Scale-free enumeration of self-avoiding walks on critical percolation clusters

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INTRODUCTION

The scaling behavior of self-avoiding walks (SAWs) on critical percolation clusters has been widely studied since the early 1980s, being of interest for both theory and praxis (see [1]). Various Monte Carlo (MC) methods [2, 3, 4] as well as exact enumeration [5, 6, 7] have been used to investigate the problem. However, neither approach proved very effective: MC methods work well for weakly diluted lattices but become inefficient at the critical concentration ($p_c \approx 0.593$ in 2D), and the computational effort for exact enumeration even scales exponentially with the number of steps.
We developed a new enumeration method, which is inspired by the ideas of renormalization theory and exploits the fractal structure of the percolation cluster. It is restricted to systems at or close to p_c, but there it outperforms even the most capable MC methods.

SELF-AVOIDING WALKS

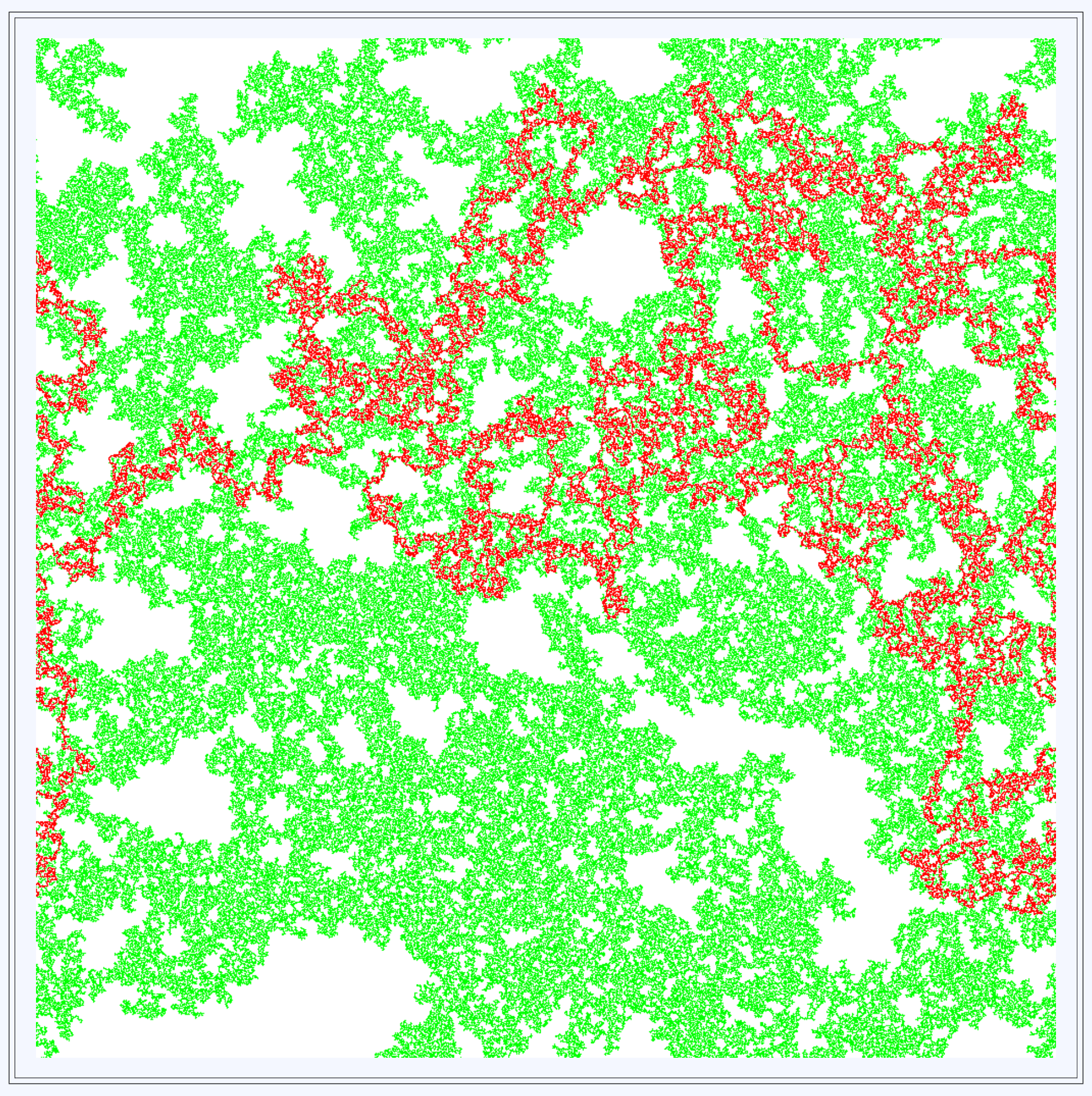
SAWs show universal scaling behavior, with "critical" exponents that are independent of system details. Most important are the exponents for the number of chains Z and the mean squared end-to-end distance $\langle R^2 \rangle$:

$$Z \sim \mu^N N^{\gamma-1}, \quad \langle R^2 \rangle \sim N^{2\nu}$$

- SAW is a simple but non-trivial model for a polymer and
- can be related to spin-systems (O(n) model).
- It is the basis for θ-polymers or the HP model.
- Exponents for fractal substrates are still controversial.

CRITICAL PERCOLATION CLUSTERS

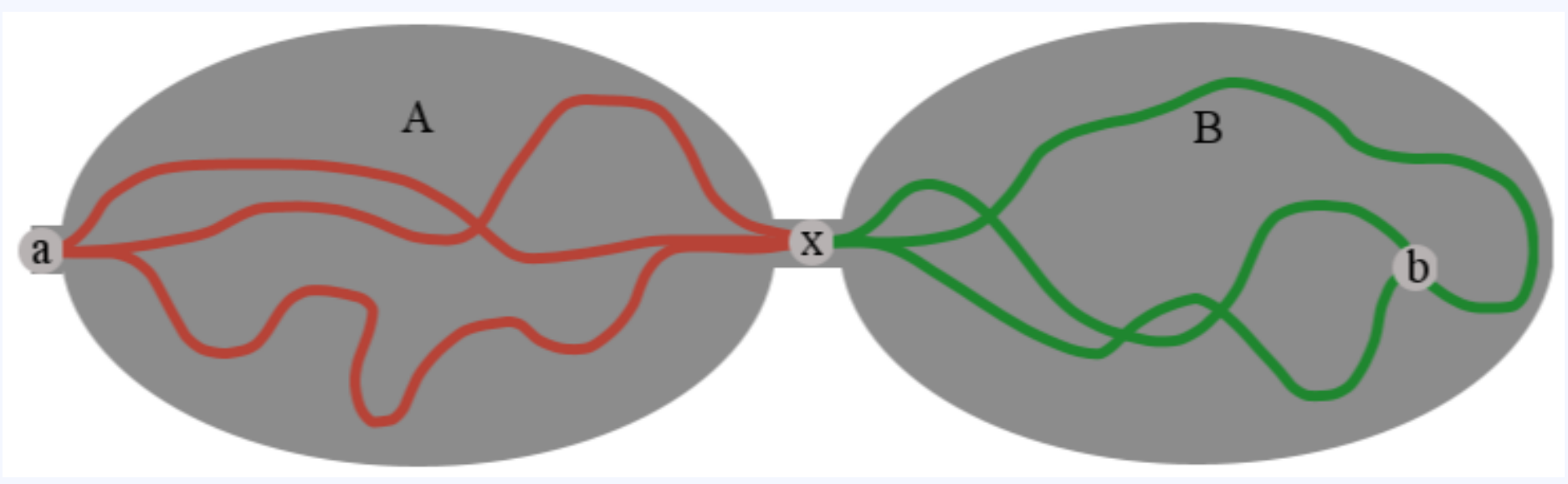
The system-spanning cluster that appears at p_c is a self-similar, fractal object. It is very fragile; removing only $O(1)$ sites is enough to divide it. This is expressed by the backbone, the part that remains when all singly connected "dangling ends" are removed.



Percolation cluster on a 1000x1000 square lattice with backbone marked in red.

