Monte Carlo calculation of the hydrodynamic radius for self-avoiding walks

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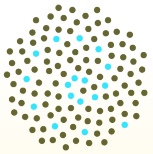
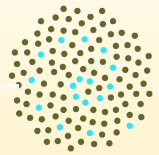
MASCOS, The University of Melbourne

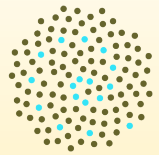
Statistical mechanics of soft matter, $(SM)^2$
RMIT University, City Campus
November 21, 2013





Self-avoiding walk model

- A walk on a lattice, step to neighbouring site provided it has not already been visited.



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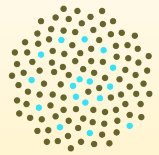
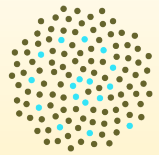


Self-avoiding walk model

- A walk on a lattice, step to neighbouring site provided it has not already been visited.
- Models polymers in good solvent limit.
- Exactly captures universal properties such as critical exponents.



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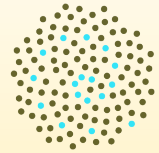

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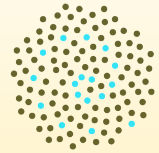

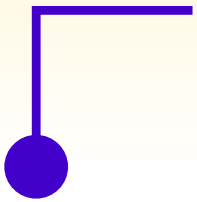

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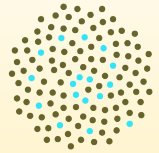

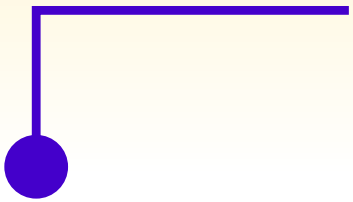

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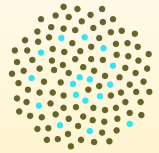

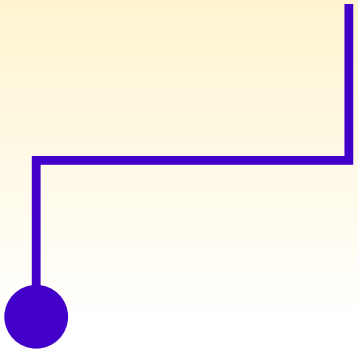

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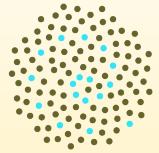

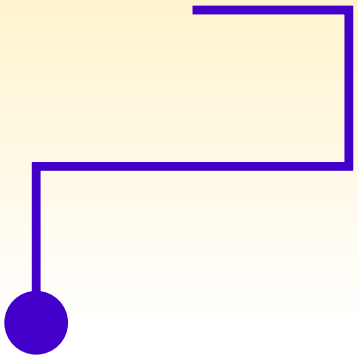

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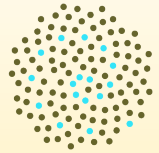

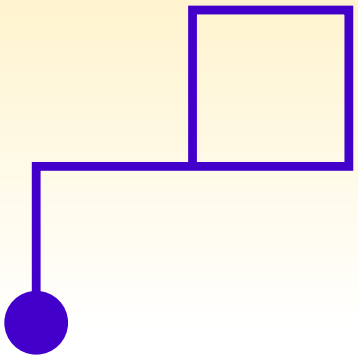

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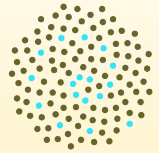

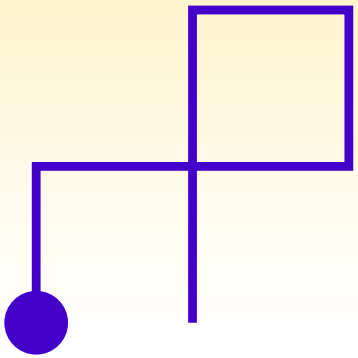

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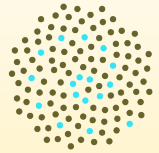

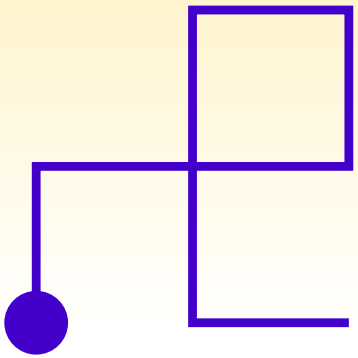

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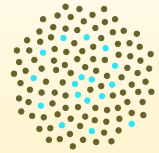

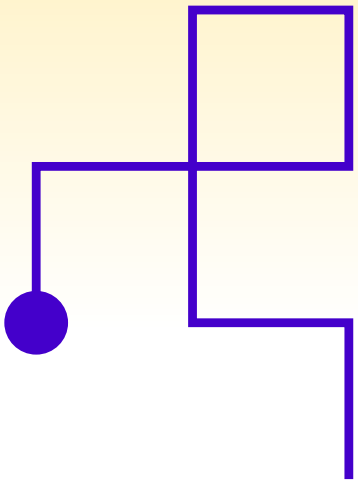

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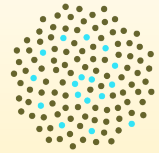

