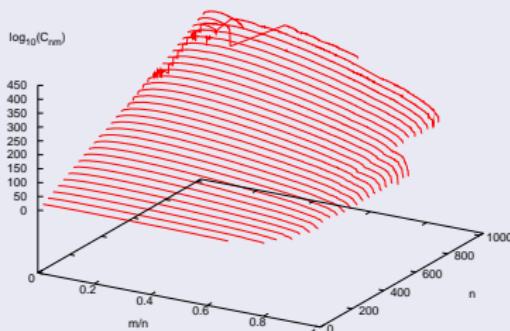
Example: 2dim ISAW simulation up to $N = 1024$

Total sample size: 140,000,000



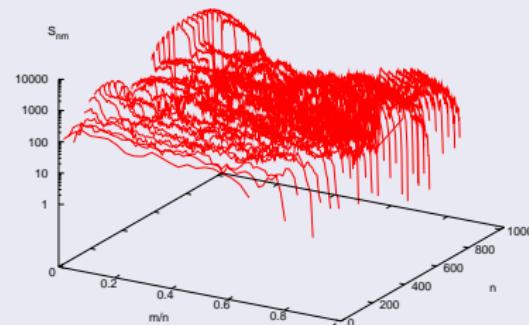
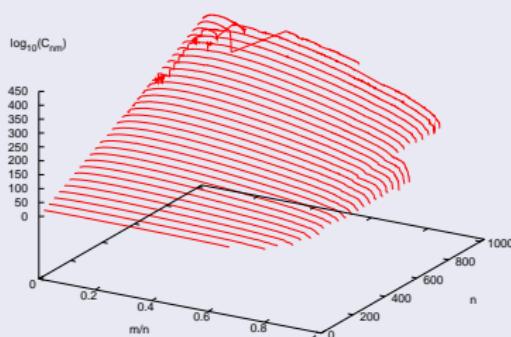
Example: 2dim ISAW simulation up to $N = 1024$

Total sample size: 150,000,000



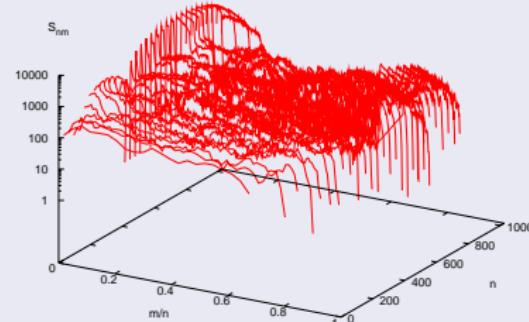
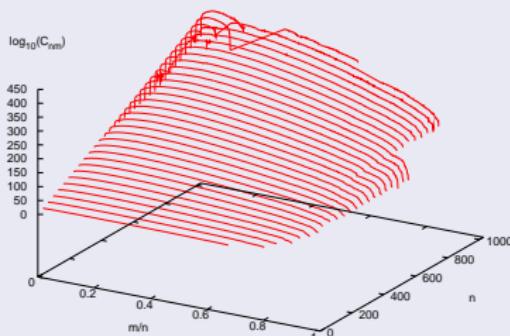
Example: 2dim ISAW simulation up to $N = 1024$

Total sample size: 160,000,000



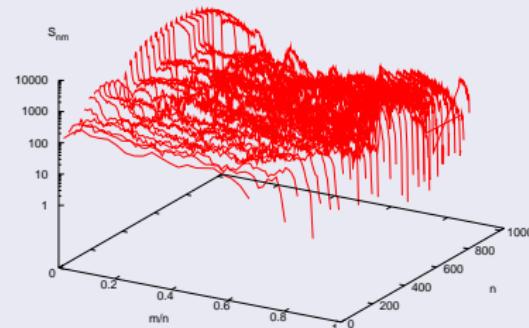
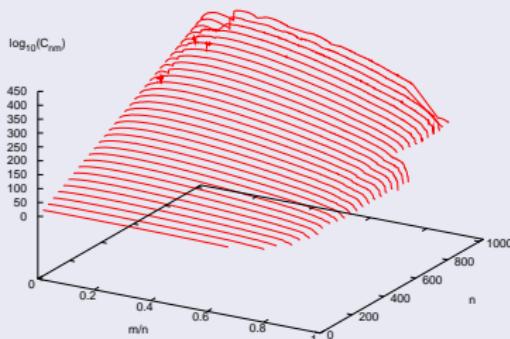
Example: 2dim ISAW simulation up to $N = 1024$

Total sample size: 170,000,000



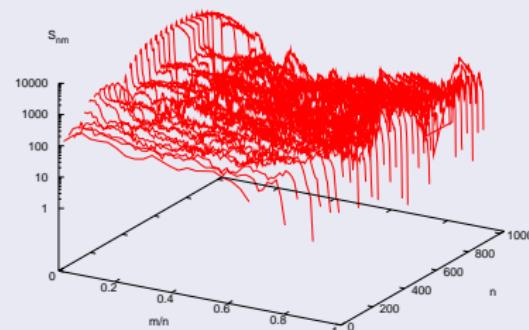
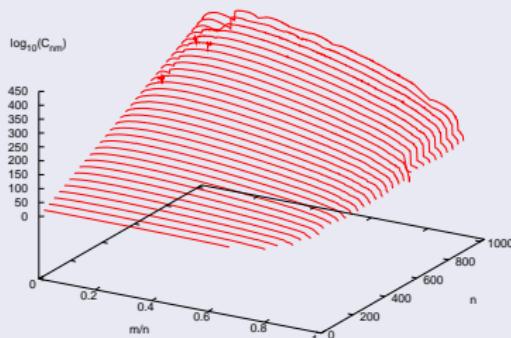
Example: 2dim ISAW simulation up to $N = 1024$

