PERM and all that

a comparison of growth algorithms

Thomas Prellberg

School of Mathematical Sciences
Queen Mary, University of London

Statistical Mechanics Study Group
November 11, 2010

Topic Outline

Outline

Acronyms and Algorithms

These days there exists a zoo of growth algorithms

- 1997: PERM
- 2003: nPERMss/nPERMis
- 2003: Multicanonical PERM
- 2004: flatPERM
- 2008: GARM/flatGARM
- 2009: GAS
- 201?: flatGAS

Acronyms and Algorithms

These days there exists a zoo of growth algorithms

- 1997: PERM
- 2003: nPERMss/nPERMis
- 2003: Multicanonical PERM
- 2004: flatPERM
- 2008: GARM/flatGARM
- 2009: GAS
- 201?: flatGAS

All of this is based on

- 1955: Rosenbluth & Rosenbluth

Which Algorithm is Best?

Which Algorithm is Best?

I don’t really know.

Which Algorithm is Best?

I don't really know.

or, perhaps slightly better,

It depends ...

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

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

- The flatPERM algorithm (and some pedagogical applications):
  - T. Prellberg and J. Krawczyk, "Flat histogram version of the pruned and enriched Rosenbluth method," Phys. Rev. Lett. 92 (2004) 120602
  - T. Prellberg, J. Krawczyk, and A. Rechnitzer, "Polymer simulations with a flat histogram stochastic growth algorithm," Computer Simulation Studies in Condensed Matter Physics XVII, pages 122-135, Springer Verlag, 2006

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

- The flatPERM algorithm (and some pedagogical applications):
  - T. Prellberg and J. Krawczyk, "Flat histogram version of the pruned and enriched Rosenbluth method," Phys. Rev. Lett. 92 (2004) 120602
  - T. Prellberg, J. Krawczyk, and A. Rechnitzer, "Polymer simulations with a flat histogram stochastic growth algorithm," Computer Simulation Studies in Condensed Matter Physics XVII, pages 122-135, Springer Verlag, 2006
- Bulk vs surface:
  - J. Krawczyk, T. Prellberg, A. L. Owczarek, and A. Rechnitzer, "Stretching of a chain polymer adsorbed at a surface," Journal of Statistical Mechanics: theory and experiment, JSTAT (2004) P10004
  - J. Krawczyk, A. L. Owczarek, T. Prellberg, and A. Rechnitzer, "Layering transitions for adsorbing polymers in poor solvents," Europhys. Lett. 70 (2005) 726-732
  - J. Krawczyk, A. L. Owczarek, T. Prellberg, and A. Rechnitzer, "Pulling absorbing and collapsing polymers off a surface," Journal of Statistical Mechanics: theory and experiment, JSTAT (2005) P05008
  - A. L. Owczarek, A. Rechnitzer, J. Krawczyk, and T. Prellberg, "On the location of the surface-attached globule phase in collapsing polymers," J. Phys. A 40 (2007) 13257-13267

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

- The flatPERM algorithm (and some pedagogical applications):
  - T. Prellberg and J. Krawczyk, "Flat histogram version of the pruned and enriched Rosenbluth method," Phys. Rev. Lett. 92 (2004) 120602
  - T. Prellberg, J. Krawczyk, and A. Rechnitzer, "Polymer simulations with a flat histogram stochastic growth algorithm," Computer Simulation Studies in Condensed Matter Physics XVII, pages 122-135, Springer Verlag, 2006
- Bulk vs surface:
  - J. Krawczyk, T. Prellberg, A. L. Owczarek, and A. Rechnitzer, "Stretching of a chain polymer adsorbed at a surface," Journal of Statistical Mechanics: theory and experiment, JSTAT (2004) P10004
  - J. Krawczyk, A. L. Owczarek, T. Prellberg, and A. Rechnitzer, "Layering transitions for adsorbing polymers in poor solvents," Europhys. Lett. 70 (2005) 726-732
  - J. Krawczyk, A. L. Owczarek, T. Prellberg, and A. Rechnitzer, "Pulling absorbing and collapsing polymers off a surface," Journal of Statistical Mechanics: theory and experiment, JSTAT (2005) P05008
  - A. L. Owczarek, A. Rechnitzer, J. Krawczyk, and T. Prellberg, "On the location of the surface-attached globule phase in collapsing polymers," J. Phys. A 40 (2007) 13257-13267
- Hydrogen-bond type interactions:
  - J. Krawczyk, A. L. Owczarek, T. Prellberg, and A. Rechnitzer, "A Lattice Model for Parallel and Orthogonal Beta-Sheets using Hydrogen-Like Bonding," Phys. Rev. E 76 (2007) 051904
  - J. Krawczyk, A. L. Owczarek, and T. Prellberg, "The competition of hydrogen-like and isotropic interactions in polymer collapse," Journal of Statistical Mechanics: theory and experiment, JSTAT (2007) P09016
  - J. Krawczyk, A. L. Owczarek, and T. Prellberg, "Semi-flexible hydrogen-bonded and non-hydrogen bonded lattice polymers," Physica A 388 (2009) 104
  - J. Krawczyk, A. L. Owczarek, and T. Prellberg, "'A Semi-flexible attracting-segment model of two-dimensional polymer collapse," Physica A 389 (2010) 1619

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

- The flatPERM algorithm (and some pedagogical applications):
  - T. Prellberg and J. Krawczyk, "Flat histogram version of the pruned and enriched Rosenbluth method," Phys. Rev. Lett. 92 (2004) 120602
  - T. Prellberg, J. Krawczyk, and A. Rechnitzer, "Polymer simulations with a flat histogram stochastic growth algorithm," Computer Simulation Studies in Condensed Matter Physics XVII, pages 122-135, Springer Verlag, 2006
- Bulk vs surface:
  - J. Krawczyk, T. Prellberg, A. L. Owczarek, and A. Rechnitzer, "Stretching of a chain polymer adsorbed at a surface," Journal of Statistical Mechanics: theory and experiment, JSTAT (2004) P10004
  - J. Krawczyk, A. L. Owczarek, T. Prellberg, and A. Rechnitzer, "Layering transitions for adsorbing polymers in poor solvents," Europhys. Lett. 70 (2005) 726-732
  - J. Krawczyk, A. L. Owczarek, T. Prellberg, and A. Rechnitzer, "Pulling absorbing and collapsing polymers off a surface," Journal of Statistical Mechanics: theory and experiment, JSTAT (2005) P05008
  - A. L. Owczarek, A. Rechnitzer, J. Krawczyk, and T. Prellberg, "On the location of the surface-attached globule phase in collapsing polymers," J. Phys. A 40 (2007) 13257-13267
- Hydrogen-bond type interactions:
  - J. Krawczyk, A. L. Owczarek, T. Prellberg, and A. Rechnitzer, "A Lattice Model for Parallel and Orthogonal Beta-Sheets using Hydrogen-Like Bonding," Phys. Rev. E 76 (2007) 051904
  - J. Krawczyk, A. L. Owczarek, and T. Prellberg, "The competition of hydrogen-like and isotropic interactions in polymer collapse," Journal of Statistical Mechanics: theory and experiment, JSTAT (2007) P09016
  - J. Krawczyk, A. L. Owczarek, and T. Prellberg, "Semi-flexible hydrogen-bonded and non-hydrogen bonded lattice polymers," Physica A 388 (2009) 104
  - J. Krawczyk, A. L. Owczarek, and T. Prellberg, "'A Semi-flexible attracting-segment model of two-dimensional polymer collapse," Physica A 389 (2010) 1619
- 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 November 10th,

- PERM (1997): 248 citations
- nPERM (2003): 66 citations
- Multicanonical PERM (2003): 47 citations
- flatPERM (2004): 37 citations
- GARM/flatGARM (2008): 4 citations
- GAS/flatGAS (2009): 2 citation

Putting Things into Perspective

As of November 10th,

- PERM (1997): 248 citations
- nPERM (2003): 66 citations
- Multicanonical PERM (2003): 47 citations
- flatPERM (2004): 37 citations
- GARM/flatGARM (2008): 4 citations
- GAS/flatGAS (2009): 2 citation

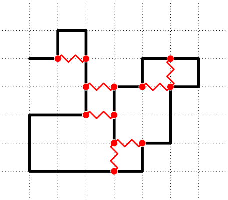
This should be compared with e.g.