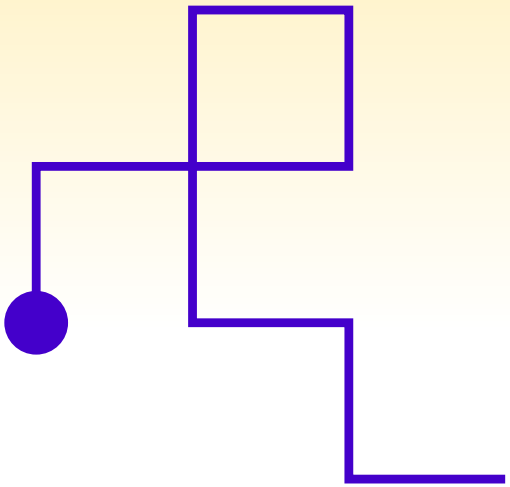

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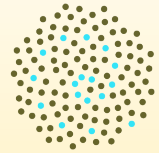

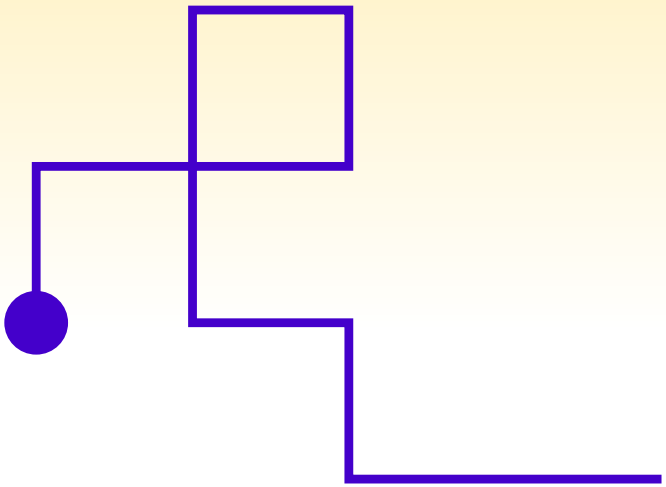

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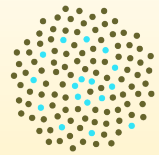

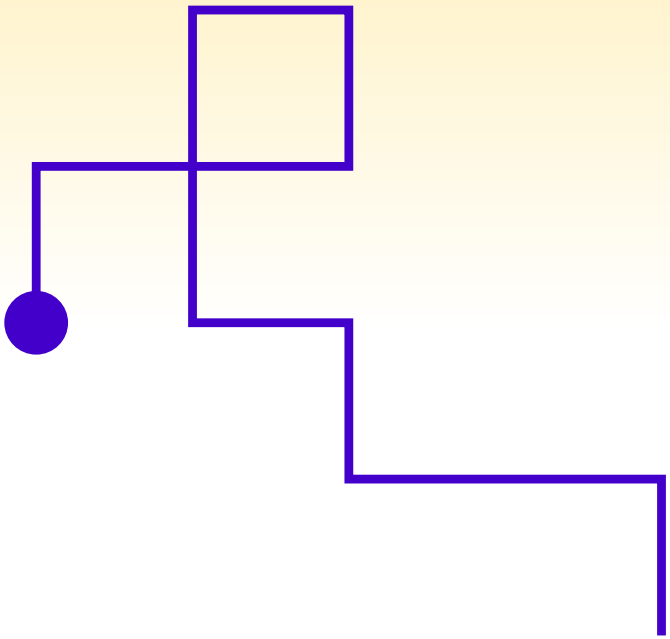

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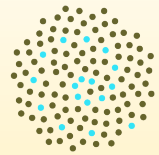

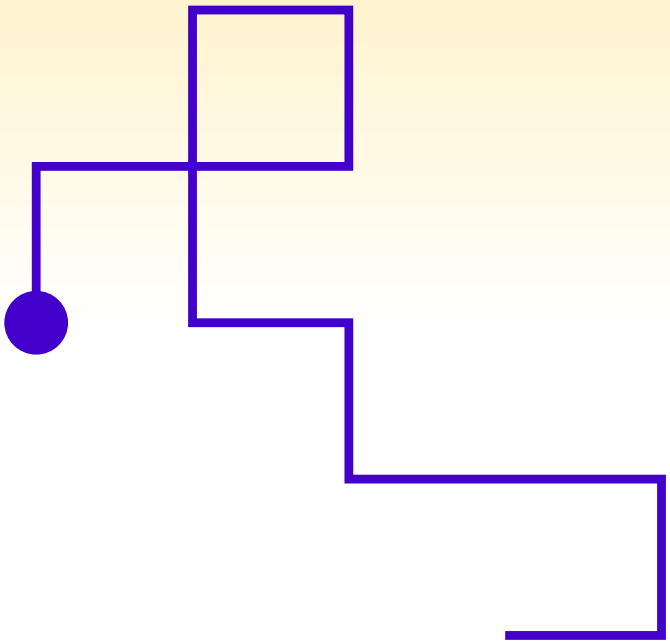

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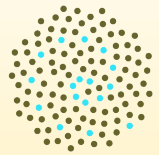

