Worm Algorithms

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AUSTRALIAN RESEARCH COUNCIL
Centre of Excellence for Mathematics
and Statistics of Complex Systems

References/Collaborators

1. Youjin Deng, Timothy M. Garoni, and Alan D. Sokal, *Dynamic Critical Behavior of the Worm Algorithm for the Ising Model*, Phys. Rev. Lett. 99, 110601 (2007).
2. Wei Zhang, Timothy M. Garoni, and Youjin Deng, *Simulating the fully-packed loop model on the honeycomb lattice with a worm algorithm*, preprint.

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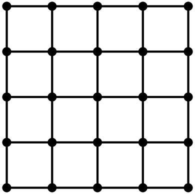
How do we efficiently simulate models near criticality?

- Problem: critical slowing-down
- The current state-of-the-art: cluster algorithms
  - Swendsen & Wang PRL 1987
  - Use global moves in clever way
- More recent idea: worm algorithms
  - Prokof'ev & Svistunov PRL 2001
  - Enlarge an Eulerian configuration space to include defects
  - Move the defects via random walk

Eulerian subgraphs

- Fix a finite graph $G = (V, E)$



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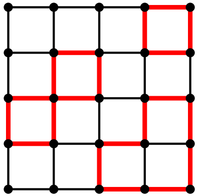
- $A \subseteq E$ is Eulerian if every vertex in (V, A) has even degree



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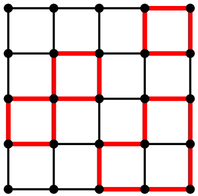
- The cycle space $\mathcal{C}(G) = \{A \subseteq E : A \text{ is Eulerian}\}$



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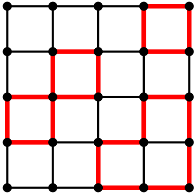

- Consider the Ising model on G

$$Z_{\text{Ising}} = \sum_{\sigma \in \{-1,+1\}^V} \prod_{ij \in E} e^{\beta \sigma_i \sigma_j}$$

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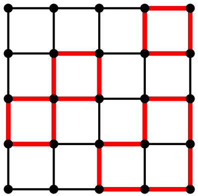

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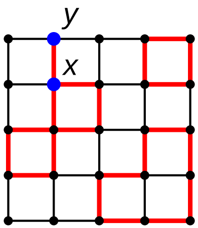
$$Z_{\text{Ising}} = \sum_{\sigma \in \{-1,+1\}^V} \prod_{ij \in E} e^{\beta \sigma_i \sigma_j}$$

- The high-temperature expansion is

$$Z_{\text{Ising}} = \left(2^{|V|} \cosh^{|E|} \beta\right) \sum_{A \in \mathcal{C}(G)} (\tanh \beta)^{|A|}$$

State space for worm dynamics

- Let ∂A be the set of all vertices with odd degree in (V, A)



- For distinct $x, y \in V$ define

$$\mathcal{S}_{x,y} = \{A \subseteq E : \partial A = \{x, y\}\}$$
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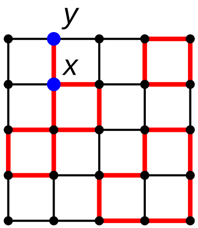

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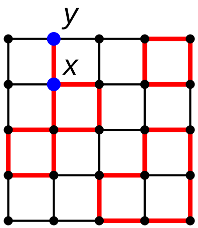

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$$\mathcal{S} = \{(A, x, y) : x, y \in V \text{ and } A \in \mathcal{S}_{x,y}\}$$

- Assign $(A, x, y) \in \mathcal{S}$ probability

$$\pi(A, x, y) \propto d_x\, d_y\, (\tanh \beta)^{|A|}$$

Ising susceptibility

- If $Z := \sum_{A \in \mathcal{C}(G)} w^{|A|}$ and $w := \tanh \beta$

$$Z_{\text{Ising}} = \left(2^{|V|} \cosh^{|E|} \beta\right) Z \qquad \text{Partition function}$$

$$Z \left\langle \sigma_x \sigma_y \right\rangle_{\text{Ising}} = \sum_{A \in \mathcal{S}_{x,y}} w^{|A|} \qquad \text{Two-point function}$$

$$Z \left\langle \mathcal{M}^2 \right\rangle_{\text{Ising}} = \sum_{A \in \mathcal{S}} w^{|A|} \qquad \text{Magnetization}$$