- Umbrella Sampling (1977): 1040 citations
- Multicanonical Sampling (1992): 778 citations
- Wang-Landau Sampling (2001): 728 citations

ISAW - the canonical lattice model

Interacting Self-Avoiding Walk (ISAW)

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



ISAW - the canonical lattice model

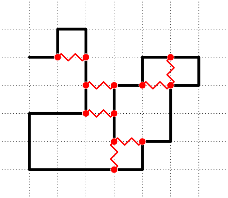
Interacting Self-Avoiding Walk (ISAW)

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

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



ISAW - the canonical lattice model

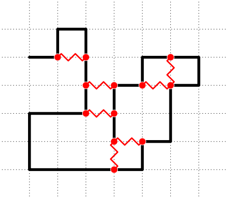
Interacting Self-Avoiding Walk (ISAW)

- 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 $E_N(\varphi) = m(\varphi)\epsilon$

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

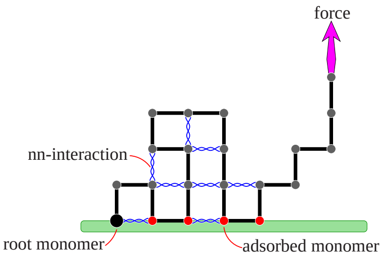


Thermodynamic Limit for a dilute solution:

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

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)

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)

Rosenbluth Sampling (for SAW)

- Choose starting vertex at the origin
- Draw one of the unoccupied neighbouring sites uniformly at random
- If there is none, reject entire walk and start again
- If unoccupied, accept and repeat (up to some maximal walk length)

MN Rosenbluth and AW Rosenbluth, J Chem Phys 23 (1955) 356

JM Hammersley J M and KW Morton, J R Stat Soc B 16 (1954) 23

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)

Rosenbluth Sampling (for SAW)

- Choose starting vertex at the origin
- Draw one of the unoccupied neighbouring sites uniformly at random
- If there is none, reject entire walk and start again
- If unoccupied, accept and repeat (up to some maximal walk length)

MN Rosenbluth and AW Rosenbluth, J Chem Phys 23 (1955) 356

JM Hammersley J M and KW Morton, J R Stat Soc B 16 (1954) 23

(Augment with Importance Sampling for ISAW)

Rosenbluth versus Simple Sampling

Simple Sampling

- Large attrition, so very inefficient
- Uniform, independent samples

Rosenbluth versus Simple Sampling

Simple Sampling

- Large attrition, so very inefficient
- Uniform, independent samples

Rosenbluth Sampling

- Less attrition (but still exponential)

Rosenbluth versus Simple Sampling

Simple Sampling

- Large attrition, so very inefficient
- Uniform, independent samples

Rosenbluth Sampling

- Less attrition (but still exponential)
- Non-uniform sampling

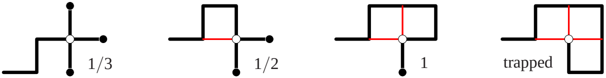
Rosenbluth versus Simple Sampling

Simple Sampling

- Large attrition, so very inefficient
- Uniform, independent samples

Rosenbluth Sampling

- Less attrition (but still exponential)
- Non-uniform sampling



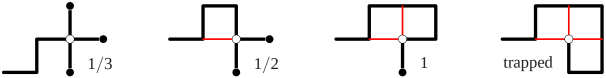
Rosenbluth versus Simple Sampling

Simple Sampling

- Large attrition, so very inefficient
- Uniform, independent samples

Rosenbluth Sampling

- Less attrition (but still exponential)
- Non-uniform sampling



- 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

- Modify Rosenbluth Sampling by controlling the weights $W_\beta(\varphi) = W(\varphi)e^{-\beta E(\varphi)}$

PERM: "Go with the Winners"

PERM = Pruned and Enriched Rosenbluth Method

P Grassberger, Phys Rev E 56 (1997) 3682

- Modify Rosenbluth Sampling by controlling the weights $W_\beta(\varphi) = W(\varphi)e^{-\beta E(\varphi)}$
  1. Combat large weights by Enrichment:
     Weight $W_\beta(\varphi)$ too large $\Rightarrow$ make copies of the walk

PERM: "Go with the Winners"

PERM = Pruned and Enriched Rosenbluth Method

P Grassberger, Phys Rev E 56 (1997) 3682

- Modify Rosenbluth Sampling by controlling the weights $W_\beta(\varphi) = W(\varphi)e^{-\beta E(\varphi)}$
  1. Combat large weights by Enrichment:
     Weight $W_\beta(\varphi)$ too large $\Rightarrow$ make copies of the walk
  2. Combat small weights by Pruning:
     Weight $W_\beta(\varphi)$ too small $\Rightarrow$ remove walks occasionally

PERM: "Go with the Winners"

PERM = Pruned and Enriched Rosenbluth Method

P Grassberger, Phys Rev E 56 (1997) 3682

- Modify Rosenbluth Sampling by controlling the weights $W_\beta(\varphi) = W(\varphi)e^{-\beta E(\varphi)}$
  1. Combat large weights by Enrichment:
     Weight $W_\beta(\varphi)$ too large $\Rightarrow$ make copies of the walk
  2. Combat small weights by Pruning:
     Weight $W_\beta(\varphi)$ too small $\Rightarrow$ remove walks occasionally
- Parameters: upper thresholds T_N and t_N, pruning probability q

PERM: "Go with the Winners"

PERM = Pruned and Enriched Rosenbluth Method

P Grassberger, Phys Rev E 56 (1997) 3682

- Modify Rosenbluth Sampling by controlling the weights $W_\beta(\varphi) = W(\varphi)e^{-\beta E(\varphi)}$
  1. Combat large weights by Enrichment:
     Weight $W_\beta(\varphi)$ too large $\Rightarrow$ make copies of the walk
  2. Combat small weights by Pruning:
     Weight $W_\beta(\varphi)$ too small $\Rightarrow$ remove walks occasionally
- Parameters: upper thresholds T_N and t_N, pruning probability q
- Adapt T_N and t_N during simulation, keep T_N/t_N roughly constant

PERM: "Go with the Winners"

PERM = Pruned and Enriched Rosenbluth Method

P Grassberger, Phys Rev E 56 (1997) 3682

- Modify Rosenbluth Sampling by controlling the weights $W_\beta(\varphi) = W(\varphi)e^{-\beta E(\varphi)}$
  1. Combat large weights by Enrichment:
     Weight $W_\beta(\varphi)$ too large $\Rightarrow$ make copies of the walk
  2. Combat small weights by Pruning:
     Weight $W_\beta(\varphi)$ too small $\Rightarrow$ remove walks occasionally
- Parameters: upper thresholds T_N and t_N, pruning probability q
- Adapt T_N and t_N during simulation, keep T_N/t_N roughly constant

nPERM = New PERM

HP Hsu et al, Phys Rev E 68 (2003) 021113

- Significant improvement: when enriching, force *distinct* copies

PERM: "Go with the Winners"

PERM = Pruned and Enriched Rosenbluth Method

P Grassberger, Phys Rev E 56 (1997) 3682

- Modify Rosenbluth Sampling by controlling the weights $W_\beta(\varphi) = W(\varphi)e^{-\beta E(\varphi)}$
  1. Combat large weights by Enrichment:
     Weight $W_\beta(\varphi)$ too large $\Rightarrow$ make copies of the walk
  2. Combat small weights by Pruning:
     Weight $W_\beta(\varphi)$ too small $\Rightarrow$ remove walks occasionally
- Parameters: upper thresholds T_N and t_N, pruning probability q
- Adapt T_N and t_N during simulation, keep T_N/t_N roughly constant

nPERM = New PERM

HP Hsu et al, Phys Rev E 68 (2003) 021113

- Significant improvement: when enriching, force *distinct* copies

(Augment with Importance Sampling: nPERMis)

