True asymptotics of self-avoiding walks on 3D percolation clusters

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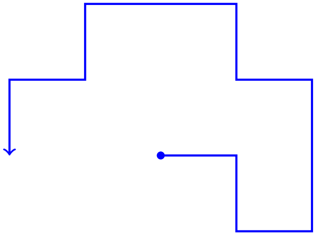
Self-avoiding walk (SAW)



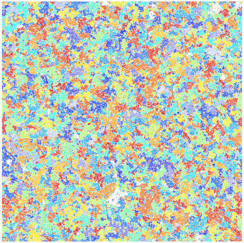
Universal scaling behavior

Number of conformations: $Z_N \sim \mu^N N^{\gamma-1}$

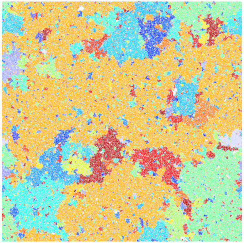
Mean end-to-end distance: $\langle R^2 \rangle = \frac{\sum_{i=1}^{Z_N} R_i^2}{Z_N} \sim N^{2\nu}$

Flory: $\nu \approx \frac{3}{2+D}$

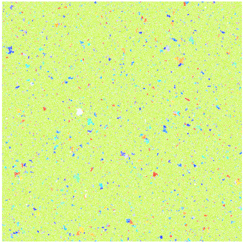
Percolation



$p = 0.55 < p_c$



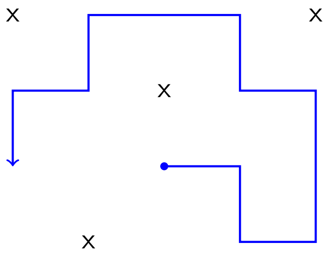
$p = 0.592746 \approx p_c$



$p = 0.62 > p_c$

D	p_c	d_f	d_l	d_{Bf}
2	0.592...	91/48	1.68...	1.64...
3	0.311...	2.52...	1.84...	1.81...
6	0.109...	4	2	2

SAWs in disorder

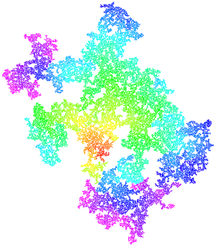


Quenched averages: same scaling laws with new exponents?

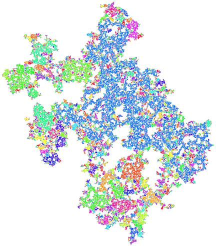
$$[Z_N] \sim \mu^N N^{\gamma-1}, \qquad \left[\left\langle R^2 \right\rangle\right] \sim N^{\nu}$$

Standard numerical tools rather inefficient to tackle this problem!

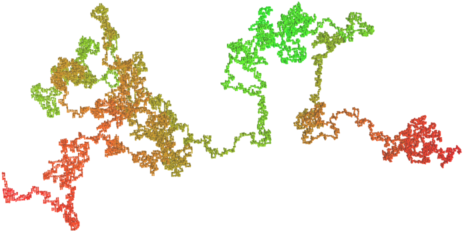
Structure of the critical cluster



10^3 chemical shells around origin

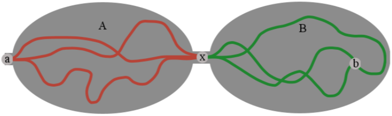


Bi-connected components

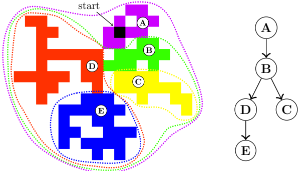


← Backbone of a 3D cluster

Hierarchical factorization



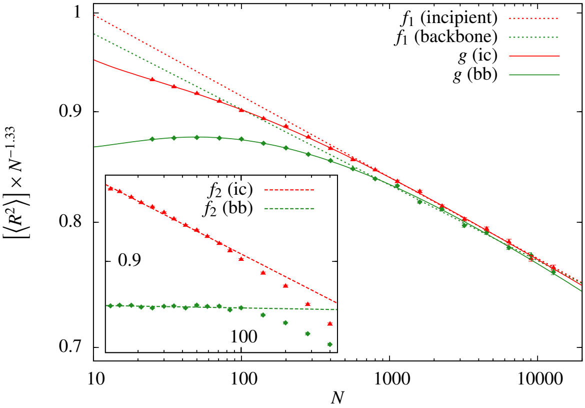
$$Z_{a\to b}[N] = \sum_{i=0}^{N} Z_{a\to x}[i] \cdot Z_{x\to b}[N-i]$$



→ Exact enumeration of SAW configurations in polynomial time.