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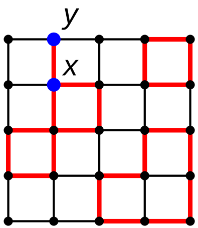
- Therefore the observable $\mathcal{D}_0(A,x,y) = \delta_{x,y}$ satisfies

$$\langle\mathcal{D}_0\rangle_\pi = 1/\chi$$

Worm dynamics



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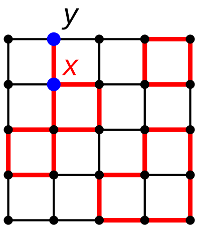

- Start in configuration (A, x, y)
- Pick x or y

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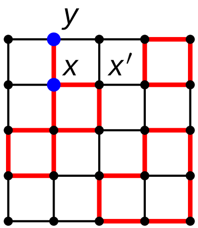

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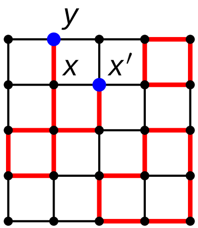

- Start in configuration (A, x, y)
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- Propose $(A, x, y) \to (A \triangle xx', x', y)$

- If transition removes an edge accept with probability 1

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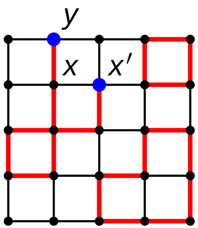

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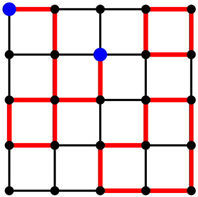

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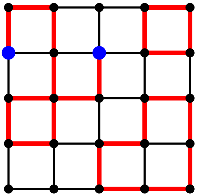

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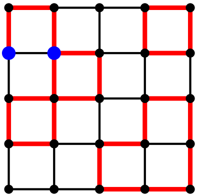

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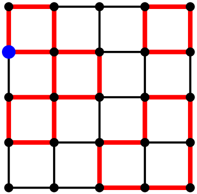

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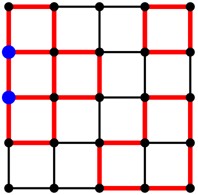

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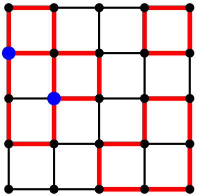

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Transition matrix

- Let G be translationally invariant with degree z
- Worm dynamics corresponds to transition matrix P on $\mathcal{S}$

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Lemma

P is in detailed balance with $\pi(A,x,y) = w^{|A|}/Z\, V\, \chi$

- Can estimate χ by running the worm dynamics

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- Empirically – measuring autocorrelations

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- Markov chain
  - State space S, with $|S| < \infty$
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- Stationary process – start “in equilibrium”

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- 1 “effectively independent” observation every $2\,\tau_{\mathrm{int},X}$ steps

Exponential autocorrelation times

- $\rho_X(t)$ typically decays exponentially as $t \to \infty$
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$$\tau_{\mathrm{exp},X} := \limsup_{t\to\infty} \frac{t}{-\log|\rho_X(t)|} \quad \text{and} \quad \tau_{\mathrm{exp}} := \sup_X \tau_{\mathrm{exp},X}$$

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Lemma

αP^t tends to π with rate bounded by $e^{-t/\tau_{\exp}}$

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- More precisely, we have a family of exponents: z_{exp}, and $z_{\text{int},X}$ for each observable X.
- Different algorithms for the same model can have very different z
- E.g. $d = 2$ Ising model
  - Glauber (Metropolis) algorithm $z \approx 2$
  - Swendsen-Wang algorithm $z \approx 0.2$

Worm simulations

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- Focus on two observables:
  - $\mathcal{N}(A, x, y) = |A|$
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- $\langle \mathcal{N} \rangle$ is "energy-like"
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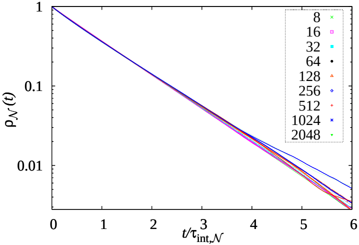
- $\langle\mathcal{N}\rangle$ is “energy-like”
- $\langle\mathcal{D}_0\rangle = 1/\chi$
- Measured observables after every hit (worm update)
- Natural unit of time is one sweep (L^d hits)

Dynamics of $\mathcal{N}$

- $\rho_{\mathcal{N}}(t)$ is almost a perfect exponential

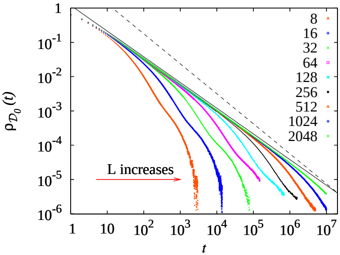


- Scaled time by $\tau_{\mathrm{int},\mathcal{N}}$
- Good data collapse suggests $z_{\mathrm{exp}} \approx z_{\mathrm{int},\mathcal{N}}$
- Fitting $\tau_{\mathrm{int},\mathcal{N}}$ gives $z_{\mathrm{int},\mathcal{N}} \approx 0.379$

- Li-Sokal bound $z_{\mathrm{exp}}, z_{\mathrm{int},\mathcal{N}} \geq \alpha/\nu$ applies to worm dynamics

Dynamics of $\mathcal{D}_0$

- $\rho_{\mathcal{D}_0}(t)$ decays significantly in $O(1)$ hits!