Multicanonical PERM

- Sample the density of states with respect to an umbrella density

GM Torrie and JP Valleau J Comput Phys 23 (1977) 187

Multicanonical PERM

- Sample the density of states with respect to an umbrella density

GM Torrie and JP Valleau J Comput Phys 23 (1977) 187

- For uniform sampling of the density of states $C_{N,m}$, we need to use weights

$$W_{flat}(\varphi) = W(\varphi)/C_{N,m}$$

Multicanonical PERM

- Sample the density of states with respect to an umbrella density

GM Torrie and JP Valleau J Comput Phys 23 (1977) 187

- For uniform sampling of the density of states $C_{N,m}$, we need to use weights

$$W_{flat}(\varphi) = W(\varphi)/C_{N,m}$$

- As $C_{N,m}$ is unknown, compute iteratively an approximation $C^{approx}_{N,m}$ and perform a final run with

$$W^{approx}_{flat}(\varphi) = W(\varphi)/C^{approx}_{N,m}$$

(Multicanonical Method)

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

Multicanonical PERM

- Sample the density of states with respect to an umbrella density

GM Torrie and JP Valleau J Comput Phys 23 (1977) 187

- For uniform sampling of the density of states $C_{N,m}$, we need to use weights

$$W_{flat}(\varphi) = W(\varphi)/C_{N,m}$$

- As $C_{N,m}$ is unknown, compute iteratively an approximation $C_{N,m}^{approx}$ and perform a final run with

$$W_{flat}^{approx}(\varphi) = W(\varphi)/C_{N,m}^{approx}$$

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

The resulting algorithm is called multicanonical PERM

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

Revisit PERM

- Exact enumeration: choose all a continuations with weight 1

Revisit PERM

- Exact enumeration: choose all a continuations with weight 1
- Rosenbluth sampling: chose one continuation with weight a

Revisit PERM

- Exact enumeration: choose all a continuations with weight 1
- Rosenbluth sampling: chose one continuation with weight a

View Rosenbluth Sampling as *approximate enumeration*

Revisit PERM

- Exact enumeration: choose all a continuations with weight 1
- Rosenbluth sampling: chose one continuation with weight a

View Rosenbluth Sampling as *approximate enumeration*

- If an N step walk φ gets assigned a weight $W(\varphi) = \prod_{k<N} a_k(\varphi)$ then S walks with weights $W(\varphi_i)$ give an estimate

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

Revisit PERM

- Exact enumeration: choose all a continuations with weight 1
- Rosenbluth sampling: chose one continuation with weight a

View Rosenbluth Sampling as *approximate enumeration*

- If an N step walk φ gets assigned a weight $W(\varphi) = \prod_{k<N} a_k(\varphi)$ then S walks with weights $W(\varphi_i)$ give an estimate

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

- Add pruning/enrichment with respect to the ratio

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

Revisit PERM

- Exact enumeration: choose all a continuations with weight 1
- Rosenbluth sampling: chose one continuation with weight a

View Rosenbluth Sampling as *approximate enumeration*

- If an N step walk φ gets assigned a weight $W(\varphi) = \prod_{k<N} a_k(\varphi)$ then S walks with weights $W(\varphi_i)$ give an estimate

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

- Add pruning/enrichment with respect to the ratio

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

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

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

From PERM to flatPERM

An important observation:

- Number of samples generated for each N is roughly constant
- We have a $\boxed{\text{flat histogram algorithm}}$ in system size

From PERM to flatPERM

An important observation:

- Number of samples generated for each N is roughly constant
- We have a $\boxed{\text{flat histogram algorithm}}$ in system size

flatPERM = flat histogram PERM

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

From PERM to flatPERM

An important observation:

- Number of samples generated for each N is roughly constant
- We have a $\boxed{\text{flat histogram algorithm}}$ in system size

flatPERM = flat histogram PERM

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

- PERM: estimate number of walks C_N
    - $C_N^{est} = \langle W \rangle_N$
    - $r = W(\varphi)/C_N^{est}$

From PERM to flatPERM

An important observation:

- Number of samples generated for each N is roughly constant
- We have a $\boxed{\text{flat histogram algorithm}}$ in system size

flatPERM = flat histogram PERM

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

- PERM: estimate number of walks C_N
  - $C_N^{est} = \langle W \rangle_N$
  - $r = W(\varphi)/C_N^{est}$
- PERM at finite temperature: estimate partition function $Z_N(\beta)$
  - $Z_N^{est}(\beta) = \langle W \exp(-\beta E) \rangle_N$
  - $r = W(\varphi) \exp(-\beta E(\varphi))/Z_N^{est}(\beta)$

From PERM to flatPERM

An important observation:

- Number of samples generated for each N is roughly constant
- We have a $\boxed{\text{flat histogram algorithm}}$ in system size

flatPERM = flat histogram PERM

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

- PERM: estimate number of walks C_N
  - $C_N^{est} = \langle W \rangle_N$
  - $r = W(\varphi)/C_N^{est}$
- PERM at finite temperature: estimate partition function $Z_N(\beta)$
  - $Z_N^{est}(\beta) = \langle W \exp(-\beta E) \rangle_N$
  - $r = W(\varphi) \exp(-\beta E(\varphi))/Z_N^{est}(\beta)$
- flatPERM: estimate density of states $C_{N,\vec{m}}$
  - $C_{N,\vec{m}}^{est} = \langle W \rangle_{N,\vec{m}}$
  - $r = W(\varphi)/C_{N,\vec{m}}^{est}$

From PERM to flatPERM

An important observation:

- Number of samples generated for each N is roughly constant
- We have a $\boxed{\text{flat histogram algorithm}}$ in system size

flatPERM = flat histogram PERM

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

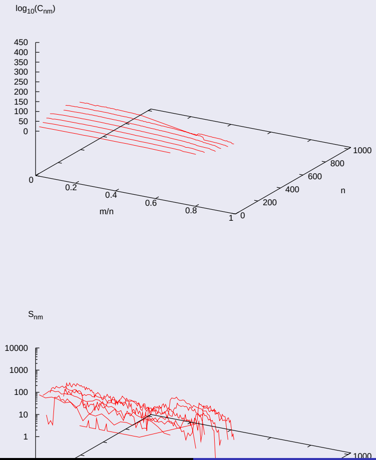
- PERM: estimate number of walks C_N
  - $C_N^{est} = \langle W \rangle_N$
  - $r = W(\varphi)/C_N^{est}$
- PERM at finite temperature: estimate partition function $Z_N(\beta)$
  - $Z_N^{est}(\beta) = \langle W \exp(-\beta E) \rangle_N$
  - $r = W(\varphi) \exp(-\beta E(\varphi))/Z_N^{est}(\beta)$
- flatPERM: estimate density of states $C_{N,\vec{m}}$
  - $C_{N,\vec{m}}^{est} = \langle W \rangle_{N,\vec{m}}$
  - $r = W(\varphi)/C_{N,\vec{m}}^{est}$
- 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

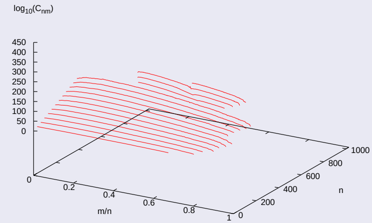
Example: 2dim ISAW simulation up to $N = 1024$