Total sample size: 180,000,000



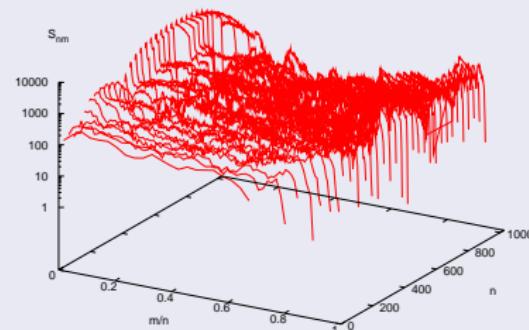
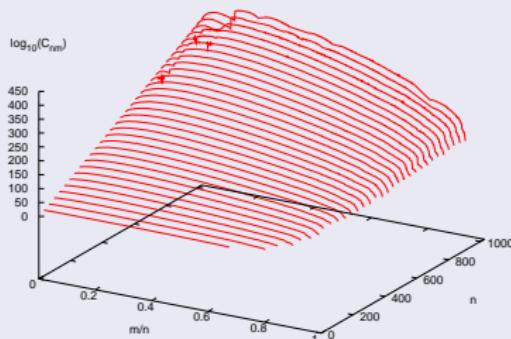
Example: 2dim ISAW simulation up to $N = 1024$

Total sample size: 190,000,000



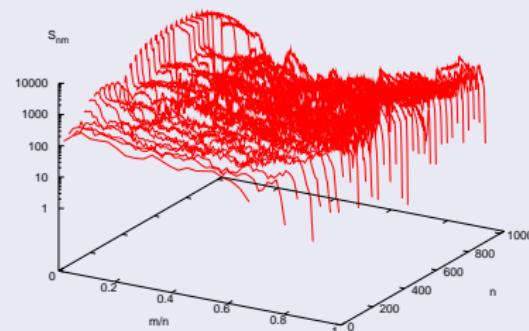
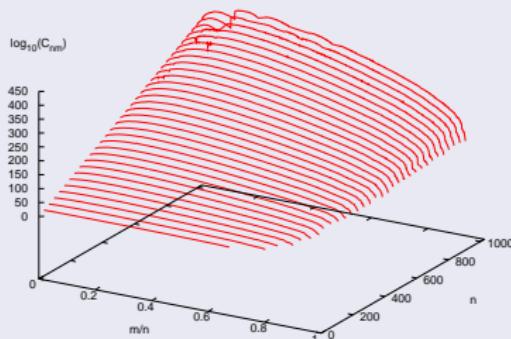
Example: 2dim ISAW simulation up to $N = 1024$

Total sample size: 200,000,000



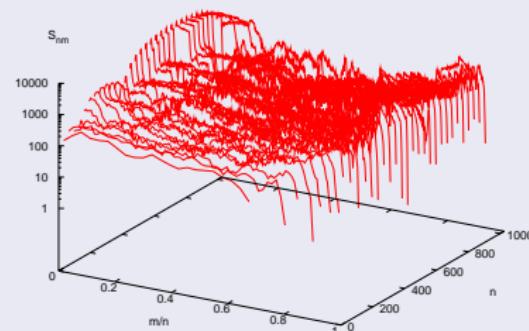
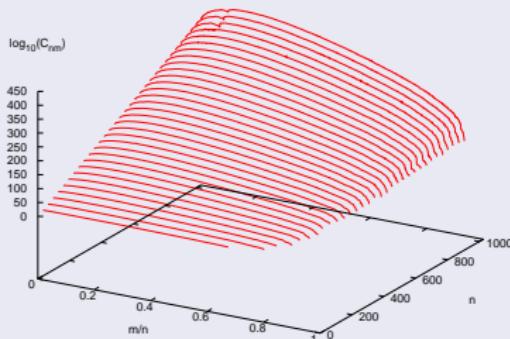
Example: 2dim ISAW simulation up to $N = 1024$

Total sample size: 210,000,000



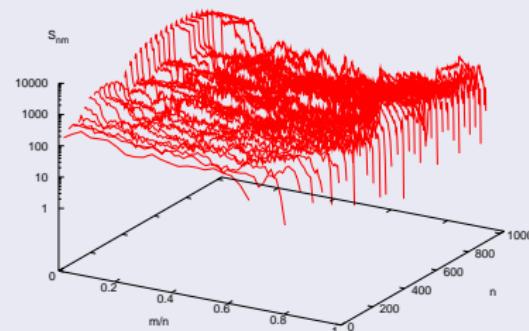
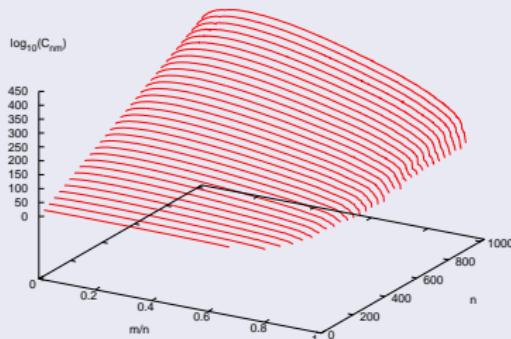
Example: 2dim ISAW simulation up to $N = 1024$