- $\rho_{\mathcal{D}_0}(t) \sim t^{-s}$ with $s \approx 0.75$

- $\mathcal{D}_0$ decorrelates on a totally different time scale to $\mathcal{N}$

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- Li-Sokal bound may be sharp for $d = 3$ worm algorithm
- Compare Swendsen-Wang $z_{SW} \approx 0.46$

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An alternative perspective on worm dynamics

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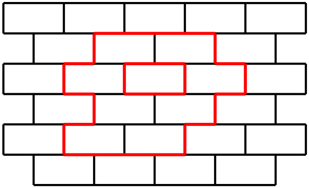
Loop models

- Honeycomb lattice Eulerian subgraphs = disjoint cycles
- Nienhuis loop model



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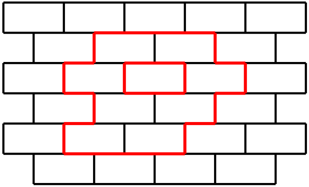

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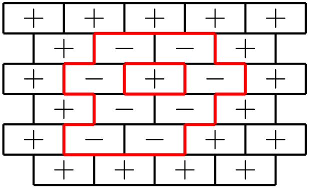

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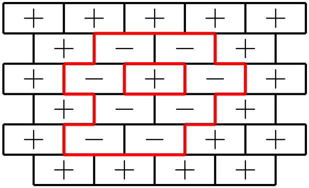

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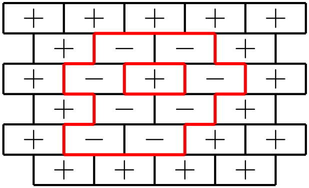

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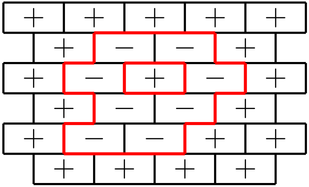

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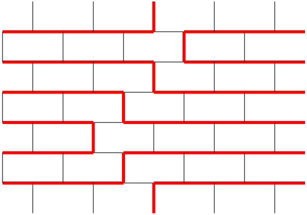
- Worm $\iff$ simulate dual Ising domain boundaries

Fully-packed loop model (FPL)



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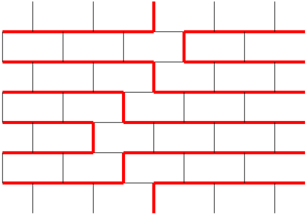

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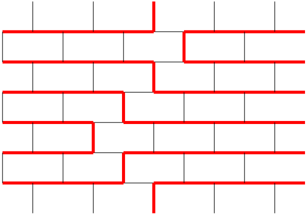

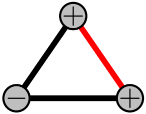

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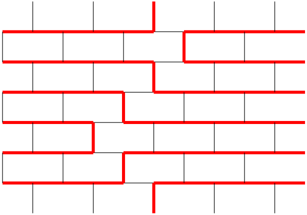

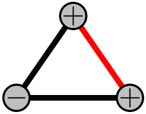

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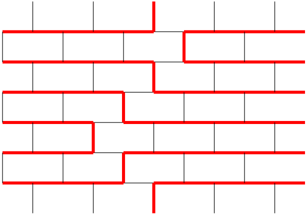

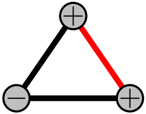

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- Can we use worm instead?

P_∞ has absorbing states

- Standard worm transitions for $w \geq 1$ on z-regular graph:

$$P_w[(A,x,y) \to (A\triangle xx', x', y)] = \frac{1}{2z}\begin{cases} 1/w & xx' \in A \\ 1 & xx' \notin A \end{cases}$$

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Worm algorithm for honeycomb-lattice FPL

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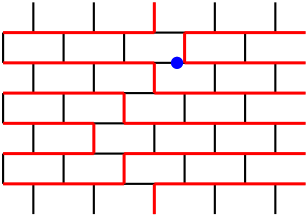

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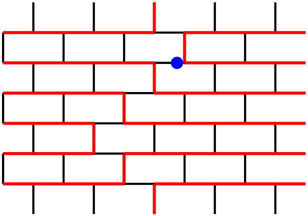