IDEA: DIVIDE AND CONQUER

If two parts of a cluster are connected through one site only, one can construct the paths on the whole cluster from the segments within the pieces.



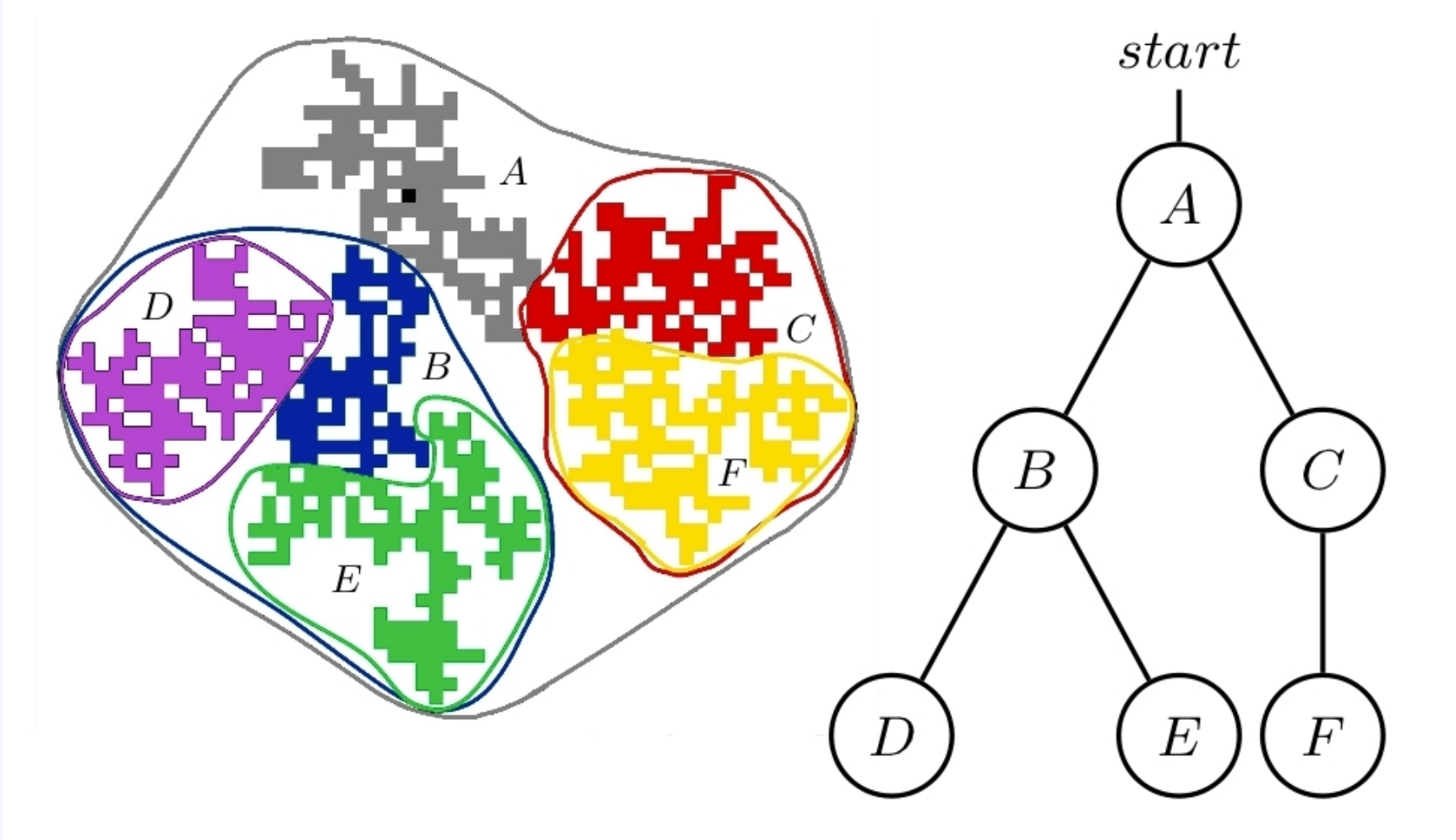
Paths $a \to b$ can be built from segments $a \to x$ and $x \to b$
The number of chains of length l from a to b is obtained via

$$Z_{a \to b}[n] = \sum_{i=0}^{n} Z_{a \to x}[i] \cdot Z_{x \to b}[n-i] \qquad (1)$$