Total sample size: 220,000,000



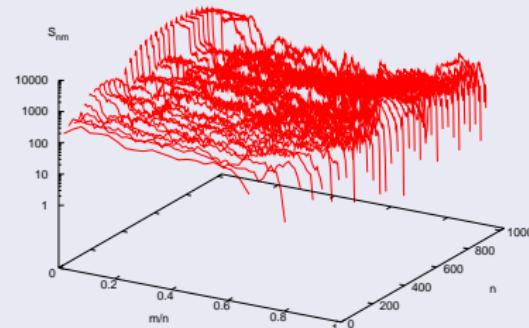
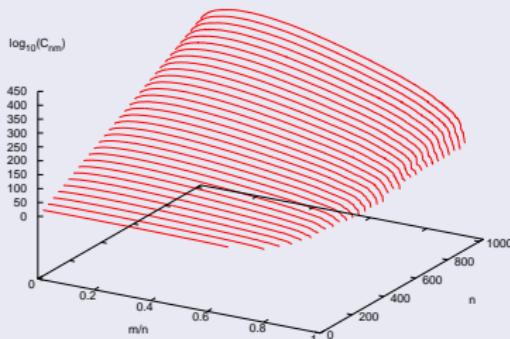
Example: 2dim ISAW simulation up to $N = 1024$

Total sample size: 230,000,000



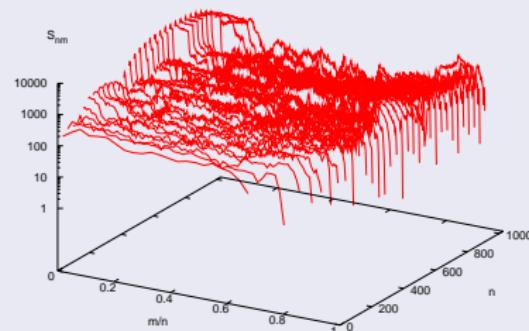
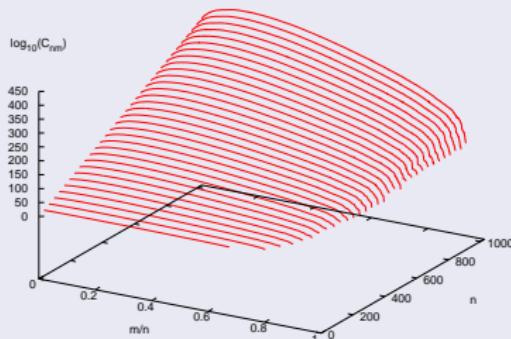
Example: 2dim ISAW simulation up to $N = 1024$

Total sample size: 240,000,000



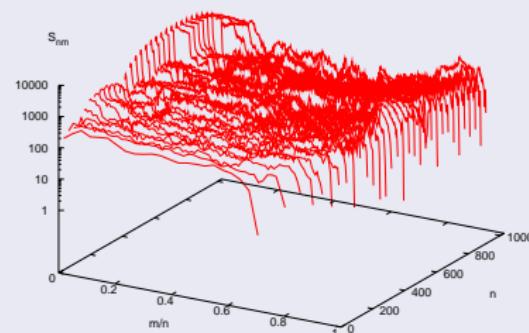
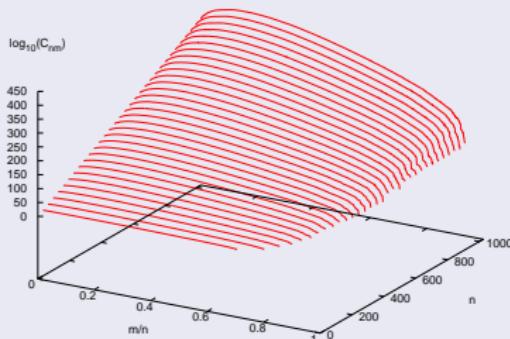
Example: 2dim ISAW simulation up to $N = 1024$

Total sample size: 250,000,000



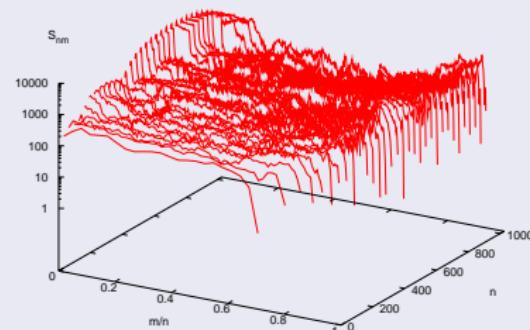
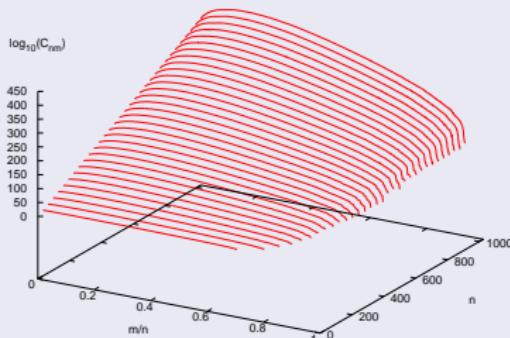
Example: 2dim ISAW simulation up to $N = 1024$

Total sample size: 260,000,000



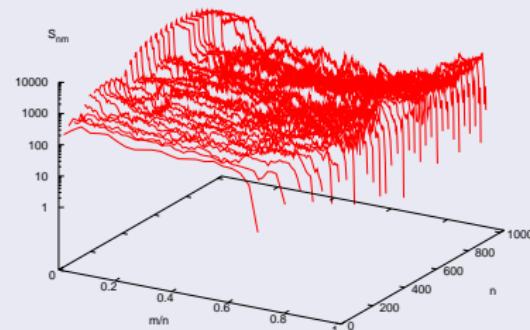
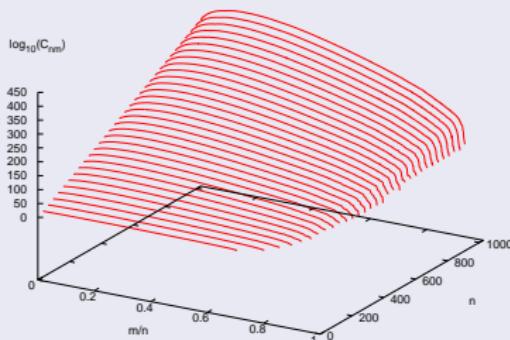
Example: 2dim ISAW simulation up to $N = 1024$