→ 10^4 steps now take ≈ 10 minutes, down from $\approx 10^{960}$ years.

End-to-end distance and Flory exponent ν



$$f(N) \cdot N^{1.33} = a \cdot N^{2\nu}$$

$$g(N) \cdot N^{1.33} = a \cdot N^{2\nu} \left(1 + b/N^{\Delta}\right)$$

Flory exponent ν – results

Our study[1]:

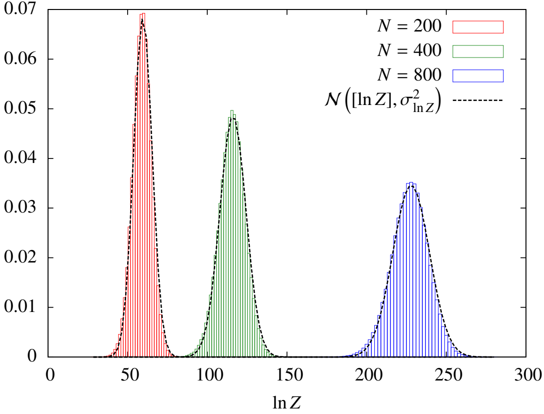
ansatz	range	$\nu_{\text{incipient}}$	ν_{backbone}
$a \cdot N^{2\nu}$	25-84	0.6547(2)	0.6646(2)
$a \cdot N^{2\nu}$	800-12800	0.6433(4)	0.643(1)
$a \cdot N^{2\nu}\left(1 + b/N^{\Delta}\right)$	25-12800	0.644(2)	0.640(3)

Previous numerical results:

study	range	$\nu_{\text{incipient}}$	ν_{backbone}
exact enum.[2]	$N \leq 30$	0.660(5)	-
exact enum.[3]	$N \leq 40$	-	0.662(6)
MC (PERM).[4]	$N < 100$	-	0.667(3)

[1] N. F. and W. Janke, PRL (in print)
[2] M. Rintoul et al., PRE *49* 2790 (1994)
[3] A. Ordemann et al., PRE *61* 6858 (2000)
[4] V. Blavatska and W. Janke, EPL *82* 66006 (2008)

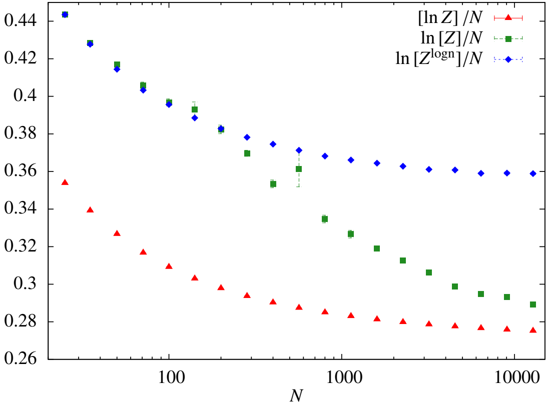
Number of walk conformations Z



$$\sigma^2_{\ln Z} = A \cdot N^{2\chi}, \quad \chi = 0.500(1)$$

Problem: distribution of Z_N almost log-normal
$\rightarrow$ large deviations make estimating $[Z_N]$ difficult.

Number of walk conformations Z



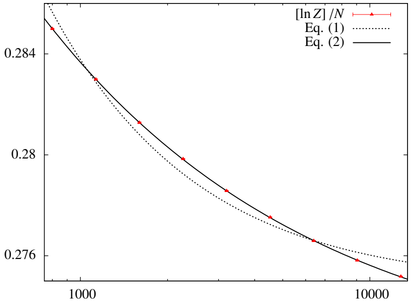
Approximation: $[Z] \approx e^{[\ln Z] + \sigma^2_{\ln Z}/2} =: [Z_{\mathrm{logn}}]$.

Scaling laws for $[Z_N]$ and $[\ln Z_N]$?