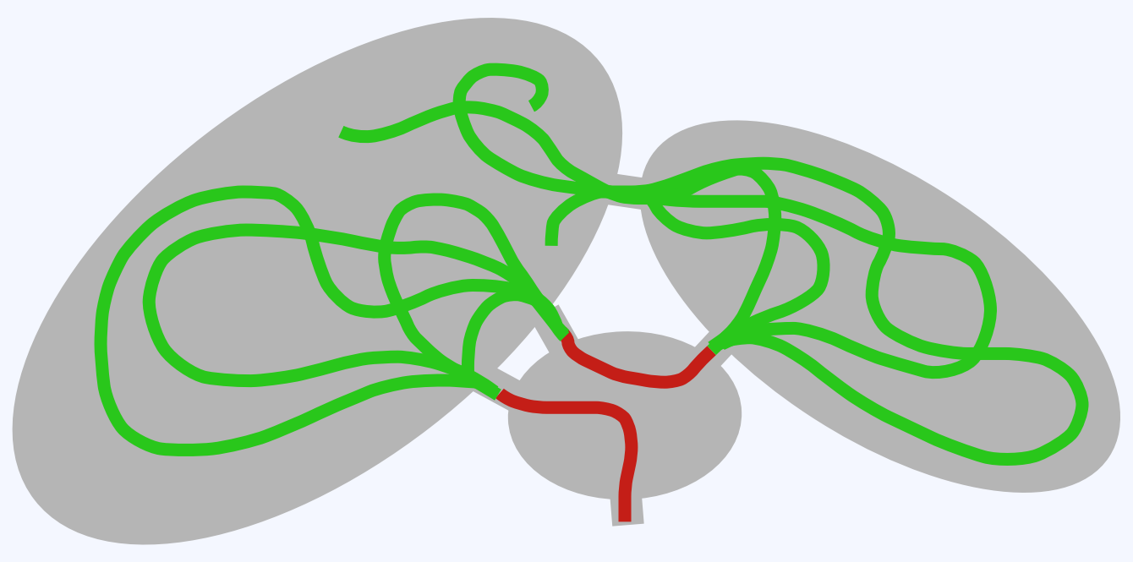
For more than one connection things are more complicated, but the principle remains the same.

BASIC STRATEGY

- Create cluster and cut off remote regions.
- Decompose cluster into nested pieces ("blobs") with few connections on all length scales and set up tree hierarchy.



- Determine paths through blobs whose "children" have already been dealt with, actively counting only in the region outside of the children.