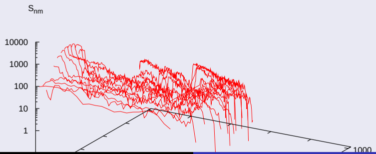
Total sample size: $1,000,000$



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

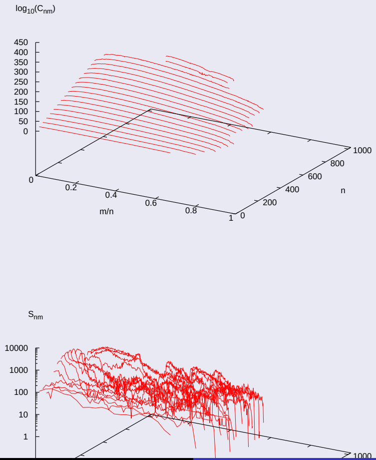
Total sample size: $10,000,000$





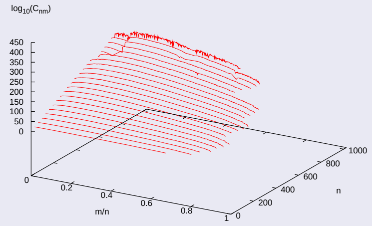
Example: 2dim ISAW simulation up to $N = 1024$

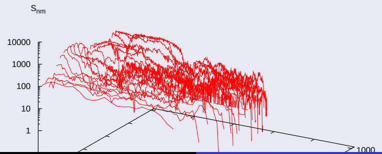
Total sample size: $20,000,000$



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

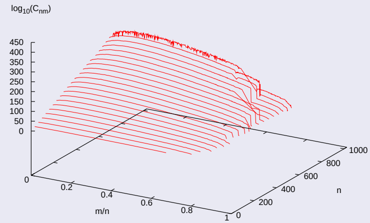
Total sample size: $30,000,000$

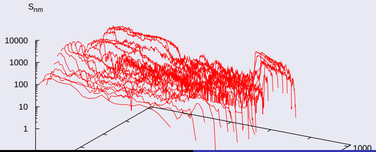




Example: 2dim ISAW simulation up to $N = 1024$

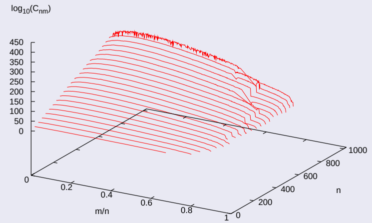
Total sample size: $40,000,000$

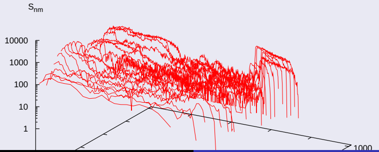




Example: 2dim ISAW simulation up to $N = 1024$

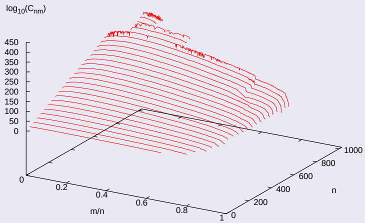
Total sample size: $50,000,000$

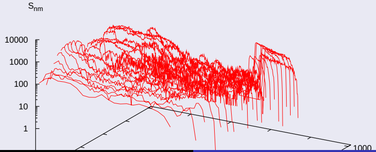




Example: 2dim ISAW simulation up to $N = 1024$

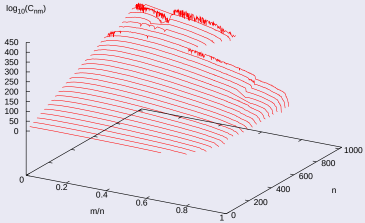
Total sample size: $60,000,000$

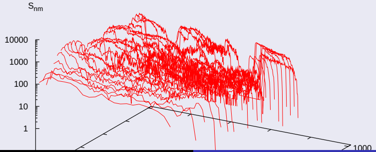




Example: 2dim ISAW simulation up to $N = 1024$

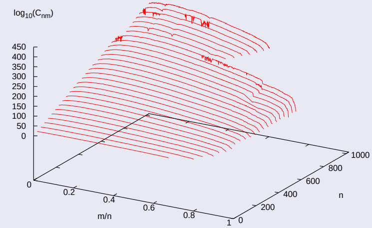
Total sample size: $70,000,000$

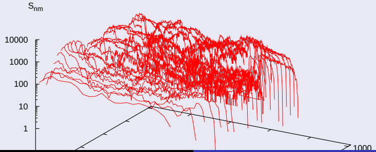




Example: 2dim ISAW simulation up to $N = 1024$

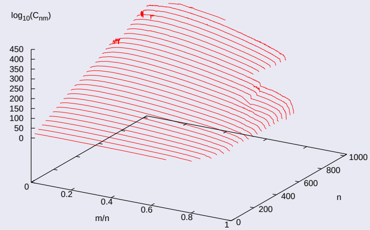
Total sample size: $80,000,000$

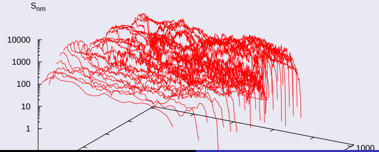




Example: 2dim ISAW simulation up to $N = 1024$

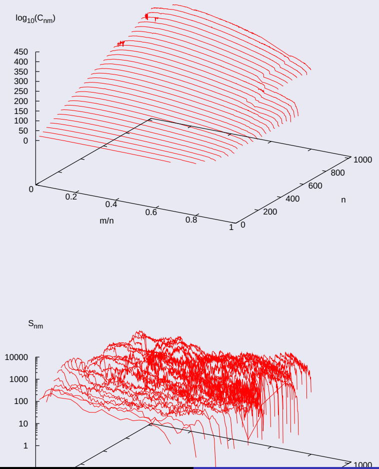
Total sample size: $90,000,000$





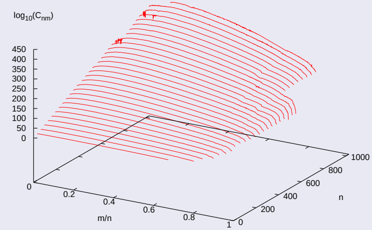
Example: 2dim ISAW simulation up to $N = 1024$

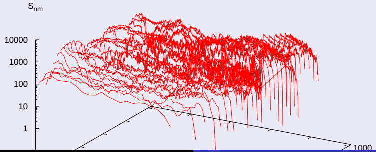
Total sample size: $100,000,000$



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

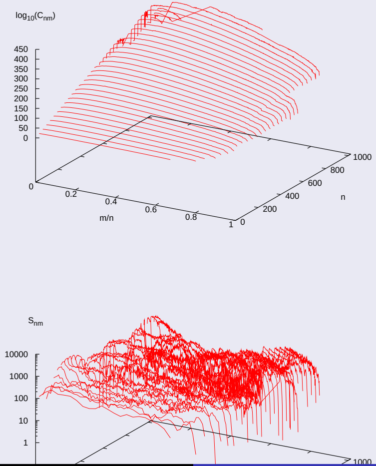
Total sample size: $110,000,000$





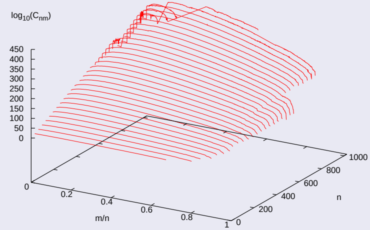
Example: 2dim ISAW simulation up to $N = 1024$

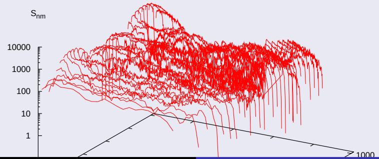
Total sample size: $120,000,000$



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

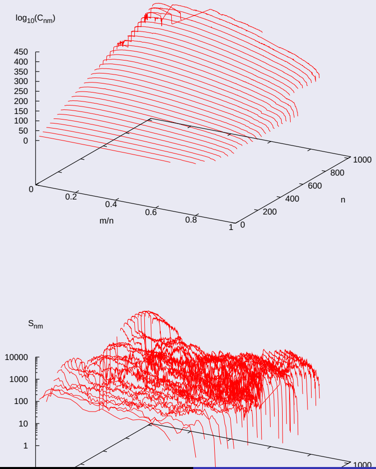
Total sample size: $130,000,000$





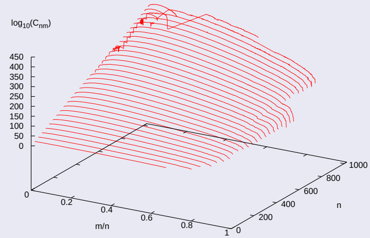
Example: 2dim ISAW simulation up to $N = 1024$