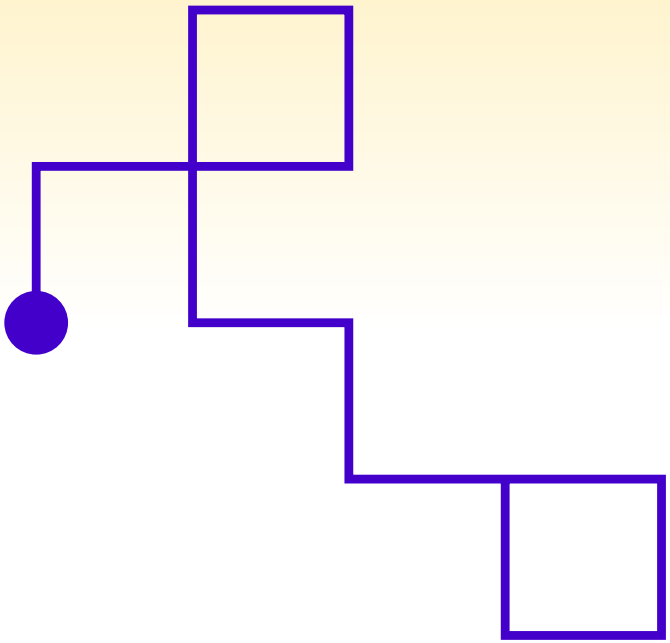

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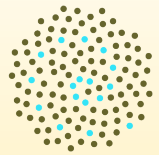

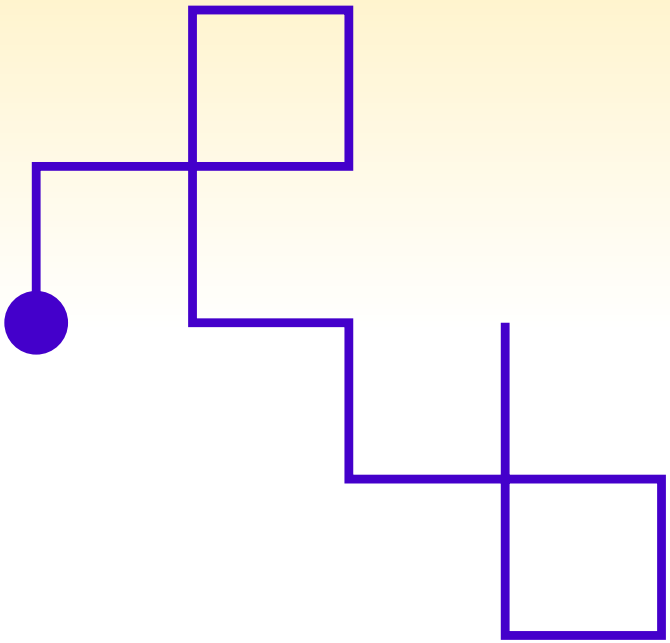

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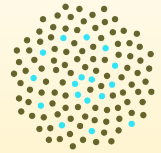

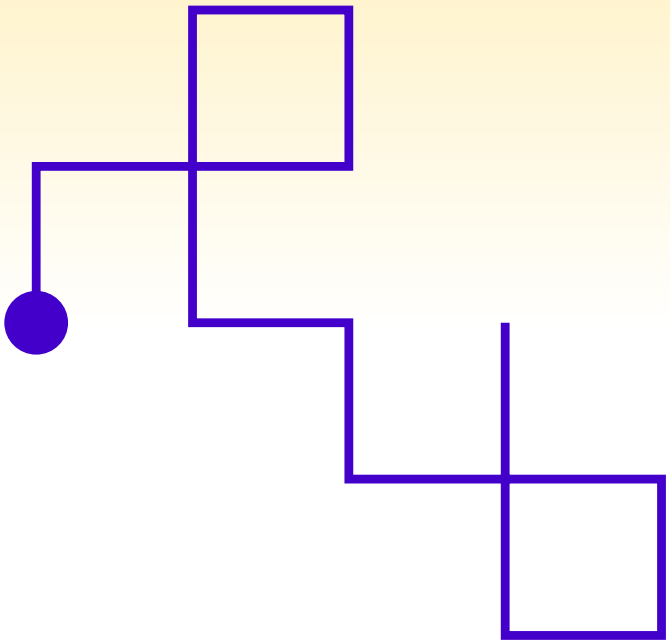

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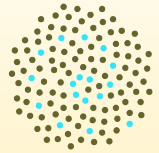