Assumption: $e^{[\ln Z_N]} \sim \mu_0^N N^{\gamma_0 - 1}$

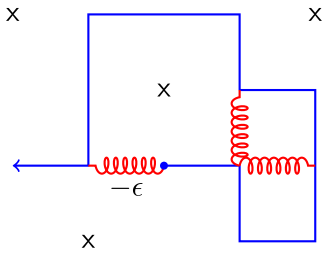
$$\longrightarrow \qquad [\ln Z_N]/N = \ln a/N + \ln \mu_0 + (\gamma - 1)\ln N/N \qquad (1)$$

$$\text{Modified:} \qquad [\ln Z_N]/N = \ln a/N + \ln \mu_0 \left(1 + bN^{-\zeta}\right) \qquad (2)$$



$$\longrightarrow \quad [Z_N] \approx [Z_{\mathrm{logn}}] \sim \cancel{\mu^N N^{\gamma - 1}} \; \mu^{N(1+b/N^{\zeta})}, \qquad \mu = e^{\ln \mu_0 + A/2} \;?$$

Self-attracting SAWs

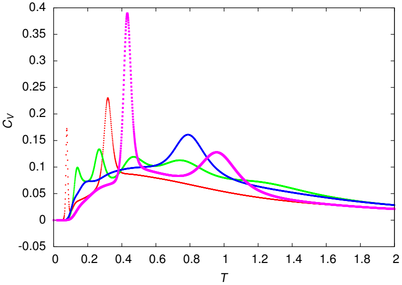


$$\langle R^2 \rangle = \frac{\sum_{i=1}^{C_N} e^{-\beta E} R_i^2}{\sum_{i=1}^{C_N} e^{-\beta E}}$$

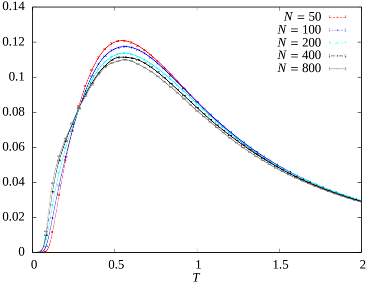
- Is there a Θ-collapse transition?[5]
- If so, at what temperature and with which exponents?

[5] see Roy et al. (1990), Barat et al. (1992), Blavatska and Janke (2009)

Specific heat



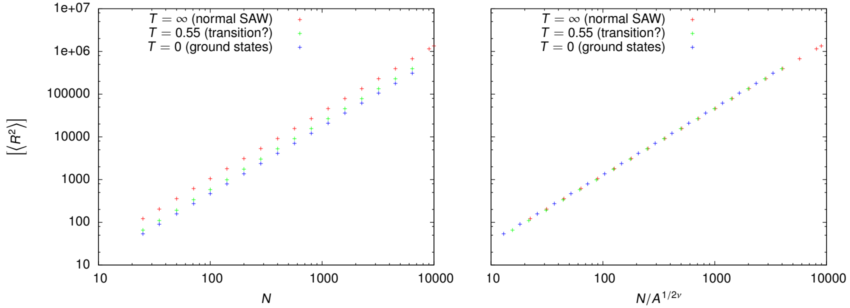
Single clusters



Quenched average

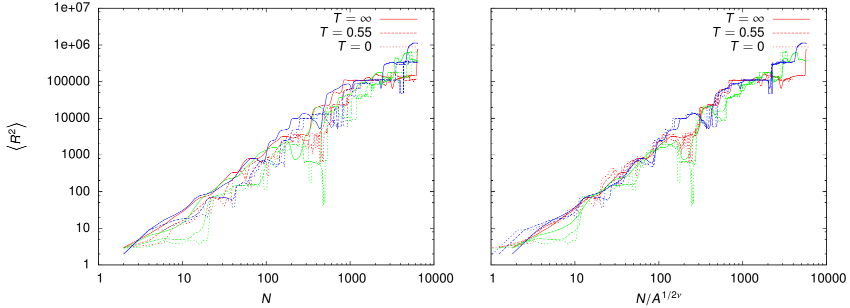
No divergence for average $[C_V] = \frac{1}{NT^2}\left[\left\langle E^2\right\rangle - \left\langle E\right\rangle^2\right]$.

End-to-end distance



Temperature only changes amplitude: $A_T \cdot [\langle R^2 \rangle] \sim N^{2\nu}$

End-to-end distance for single clusters



With rescaled N-axis, patterns for different T look very similar!

For once, energy and entropy have shared interests!

Summary

- SAWs on critical percolation clusters: basic model for polymers in disordered media.
- Fractal nature of critical clusters enables SAW enumeration in polynomial time.
- True (?) asymptotic behavior only visible after $\sim 10^3$ steps.
- Flory exponent ν smaller than previously thought, but assumption $\nu_{\text{backbone}} = \nu_{\text{full cluster}}$ holds.
- $[Z_N] \sim \mu^N N^{\gamma-1}$ wrong, instead: $[Z_N] \sim \mu^{N(1+b/N^{\zeta})}$?
- Identical scaling behavior for SAWs with short-range attractions at any temperature – no Θ-transition.

Thank you for the attention!

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