Total sample size: 270,000,000



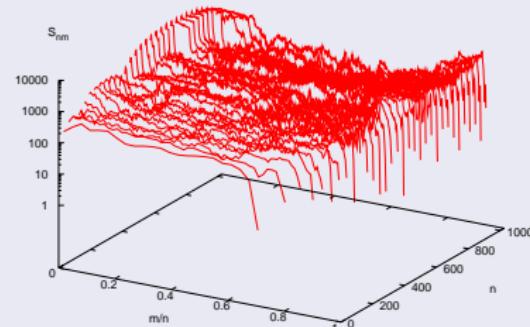
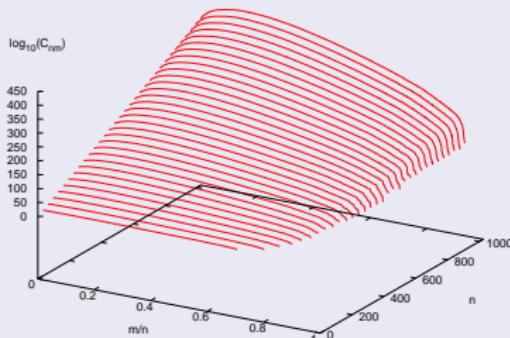
Example: 2dim ISAW simulation up to $N = 1024$

Total sample size: 280,000,000



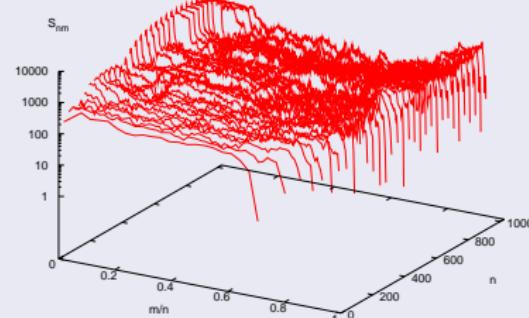
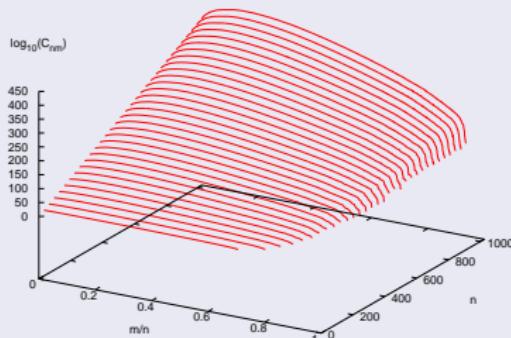
Example: 2dim ISAW simulation up to $N = 1024$

Total sample size: 290,000,000



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

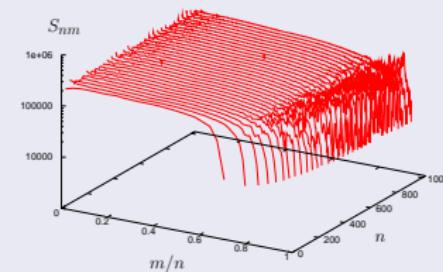
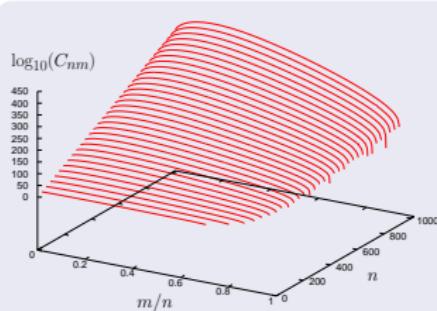
Total sample size: 300,000,000



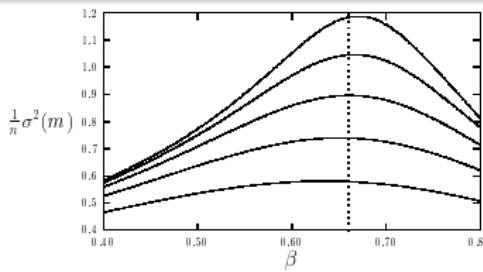
ISAW simulations

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

1 Introduction

- A Zoology of Growth Algorithms
- Which Algorithm is Best?
- ISAW - the canonical lattice model