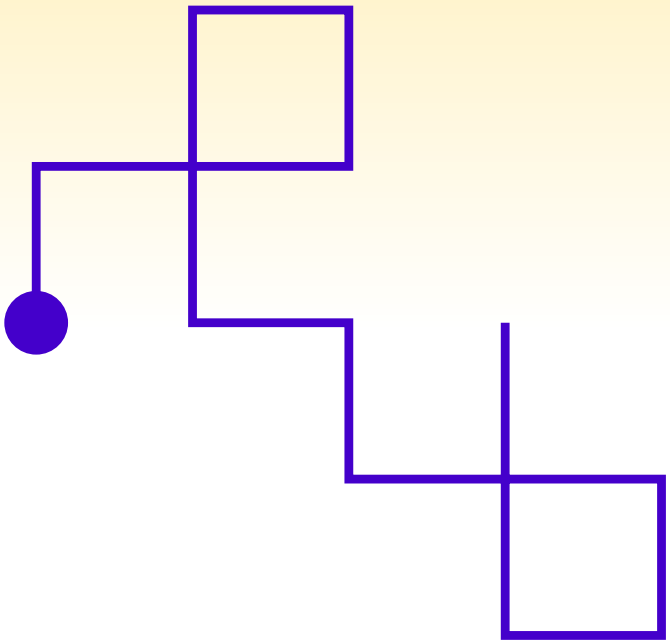

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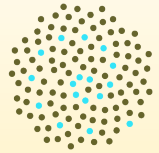

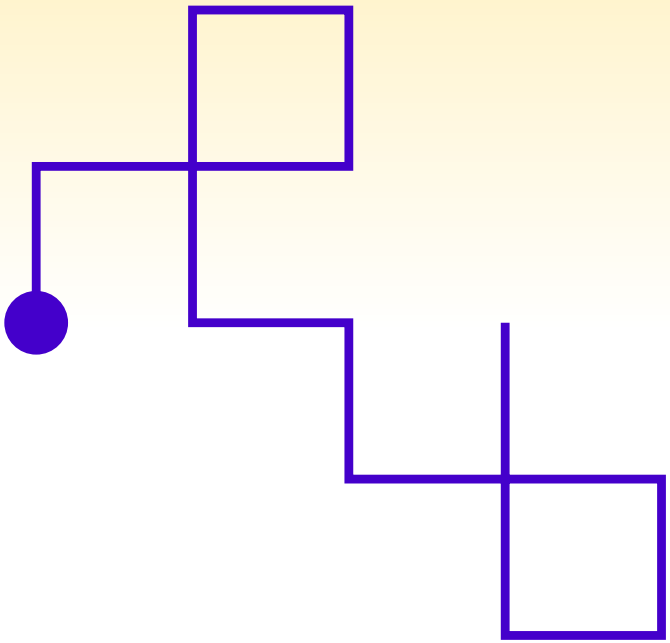

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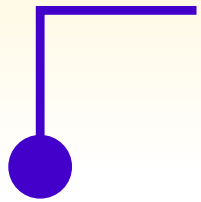

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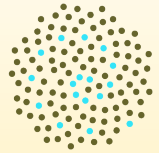

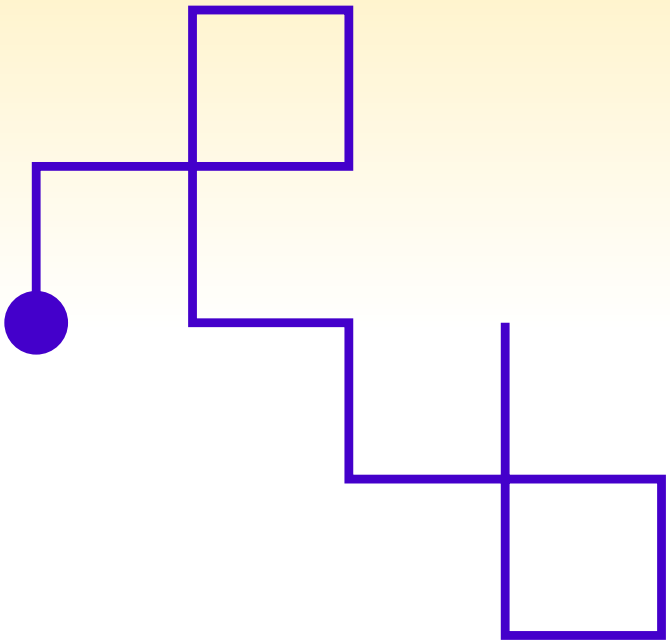

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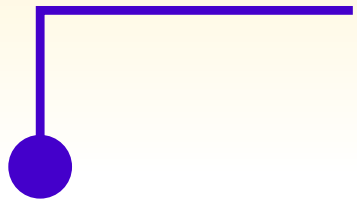