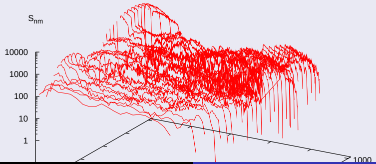
Total sample size: $140,000,000$



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

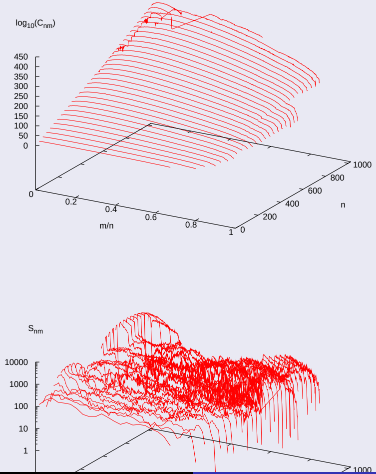
Total sample size: $150,000,000$





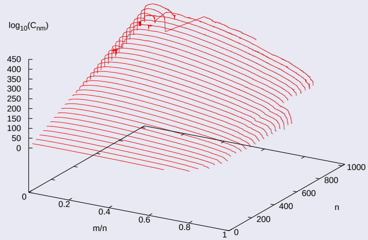
Example: 2dim ISAW simulation up to $N = 1024$

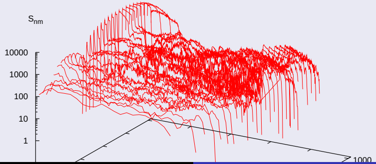
Total sample size: $160,000,000$



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

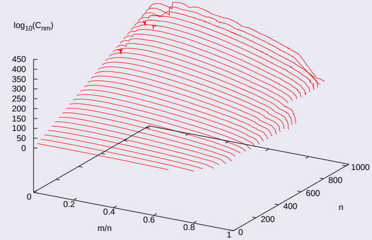
Total sample size: $170,000,000$

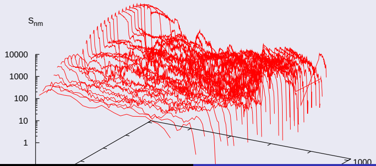




Example: 2dim ISAW simulation up to $N = 1024$

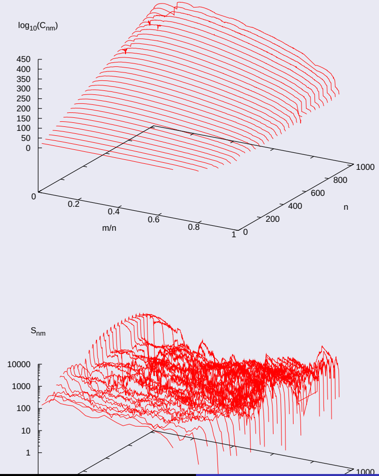
Total sample size: $180,000,000$





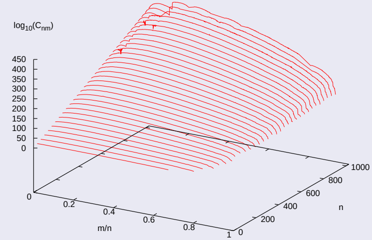
Example: 2dim ISAW simulation up to $N = 1024$

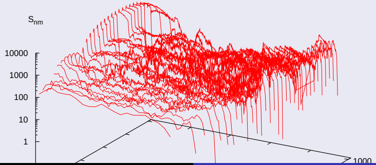
Total sample size: $190,000,000$



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

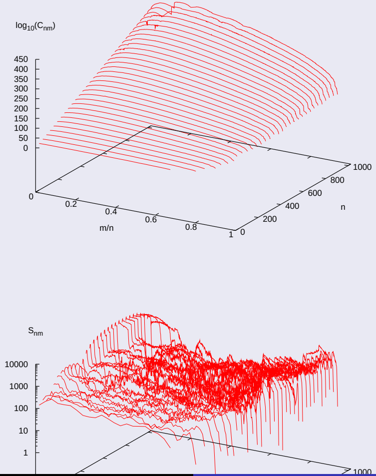
Total sample size: $200,000,000$





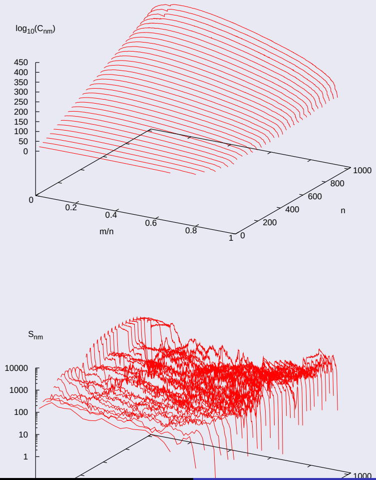
Example: 2dim ISAW simulation up to $N = 1024$

Total sample size: $210,000,000$



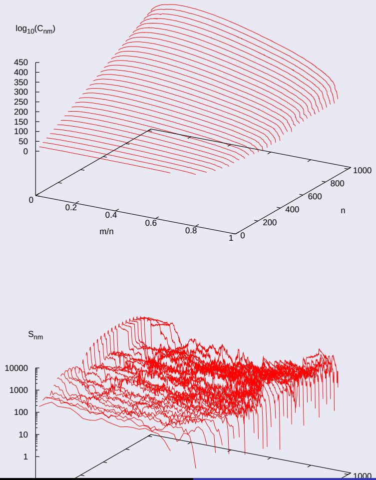
Example: 2dim ISAW simulation up to $N = 1024$

Total sample size: $220,000,000$



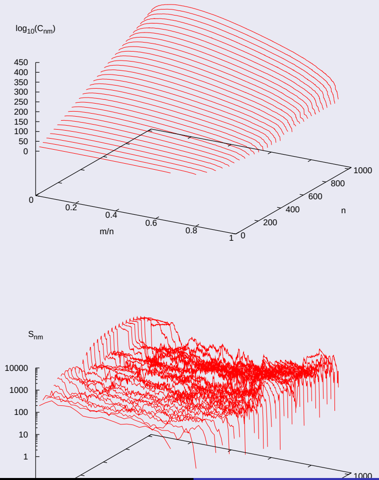
Example: 2dim ISAW simulation up to $N = 1024$

Total sample size: $230,000,000$



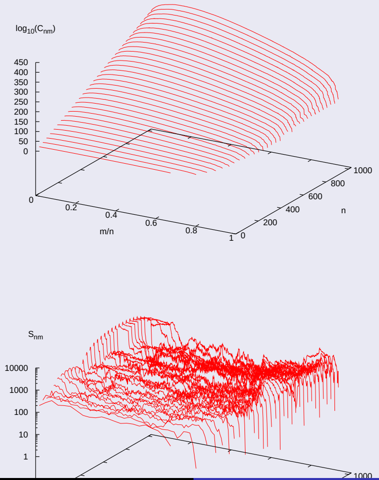
Example: 2dim ISAW simulation up to $N = 1024$

Total sample size: $240,000,000$



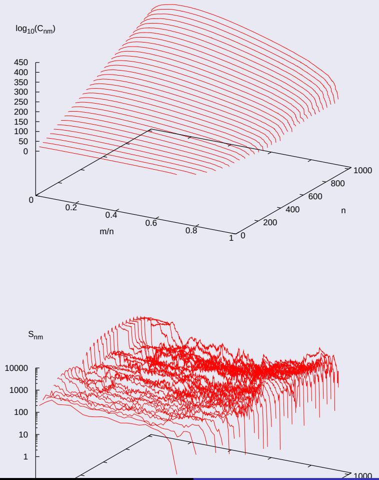
Example: 2dim ISAW simulation up to $N = 1024$