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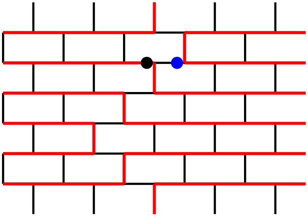

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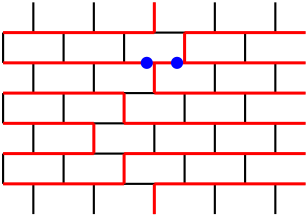

- Start in configuration (A, x, y)
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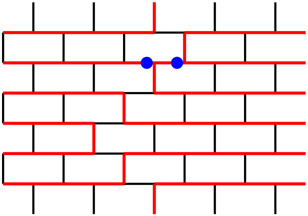

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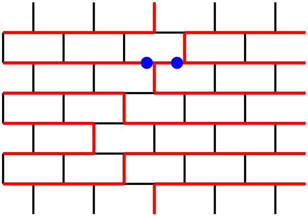

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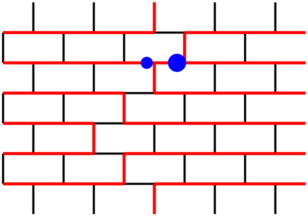

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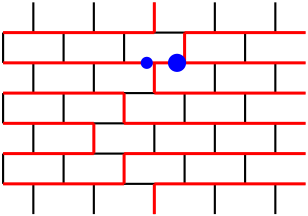

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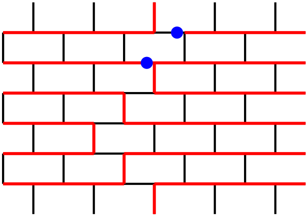

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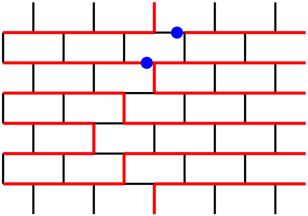

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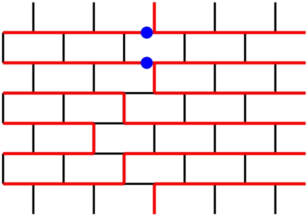

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  - Pick x or y (say x)
  - If $d_x(A) = 3$
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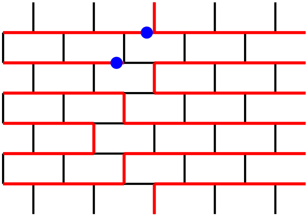
Worm algorithm for honeycomb-lattice FPL



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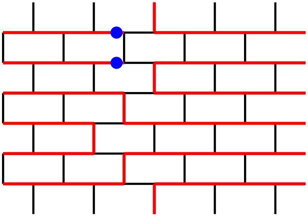

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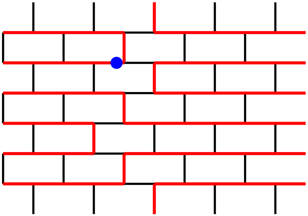

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Transition matrix

- $x \neq y$

$$P'_\infty[(A,x,y) \to (A \triangle xx', x', y)] = \begin{cases} 1/6 & d_x(A) = 3 \\ 1/4 & xx' \notin A \end{cases}$$

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- Therefore P'_∞ correctly simulates the FPL

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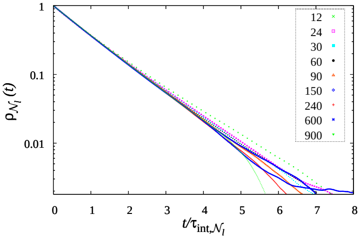
- $\langle \mathcal{N}_l \rangle$ is "energy-like"
- $\mathcal{N}_l$ is the slowest mode observed

Dynamics of $\mathcal{N}_l$

- $\rho_{\mathcal{N}_l}(t)$ is almost a perfect exponential



- Scaled time by $\tau_{\mathrm{int},\mathcal{N}_l}$
- Good data collapse suggests $z_{\mathrm{exp}} \approx z_{\mathrm{int},\mathcal{N}_l}$
- Fitting $\tau_{\mathrm{int},\mathcal{N}_l}$ gives $z_{\mathrm{int},\mathcal{N}_l} = 0.515(8)$

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Summary

- Standard worm algorithm for Ising high-temperature graphs outperforms SW in three dimensions
- Worm decorrelates on different time scales – depends on observable
- Modified worm algorithm is demonstrated to be valid for honeycomb lattice FPL
- Dynamic exponent $z \approx 0.5$
- By contrast, even the best cluster algorithms for frustrated Ising models are thought to be non-ergodic at $T = 0$