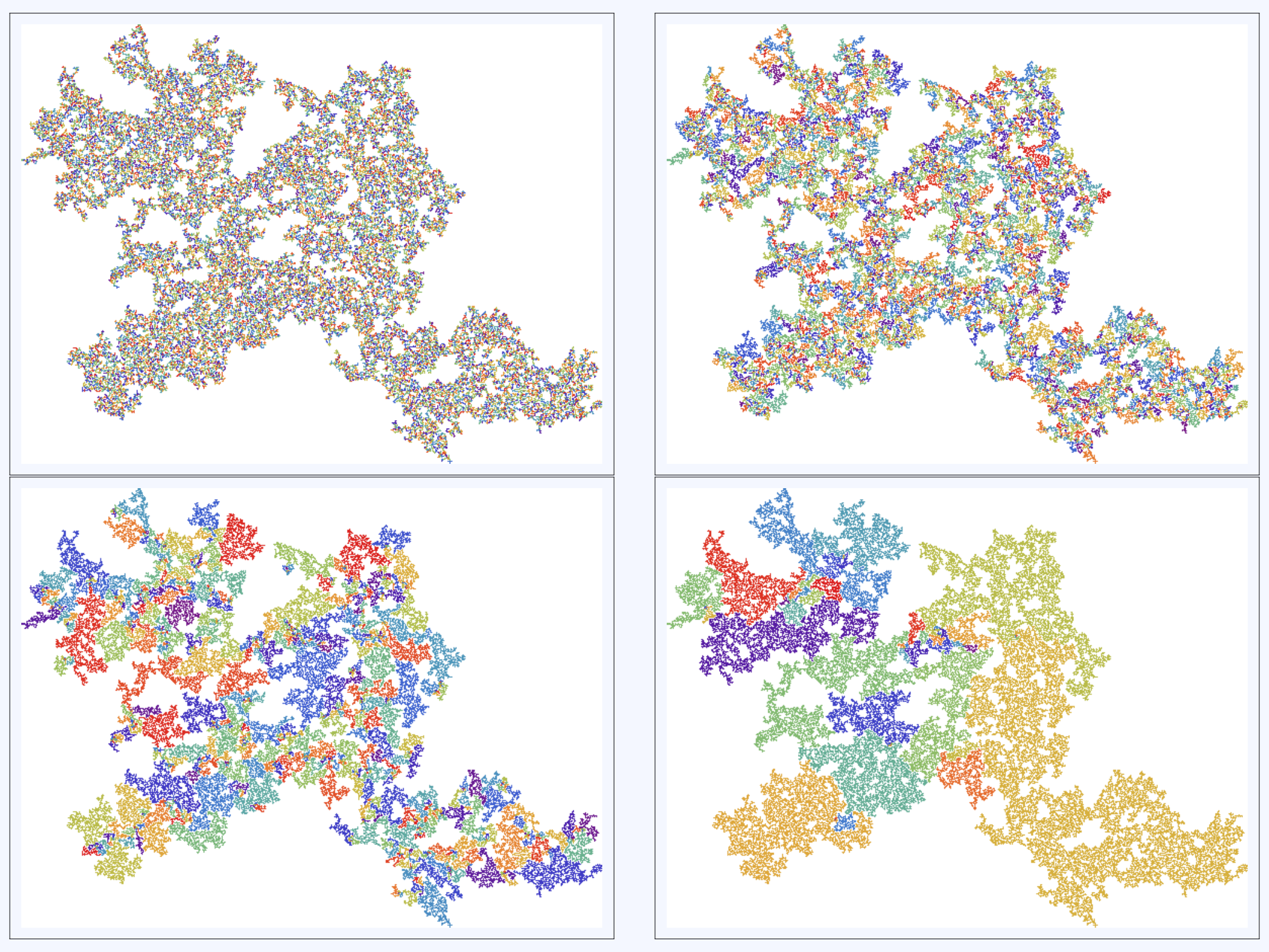


- The true numbers of paths are calculated after the counting by correctly combining the counted paths with those through the children (as in Eq. 1).

HIERARCHICAL DECOMPOSITION

Blobs must fulfill two requirements in order to keep storage and CPU time low:

1. The number of links to children and parent must be small.
2. The number of "bare" sites outside of the children must be small.