Total sample size: $250,000,000$



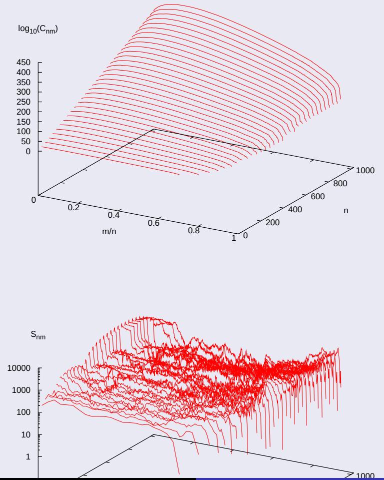
Example: 2dim ISAW simulation up to $N = 1024$

Total sample size: $260,000,000$



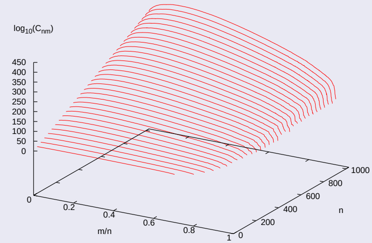
Example: 2dim ISAW simulation up to $N = 1024$

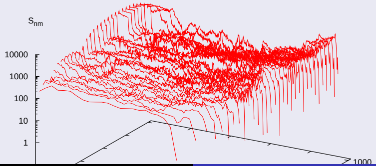
Total sample size: $270,000,000$



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

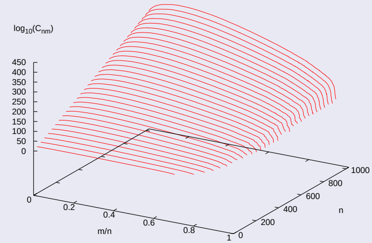
Total sample size: $280,000,000$

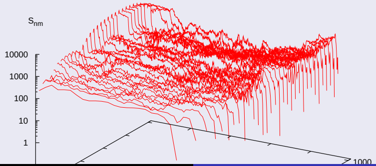




Example: 2dim ISAW simulation up to $N = 1024$

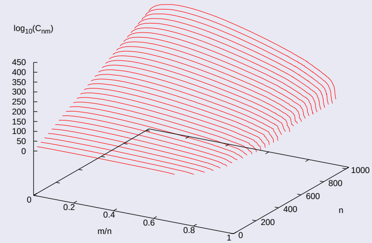
Total sample size: $290,000,000$

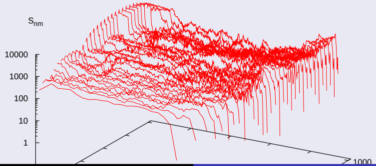




Example: 2dim ISAW simulation up to $N = 1024$

Total sample size: $300,000,000$



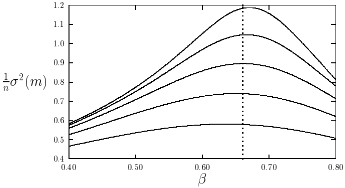


ISAW simulations

2dim ISAW density of states

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

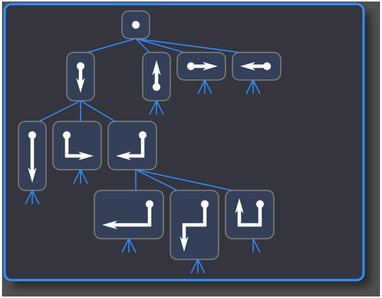
- 2d ISAW up to $n = 1024$
- One simulation suffices
- 400 orders of magnitude



Outline

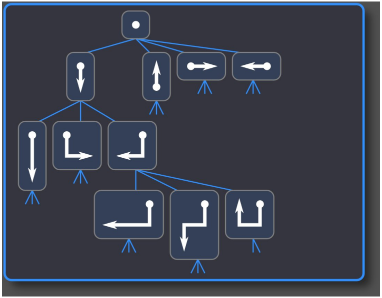
Revisit Rosenbluth Sampling

- Each configuration grown uniquely by appending edges to endpoint



Revisit Rosenbluth Sampling

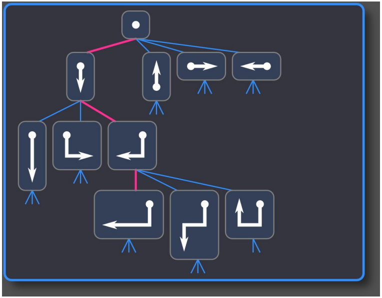
- Each configuration grown uniquely by appending edges to endpoint



- Generating tree
    - Each node of tree is a configuration

Revisit Rosenbluth Sampling

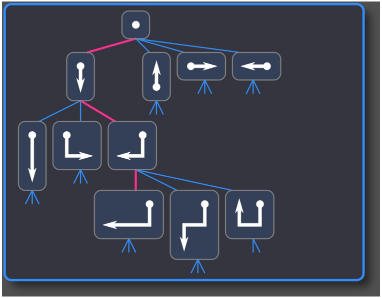
- Each configuration grown uniquely by appending edges to endpoint



- Generating tree
    - Each node of tree is a configuration
    - Sample by growing unique "sample path" down the tree

Revisit Rosenbluth Sampling

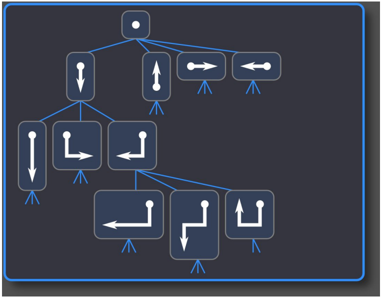
- Each configuration grown uniquely by appending edges to endpoint



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

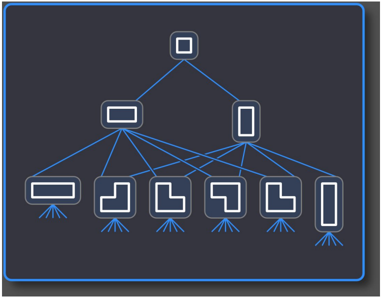
From Generating Trees to Generating Graphs

- Unique way to construct walks



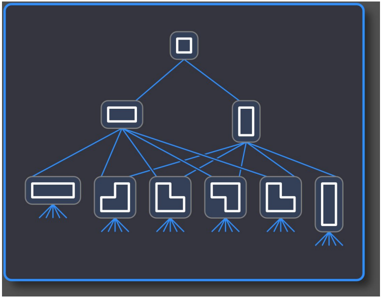
From Generating Trees to Generating Graphs

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



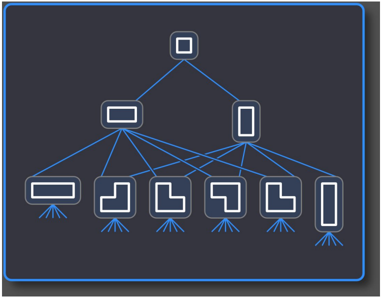
From Generating Trees to Generating Graphs

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



From Generating Trees to Generating Graphs

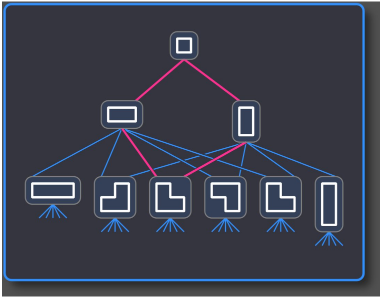
- Unique way to construct walks
- No obvious unique way to construct polygons
- Can we generalize from generating trees?



- Generating graph
  - Each node of graph is a configuration

From Generating Trees to Generating Graphs

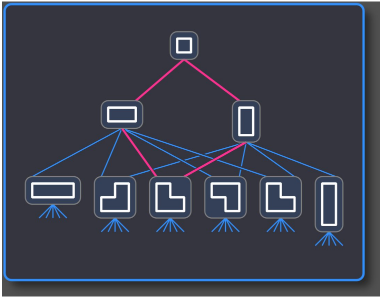
- Unique way to construct walks
- No obvious unique way to construct polygons
- Can we generalize from generating trees?