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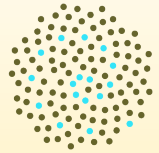

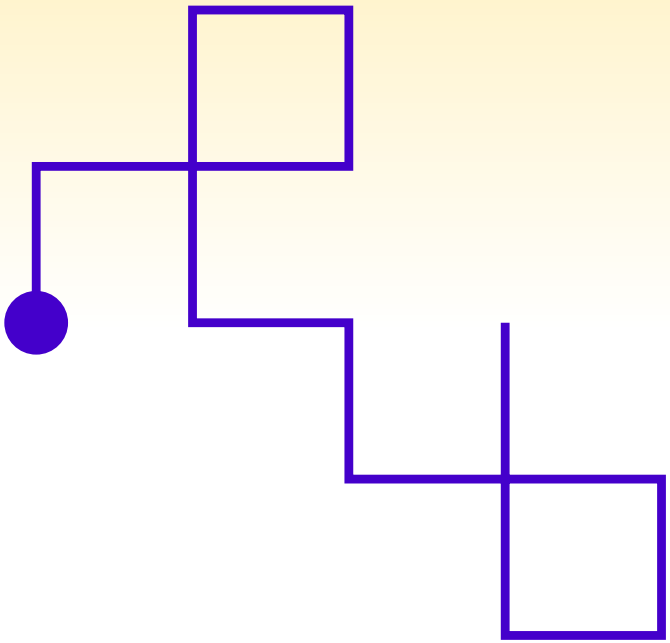

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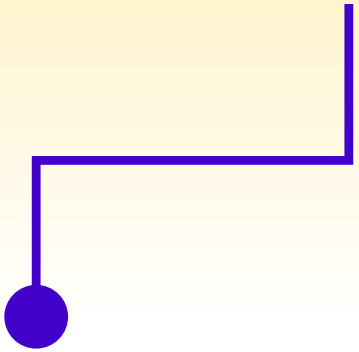

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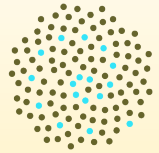

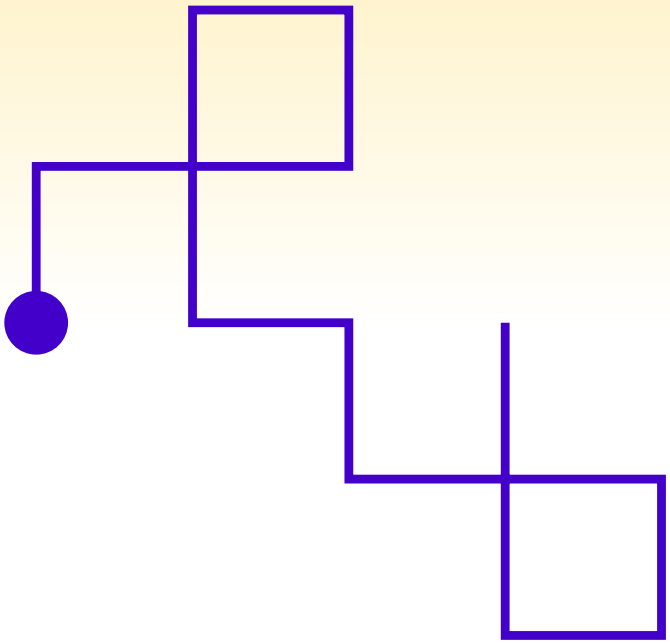

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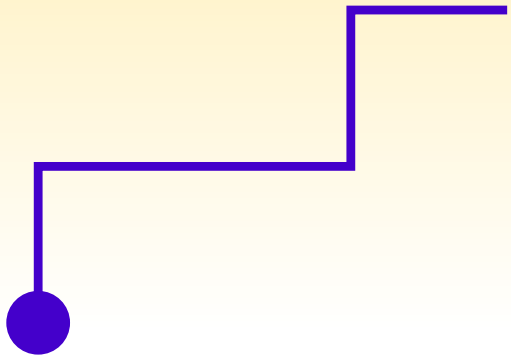

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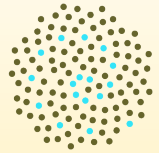