2 The 'Old' Algorithms

- Rosenbluth²
- PERM
- Multicanonical PERM
- FlatPERM

3 The 'New' Algorithms

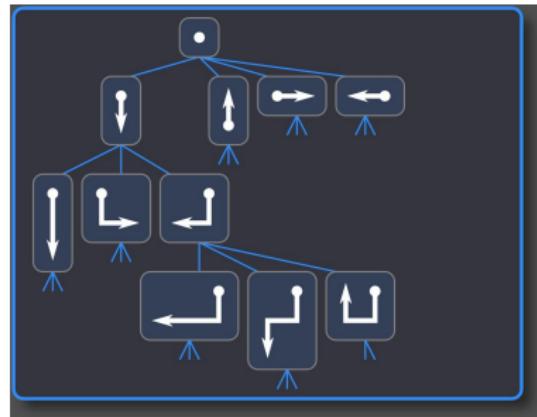
- New Ideas
- GARM
- GAS

4 Conclusion

- Outlook
- Thanks

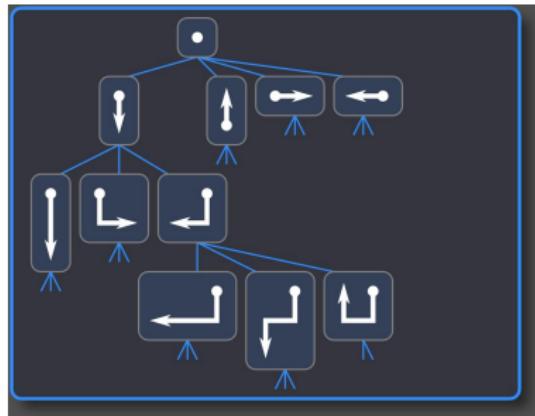
Revisit Rosenbluth Sampling

- Each configuration grown uniquely by appending edges to endpoint



Revisit Rosenbluth Sampling

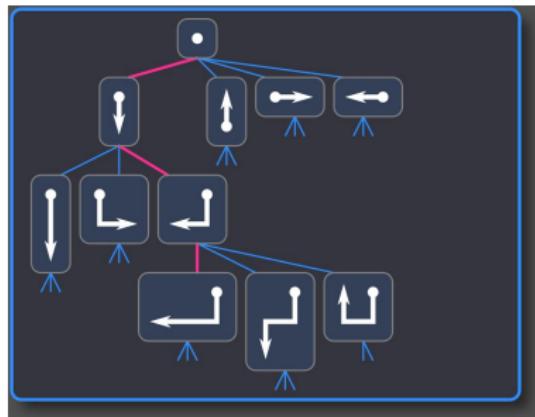
- Each configuration grown uniquely by appending edges to endpoint



- Generating tree
 - Each node of tree is a configuration

Revisit Rosenbluth Sampling

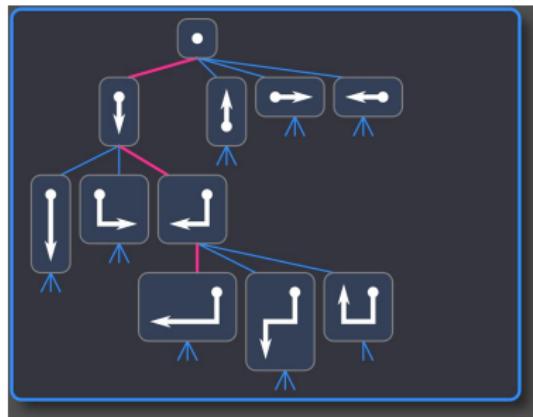
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Revisit Rosenbluth Sampling

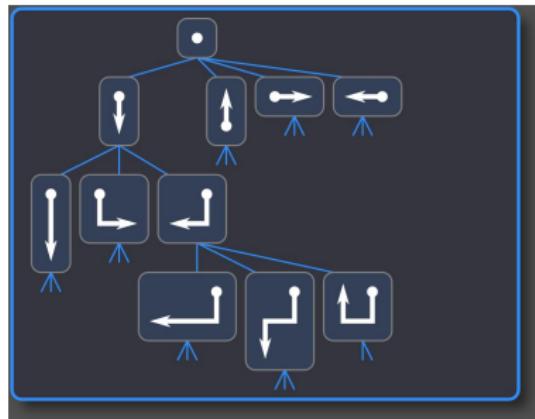
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 - Sample by growing unique “sample path” down the tree
 - The weight of sample path is $W(\varphi) = \prod_{k < N} a_k(\varphi)$

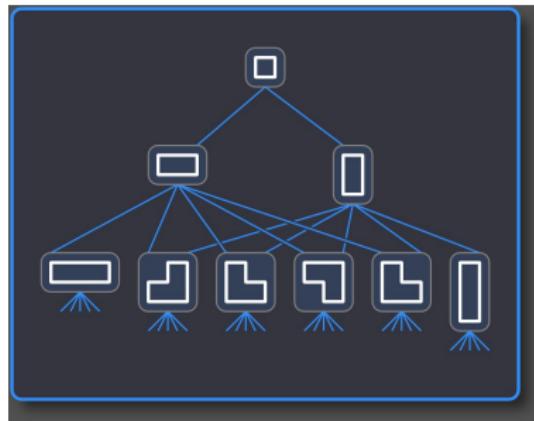
From Generating Trees to Generating Graphs

- Unique way to construct walks



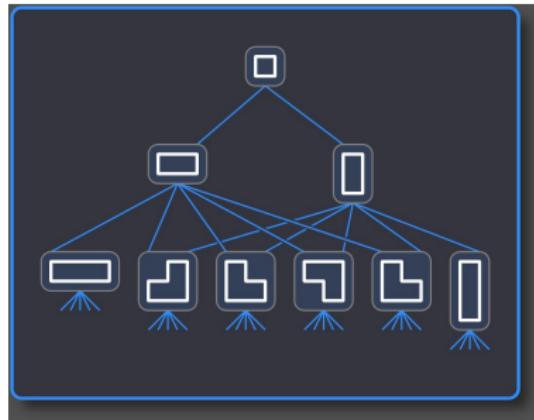
From Generating Trees to Generating Graphs

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



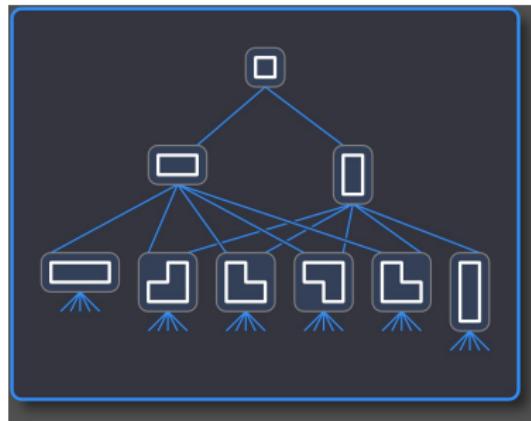
From Generating Trees to Generating Graphs