- Generating graph
  - Each node of graph is a configuration
  - Sample by growing non-unique path down the graph

From Generating Trees to Generating Graphs

- Unique way to construct walks
- 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

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
- Generating tree: bijection between sample paths and configurations

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
- Generating tree: bijection between sample paths and configurations
- Rosenbluth Sampling (with $a^- = 1$)
  - The weight $W(\varphi)$ and probability $\Pr(\varphi)$ of a sample path φ are

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

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
- Generating tree: bijection between sample paths and configurations
- Rosenbluth Sampling (with $a^- = 1$)
  - The weight $W(\varphi)$ and probability $\Pr(\varphi)$ of a sample path φ are

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

  - 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

- Generating tree: bijection between sample paths and configurations

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

- Generating graph: many sample paths give the same configuration

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

From Rosenbluth Sampling to GARM

- Generating tree: bijection between sample paths and configurations

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

- Generating graph: many sample paths give the same configuration

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

- The correct weight

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

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

From Rosenbluth Sampling to GARM

- Generating tree: bijection between sample paths and configurations

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

- Generating graph: many sample paths give the same configuration

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

- The correct weight

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

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

- GARM = Generalized Atmospheric Rosenbluth Method

Features of GARM

GARM is a genuine generalization of Rosenbluth sampling

Features of GARM

GARM is a genuine generalization of Rosenbluth sampling

- Can easily substitute GARM for Rosenbluth sampling
    - Thermal GARM
    - Pruned Enriched GARM
    - Multicanonical GARM (not done yet!)
    - Flat Histogram GARM

Features of GARM

GARM is a genuine generalization of Rosenbluth sampling

- Can easily substitute GARM for Rosenbluth sampling
  - Thermal GARM
  - Pruned Enriched GARM
  - Multicanonical GARM (not done yet!)
  - Flat Histogram GARM
- Applicable to polygons, branched polymers, lattice animals, ...
- Drawback: atmospheres may be expensive to calculate

Features of GARM

GARM is a genuine generalization of Rosenbluth sampling

- Can easily substitute GARM for Rosenbluth sampling
  - Thermal GARM
  - Pruned Enriched GARM
  - Multicanonical GARM (not done yet!)
  - Flat Histogram GARM
- Applicable to polygons, branched polymers, lattice animals, ...
- Drawback: atmospheres may be expensive to calculate

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

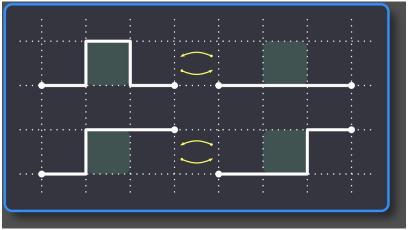
- GARM works for 2d polygons, but not 3d polygons

Grow and Shrink

- GARM works for 2d polygons, but not 3d polygons
- There are 3 minimal 3d unknots on $\mathbb{Z}^3$ and 3328 minimal trefoils cannot reach one minimal configuration from another by growing

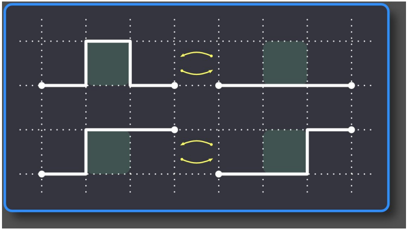
Grow and Shrink

- GARM works for 2d polygons, but not 3d polygons
- There are 3 minimal 3d unknots on $\mathbb{Z}^3$ and 3328 minimal trefoils cannot reach one minimal configuration from another by growing
- Use moves that grow and shrink



Grow and Shrink

- GARM works for 2d polygons, but not 3d polygons
- There are 3 minimal 3d unknots on $\mathbb{Z}^3$ and 3328 minimal trefoils cannot reach one minimal configuration from another by growing
- Use moves that grow and shrink



- Moves from the BFACF algorithm

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

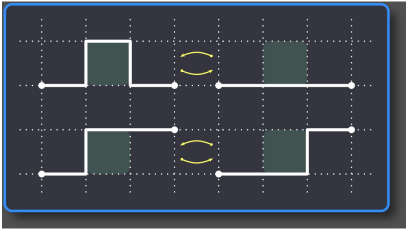
C Aragão de Carvalho, S Caracciolo and J Fröhlich, Nucl Phys B 215 (1983) 209

- Ergodic on each knot-type

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

Grow and Shrink

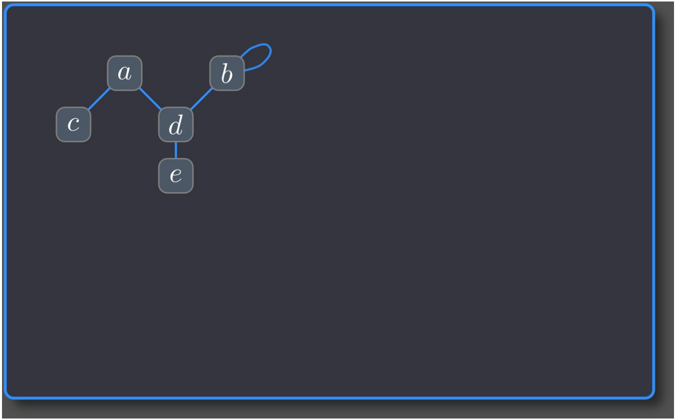
- GARM works for 2d polygons, but not 3d polygons
- There are 3 minimal 3d unknots on $\mathbb{Z}^3$ and 3328 minimal trefoils cannot reach one minimal configuration from another by growing
- Use moves that grow and shrink