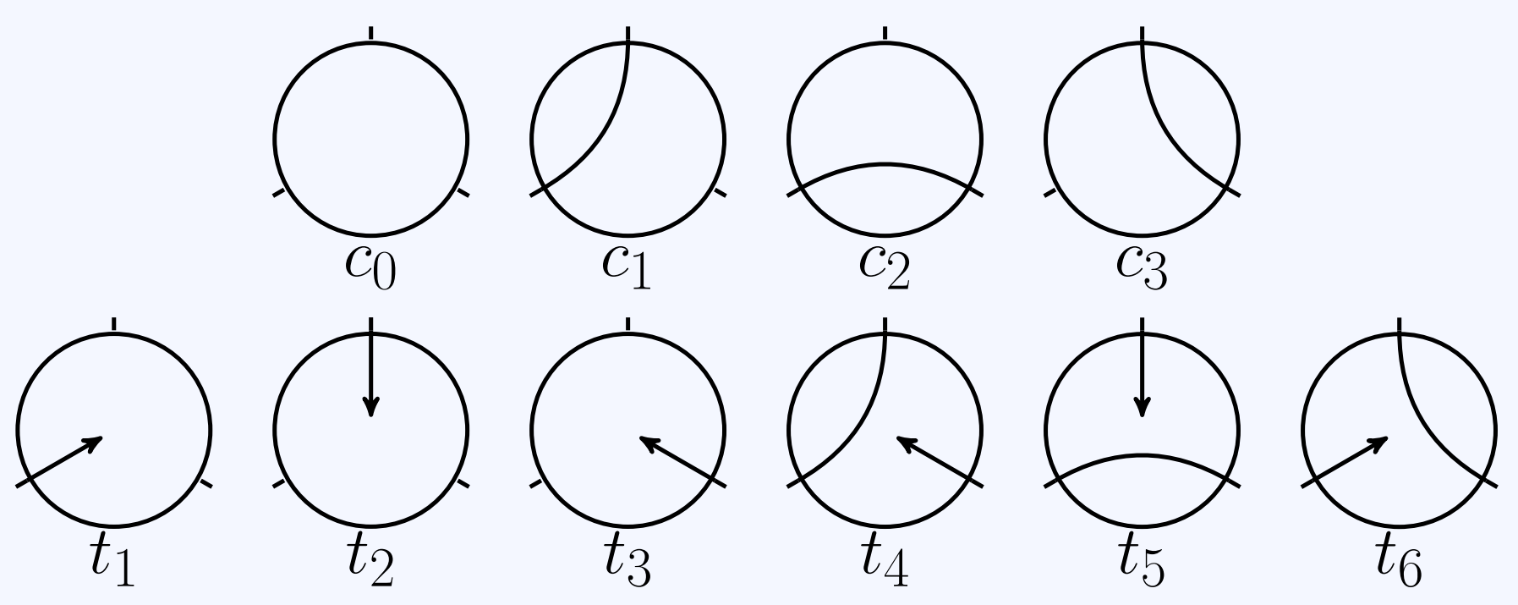


Hierarchy of the pieces is created bottom-up:

1. Define smallest blobs.
2. Judge all options ("moves") to merge neighboring blobs.
3. Perform "best" move (if possible).
4. Judge new moves, go back to 3.

TOPOLOGICALLY DIFFERENT PATHS

"Topologically different" ways to traverse a blob need to be kept in separate classes ("states").