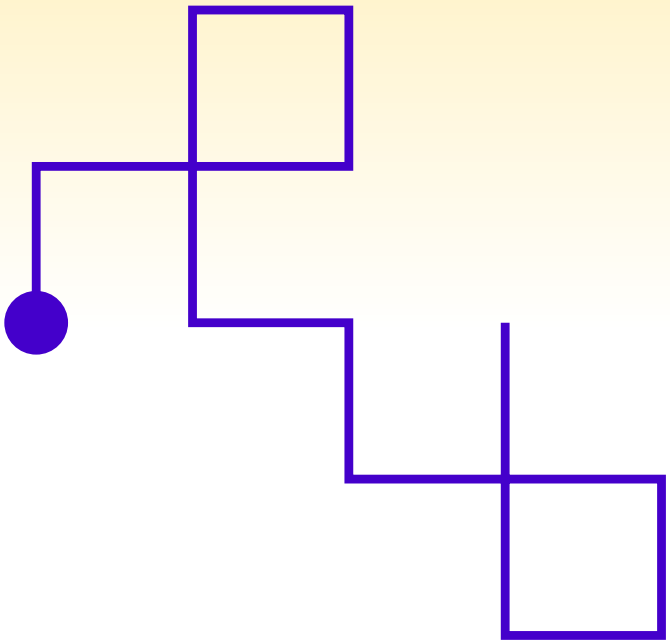

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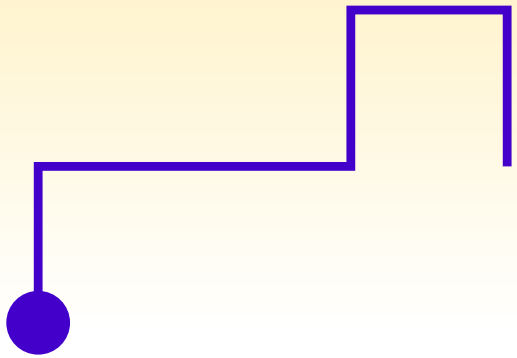

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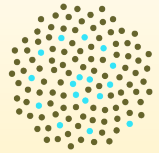

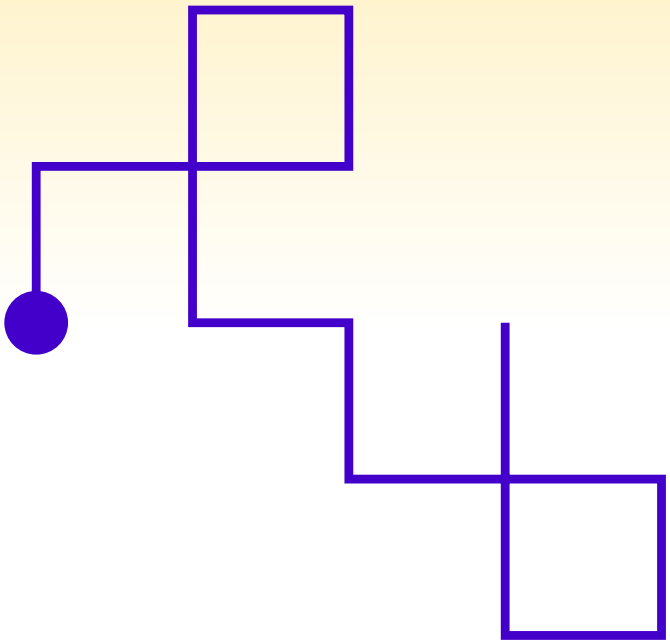

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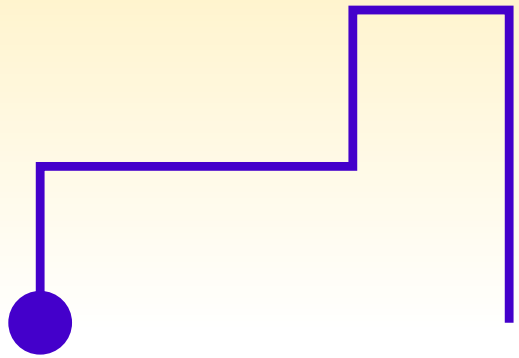

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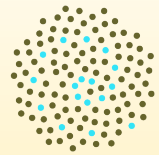