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

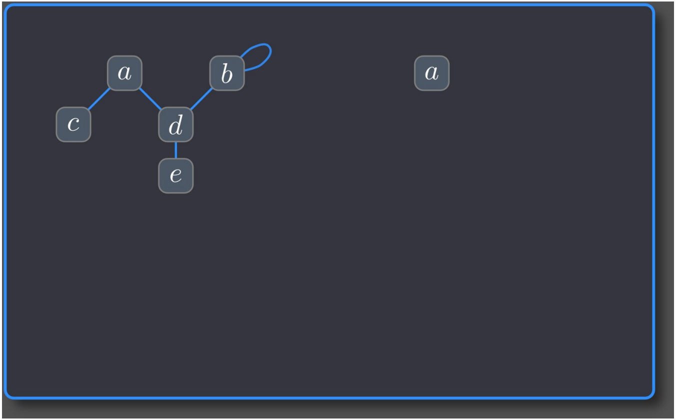
Derivative graph

- Take an arbitrary generating graph



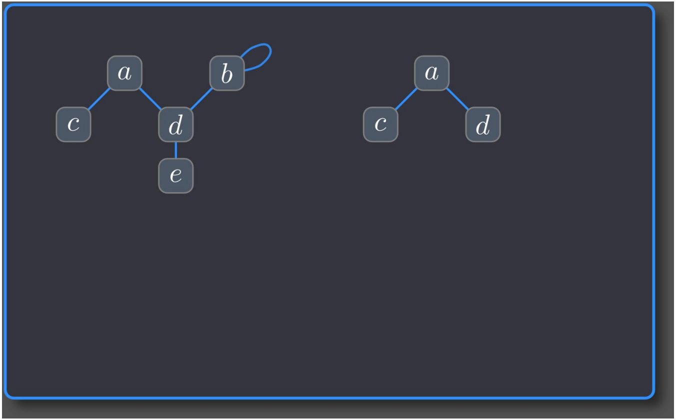
Derivative graph

- Copy the initial vertex



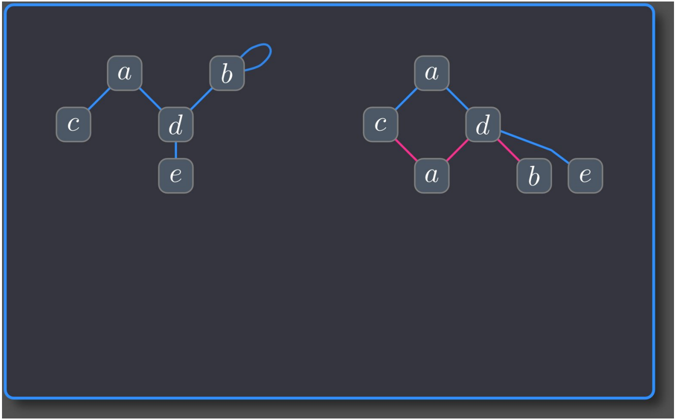
Derivative graph

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



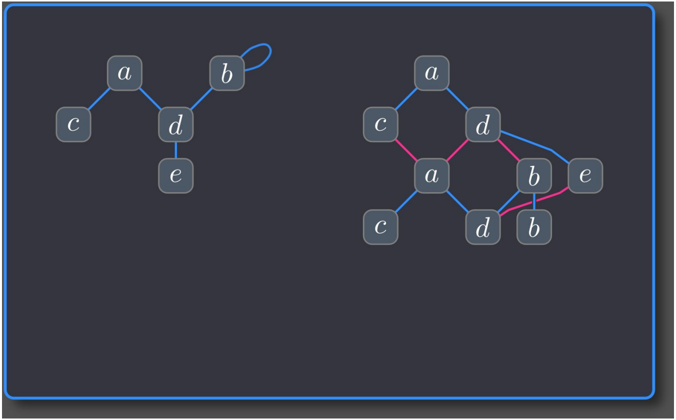
Derivative graph

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



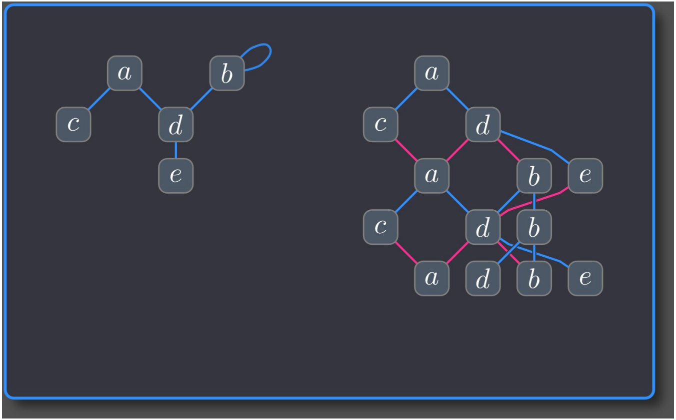
Derivative graph

- Keep adding new rows in this way



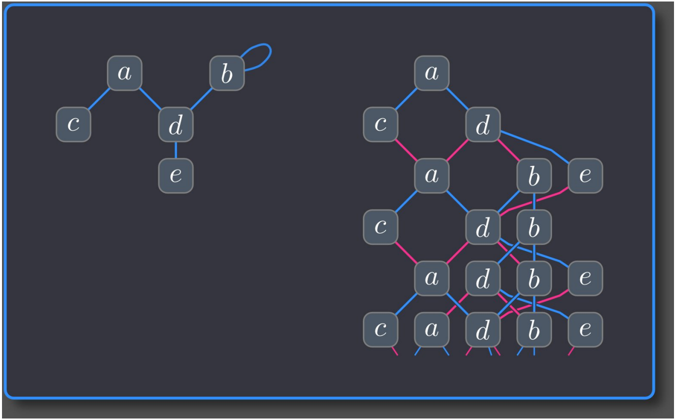
Derivative graph

- Keep adding new rows in this way



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

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
- Weight is a simple function of $a^{\pm}(\varphi), a^{0}(\varphi)$

$$\frac{\langle W(\varphi)\rangle_N}{\langle W(\varphi)\rangle_M} = \frac{C_N}{C_M}$$

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
- Weight is a simple function of $a^{\pm}(\varphi), a^{0}(\varphi)$

$$\frac{\langle W(\varphi)\rangle_N}{\langle W(\varphi)\rangle_M} = \frac{C_N}{C_M}$$

- Generalizes to Thermal GAS and Pruned Enriched GAS

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
- Weight is a simple function of $a^{\pm}(\varphi), a^{0}(\varphi)$

$$\frac{\langle W(\varphi)\rangle_N}{\langle W(\varphi)\rangle_M} = \frac{C_N}{C_M}$$

- 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

GAS Application: Minimal Polygons

- Known exactly for trefoil $C_{24}(3_1) = 3328$ — Y Diao, JKTR 2 (1993) 413
- Need to estimate numerically for other knot types
  - Draw a knot K on the cubic lattice
  - Run GAS with BFACF moves and extract the minimal polygons

EJJ van Rensburg and A Rechnitzer, JKTR, in print

GAS Application: Minimal Polygons

- Known exactly for trefoil $C_{24}(3_1) = 3328$ — Y Diao, JKTR 2 (1993) 413
- Need to estimate numerically for other knot types
  - Draw a knot K on the cubic lattice
  - Run GAS with BFACF moves and extract the minimal polygons

EJJ van Rensburg and A Rechnitzer, JKTR, in print

- Resulting numbers — see also R Scharein et al, J Phys A 42 (2009) 475006

$$C_{24}(3_1) = 3328 \qquad C_{30}(4_1) = 2648$$
$$C_{34}(5_1) = 6672 \qquad C_{36}(5_2) = 114912$$

GAS Application: Minimal Polygons

- Known exactly for trefoil $C_{24}(3_1) = 3328$ Y Diao, JKTR 2 (1993) 413
- Need to estimate numerically for other knot types
  - Draw a knot K on the cubic lattice
  - Run GAS with BFACF moves and extract the minimal polygons

EJJ van Rensburg and A Rechnitzer, JKTR, in print

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

$$C_{24}(3_1) = 3328 \qquad C_{30}(4_1) = 2648$$
$$C_{34}(5_1) = 6672 \qquad C_{36}(5_2) = 114912$$

- 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

Comparing the Algorithms?

- Testing flatPERM using 1-dim random walk

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

- Difference between multicanonical PERM and flatPERM?

Comparing the Algorithms?

- Testing flatPERM using 1-dim random walk

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

- Difference between multicanonical PERM and flatPERM?

  About the same... M Bachmann, private communication

Comparing the Algorithms?

- Testing flatPERM using 1-dim random walk

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

- Difference between multicanonical PERM and flatPERM?

  About the same... M Bachmann, private communication

- More importantly, are GARM/GAS better?

Comparing the Algorithms?

- Testing flatPERM using 1-dim random walk

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

- Difference between multicanonical PERM and flatPERM?

  About the same... M Bachmann, private communication

- More importantly, are GARM/GAS better?

  YES, as GARM/GAS works where Rosenbluth does not

  NO, as large atmospheres might be very expensive to compute (but maybe a trade-off with better sampling?)

Comparing the Algorithms?

- Testing flatPERM using 1-dim random walk

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

- Difference between multicanonical PERM and flatPERM?

  About the same... M Bachmann, private communication

- More importantly, are GARM/GAS better?

  YES, as GARM/GAS works where Rosenbluth does not

  NO, as large atmospheres might be very expensive to compute (but maybe a trade-off with better sampling?)

- Algorithms are 'dirty' (highly correlated data)

Comparing the Algorithms?

- Testing flatPERM using 1-dim random walk

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

- Difference between multicanonical PERM and flatPERM?

  About the same... M Bachmann, private communication

- More importantly, are GARM/GAS better?

  YES, as GARM/GAS works where Rosenbluth does not

  NO, as large atmospheres might be very expensive to compute (but maybe a trade-off with better sampling?)

- Algorithms are 'dirty' (highly correlated data)

  Can one prove anything useful?

Comparing the Algorithms?

- Testing flatPERM using 1-dim random walk

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

- Difference between multicanonical PERM and flatPERM?

  About the same... M Bachmann, private communication

- More importantly, are GARM/GAS better?

  YES, as GARM/GAS works where Rosenbluth does not

  NO, as large atmospheres might be very expensive to compute (but maybe a trade-off with better sampling?)

- Algorithms are 'dirty' (highly correlated data)

  Can one prove anything useful?

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

Special thanks to Andrew for the GARM/GAS figures