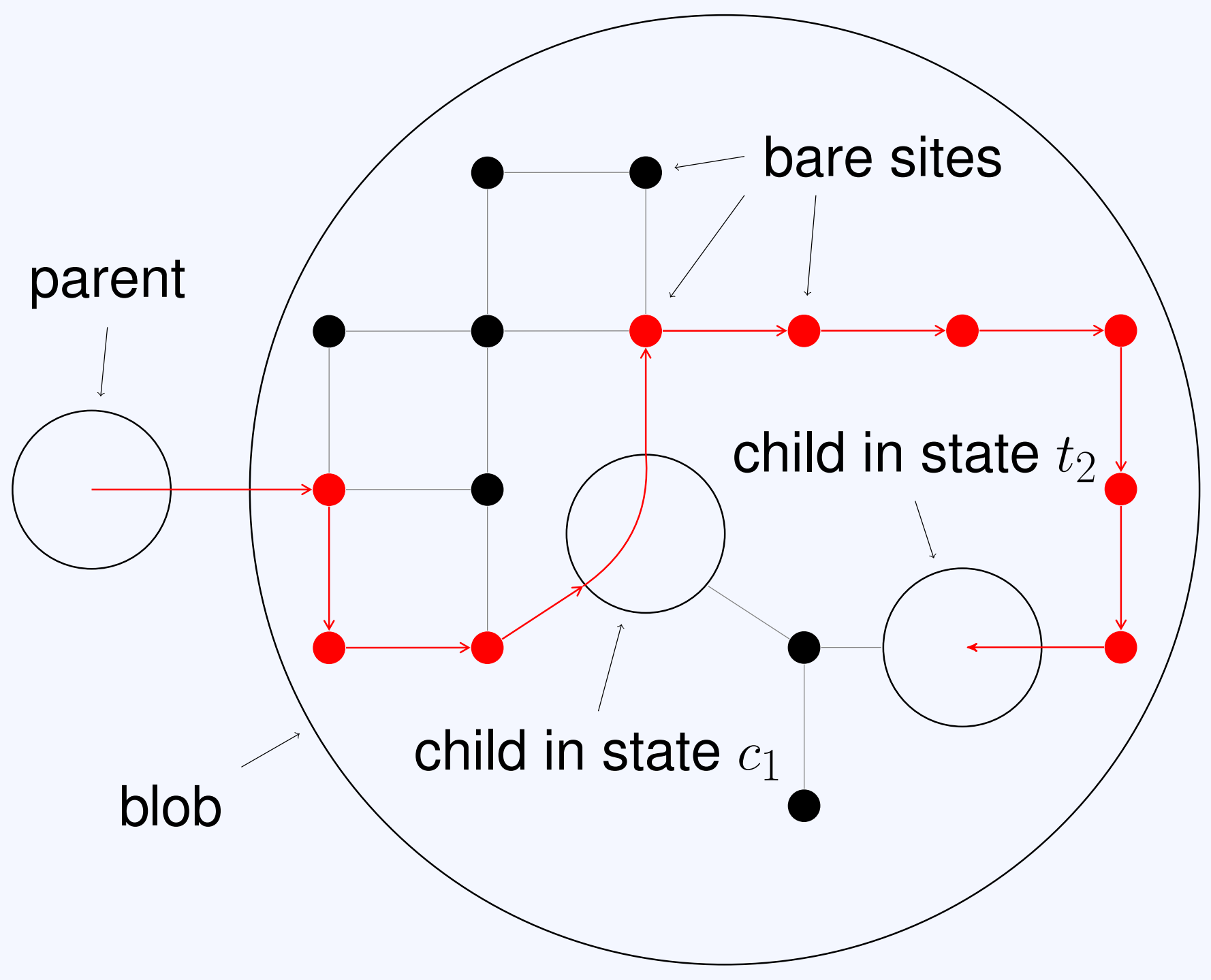
All states for a (2D) blob with three links

Number of states S increases rapidly with number of links L:

$$S(L) = \sum_{i=0}^{\lfloor L/2 \rfloor} \frac{L-2i+1}{i+1} \binom{2i}{i} \binom{L}{2i}$$

SCALE-FREE ENUMERATION

Central problem: counting of paths for each state of a blob whose children have already been dealt with.



Depth-first recursion (backtracking method):

- Start enumerating from the parent site.
- Treat children and parent as "special" sites that change state when visited.
- Store numbers of paths separately for each distinct combination of states.
- Once done, calculate real number of paths for each state of the blob by fitting the right segments together.

Afterwards, all information concerning the children can be discarded, and the blob will itself shrink to a single site when its parent is treated in the same manner.

PERFORMANCE

So far, SAWs of up to 1000 steps have been enumerated on 2×10^5 clusters. The number of SAWs of length $N = 1000$ is typically around 10^{170}.

- Decomposition and enumeration of a cluster took about 8 minutes on average.
- Best MC methods would need weeks (maybe months) to get reliable estimates.
- Normal exact enumeration would take about 10^{150} years.

Some results:

Steps N	$\langle\langle R^2 \rangle\rangle$	$\langle \ln Z \rangle$
50	$3.572(3) \times 10^2$	20.666(6)
100	$1.054(1) \times 10^3$	39.831(9)
200	$3.104(3) \times 10^3$	77.79(1)
500	$1.293(2) \times 10^4$	190.76(2)
1000	$3.788(5) \times 10^4$	378.00(3)

Estimates for the exponents: $\nu = 0.7754(15)$, $\gamma \approx 1.35(3)$.

CURRENT AND FUTURE PROJECTS

- Adaptation of the program to higher dimensions.
- Backbone vs. full cluster: are the exponents the same?
- Crossover behavior to $p < p_c$ ("lattice animals") and $p > p_c$.
- Extensions of the SAW: self-avoiding rings, star polymers, or SAWs with short-range attraction (θ-polymers).

References

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