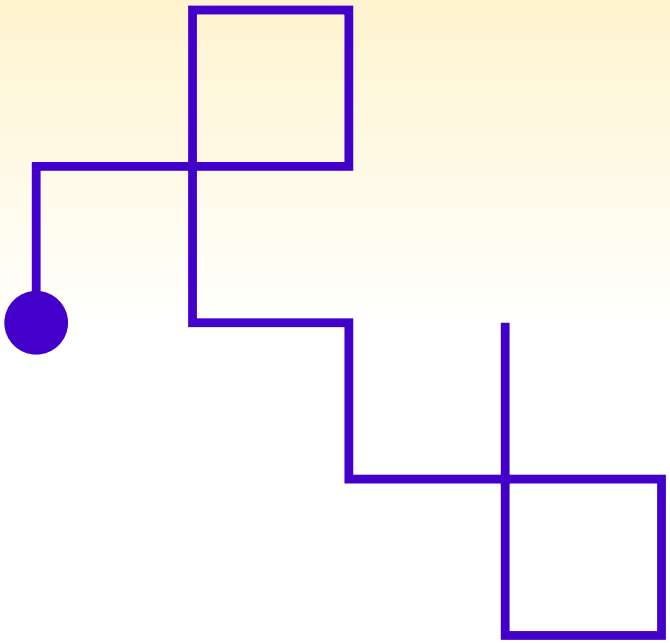

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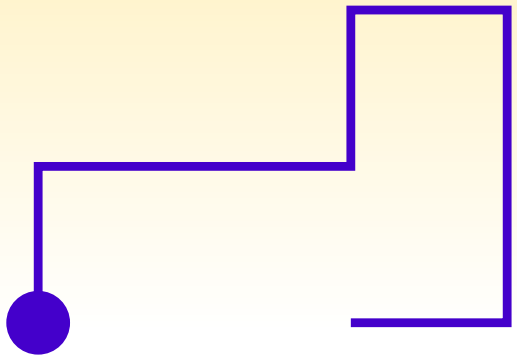
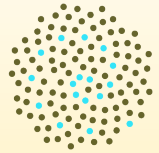
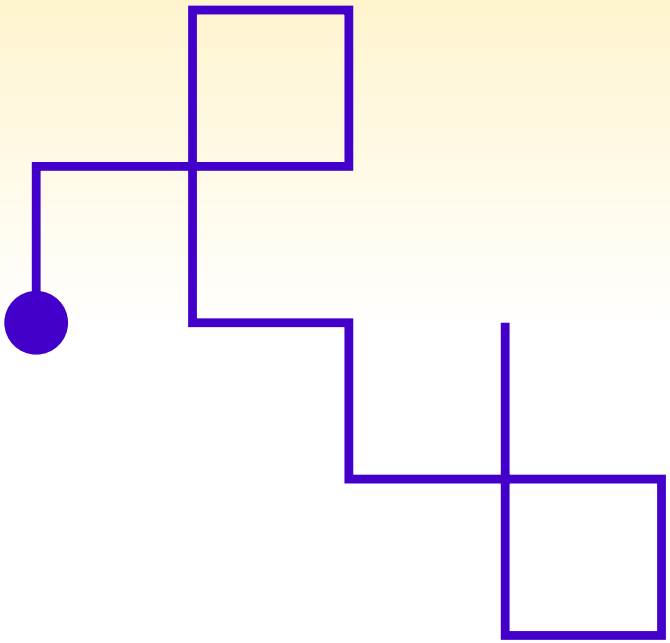
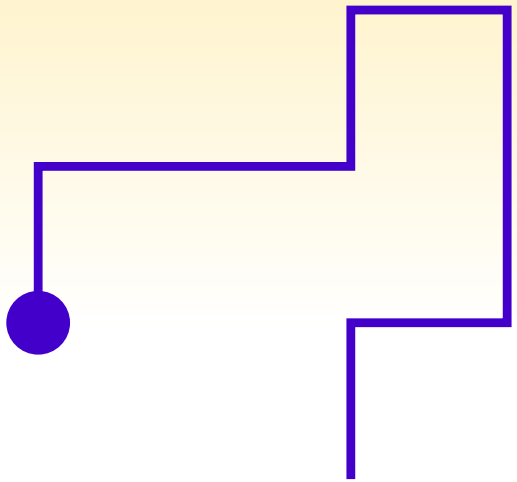


Self-avoiding walk





Simple random walk



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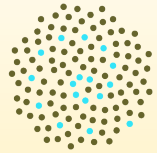