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



From Generating Trees to Generating Graphs

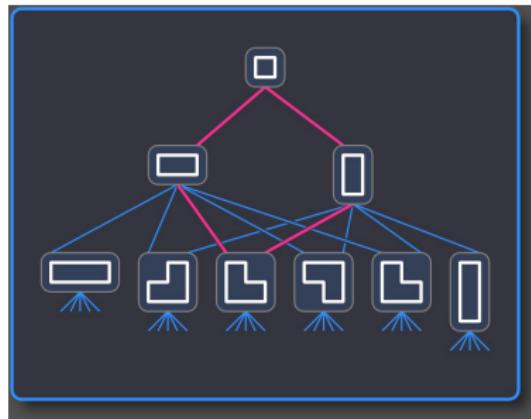
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- No obvious unique way to construct polygons
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- Generating graph
 - Each node of graph is a configuration

From Generating Trees to Generating Graphs

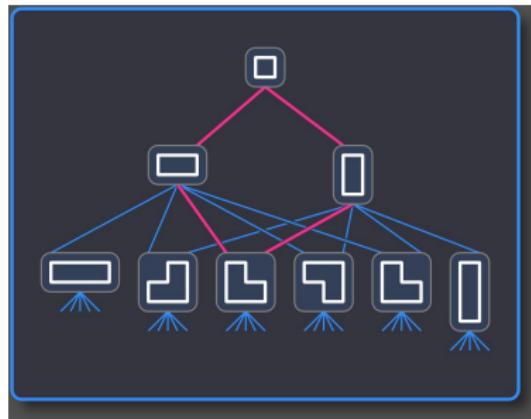
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- No obvious unique way to construct polygons
- Can we generalize from generating trees?



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

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- 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

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

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 - Thermal GARM
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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

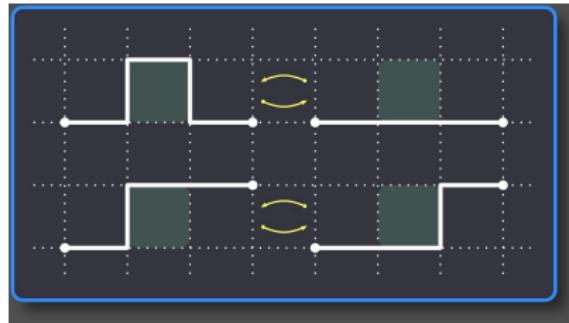
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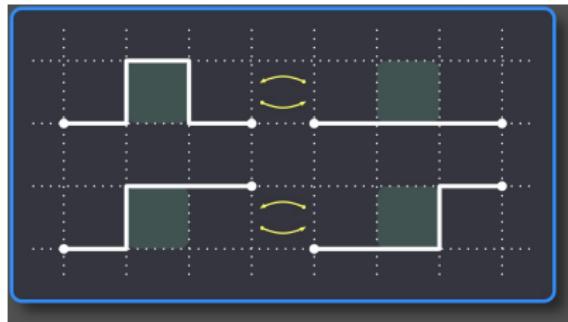
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- Moves from the BFACF algorithm

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

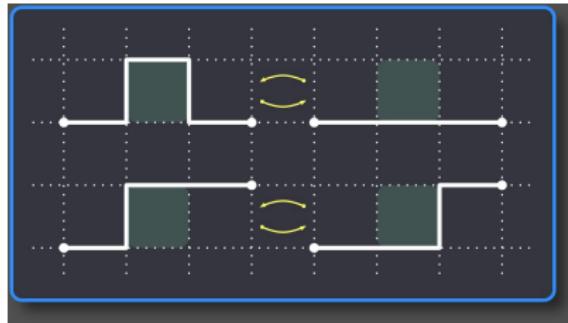
C Aragão de Carvalho, S Caracciolo and J Fröhlich, Nucl Phys B 215 (1983) 209

- Ergodic on each knot-type

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

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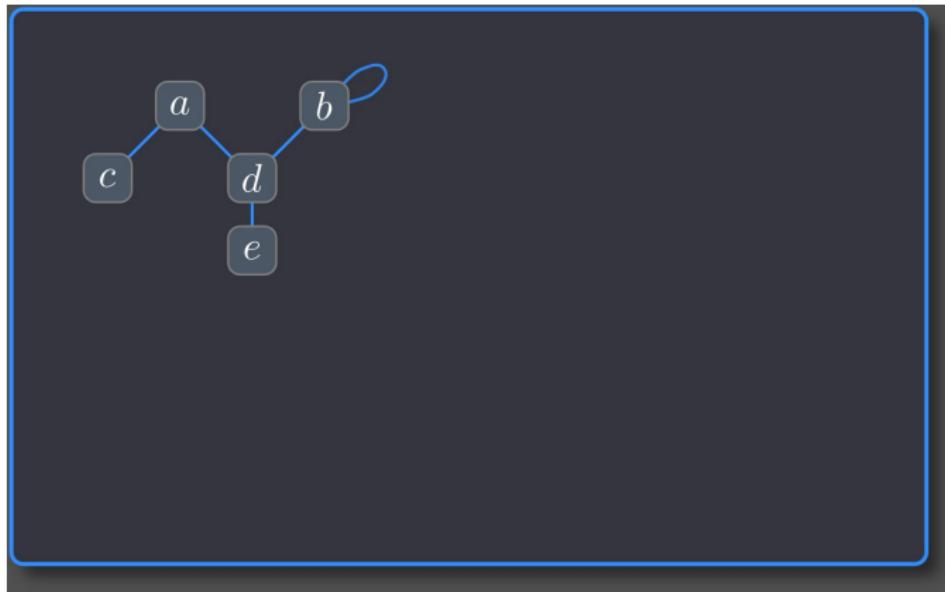
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- Generating graph still exists, but now sample paths are not directed
- Need to “redirect” the graph

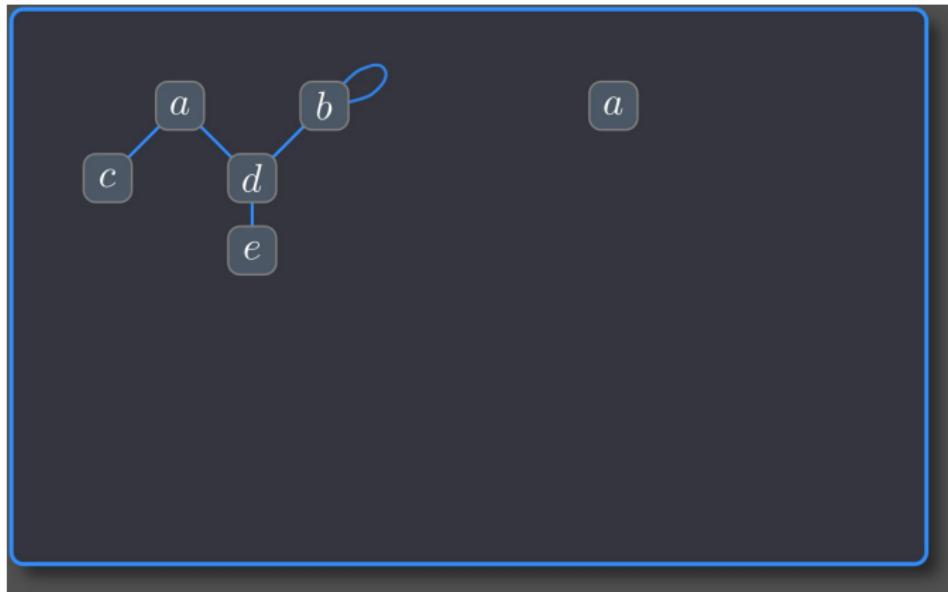
Derivative graph

- Take an arbitrary generating graph



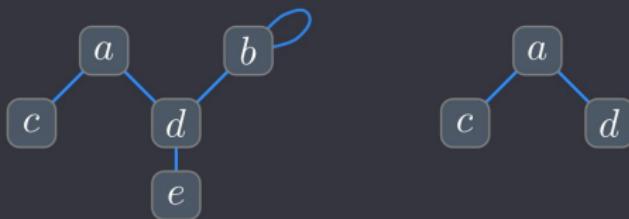
Derivative graph

- Copy the initial vertex



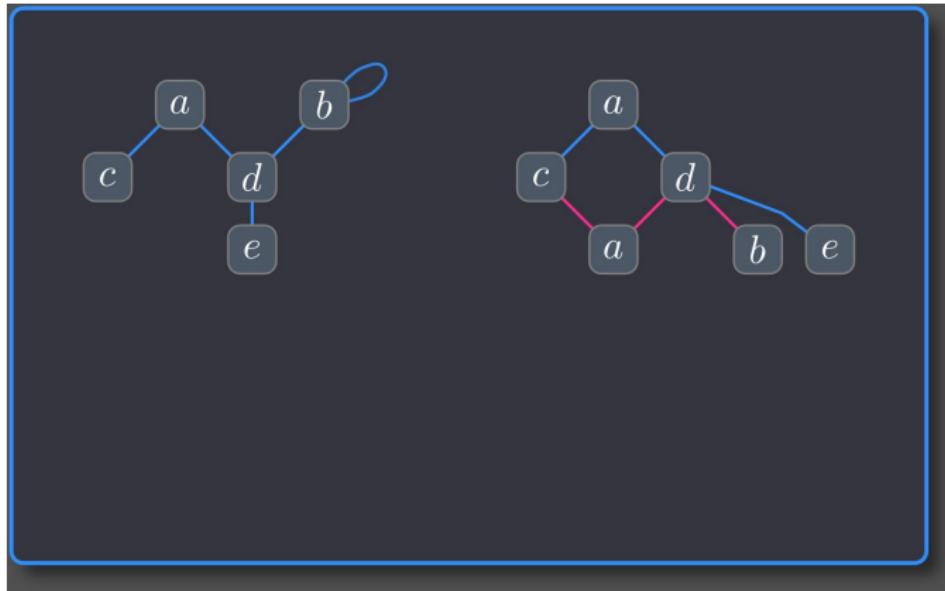
Derivative graph

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



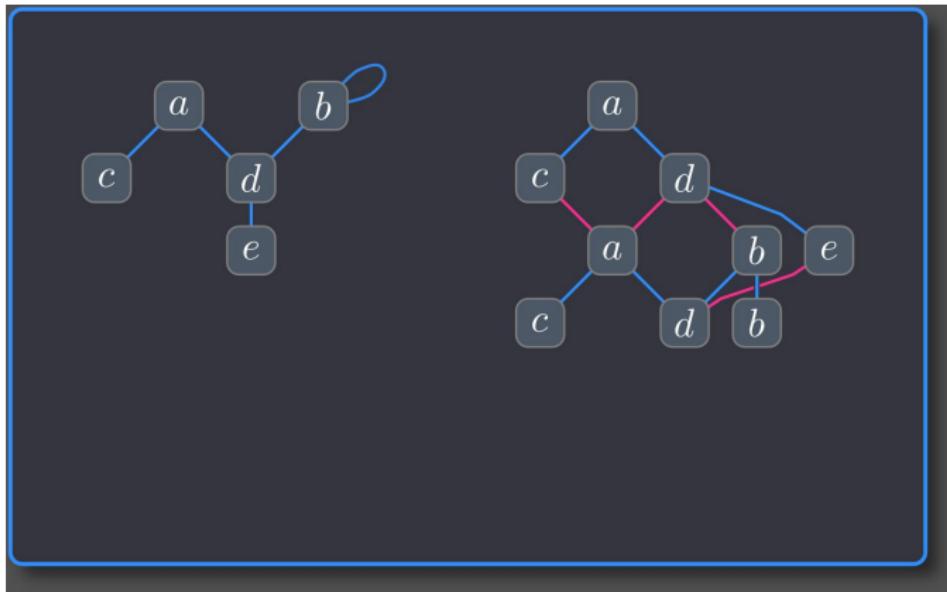
Derivative graph

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



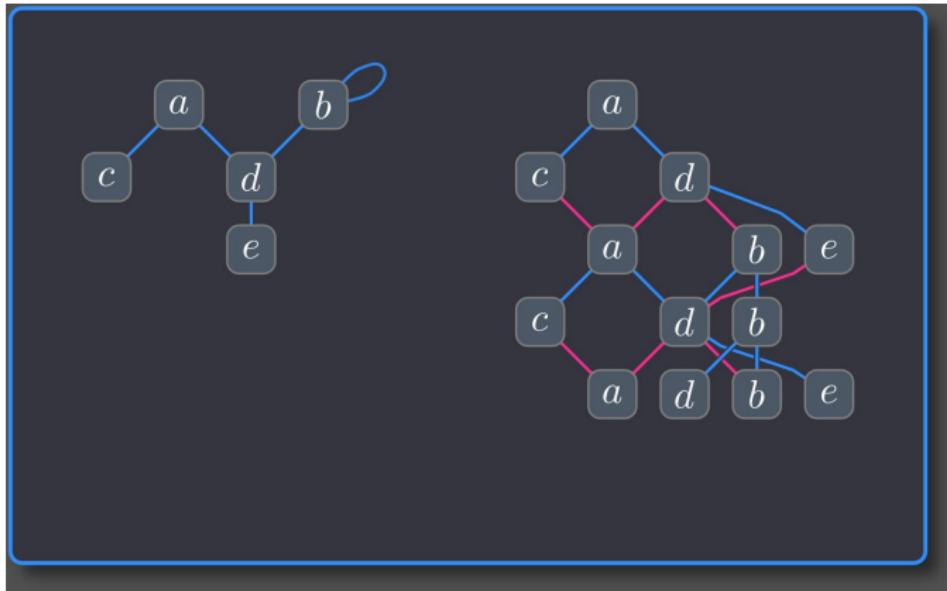
Derivative graph

- Keep adding new rows in this way



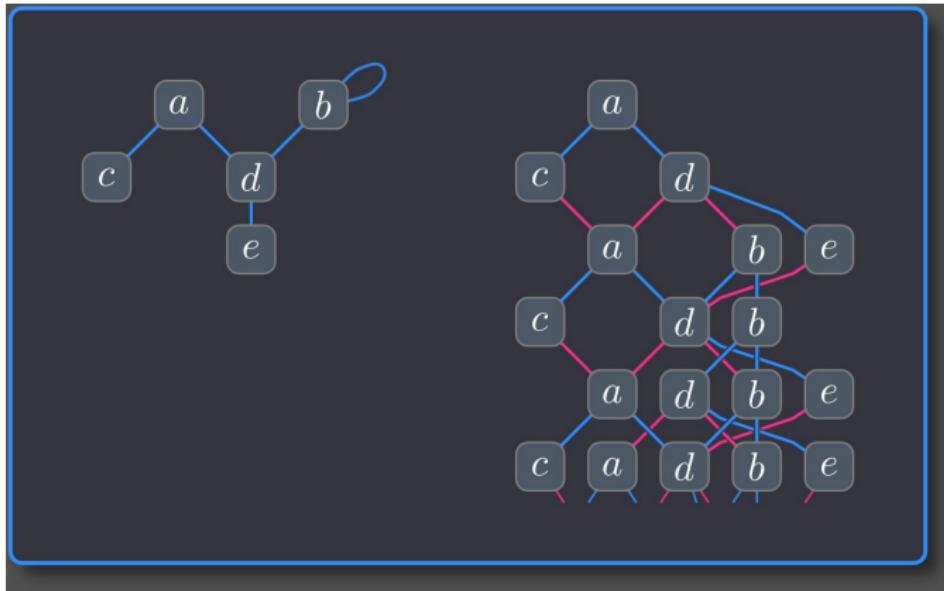
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Derivative graph

- This gives the “derivative graph”



From GARM to GAS

GAS = Generalized Atmospheric Sampling = Grow And Shrink

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

- Do GARM sampling on the derivative graph

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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

- Known exactly for trefoil $C_{24}(3_1) = 3328$

Y Diao, JKTR 2 (1993) 413

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- Run GAS with BFACF moves and extract the minimal polygons

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- Resulting numbers

see also R Scharein et al, J Phys A 42 (2009) 475006

$$C_{24}(3_1) = 3328$$

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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

1 Introduction

- A Zoology of Growth Algorithms
- Which Algorithm is Best?
- ISAW - the canonical lattice model

2 The 'Old' Algorithms

- Rosenbluth²
- PERM
- Multicanonical PERM
- FlatPERM

3 The 'New' Algorithms

- New Ideas
- GARM
- GAS

4 Conclusion

- Outlook
- Thanks

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 (Dresden)
- Aleks Owzcarek (Melbourne)
- Andrew Rechnitzer (Vancouver)

- Buks van Rensburg (Toronto)

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

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- Royal Society

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