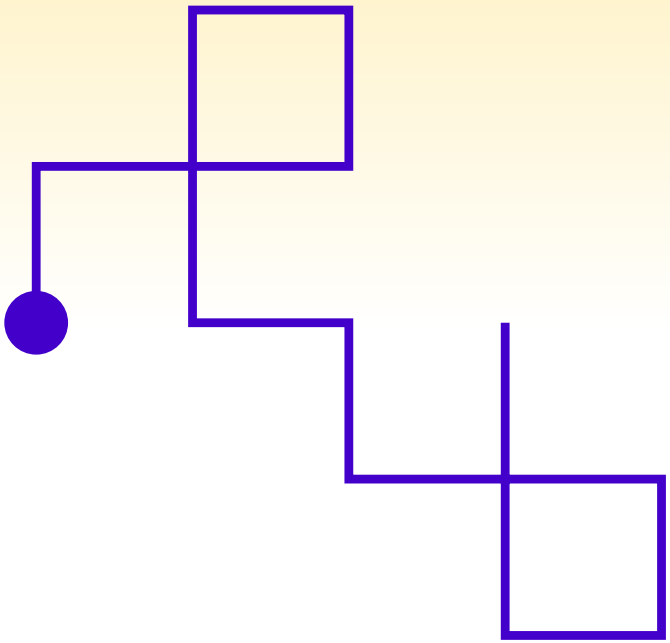

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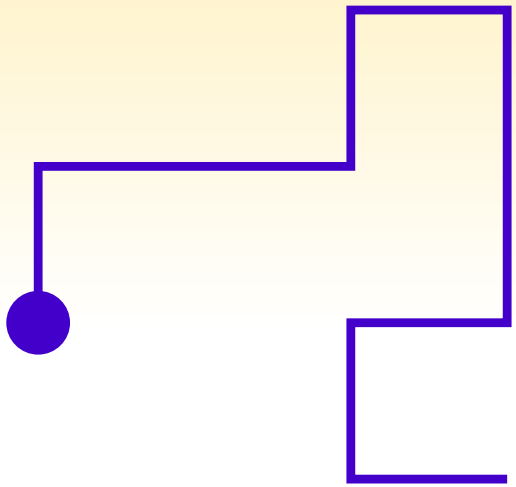

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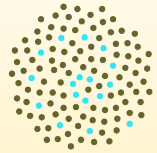

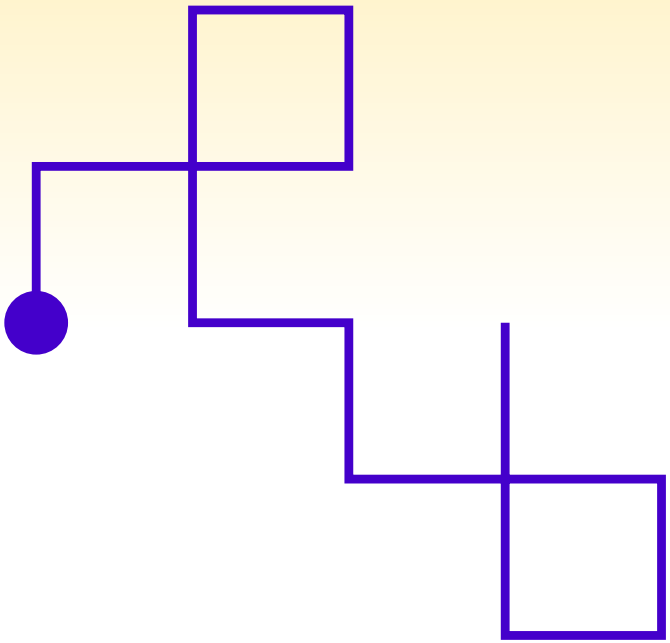

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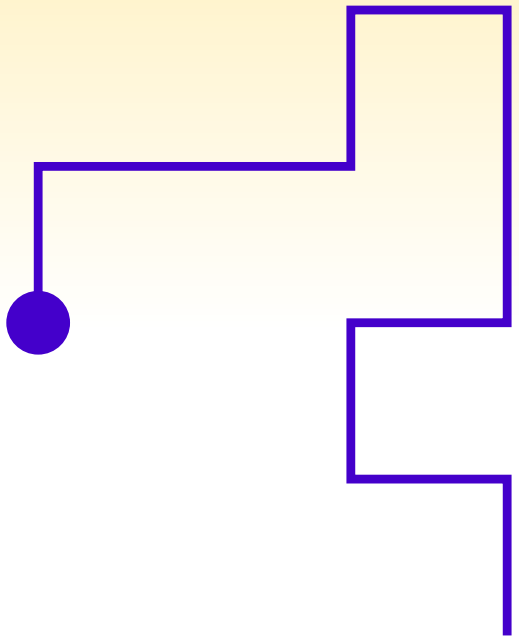

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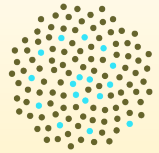

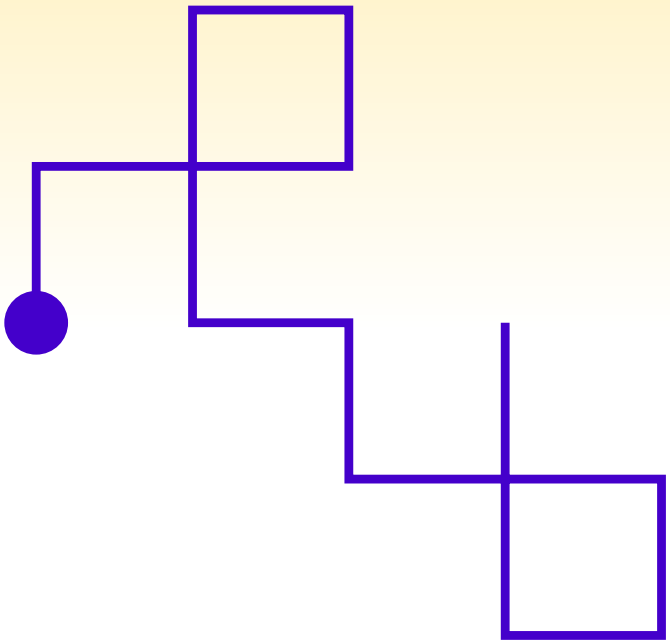

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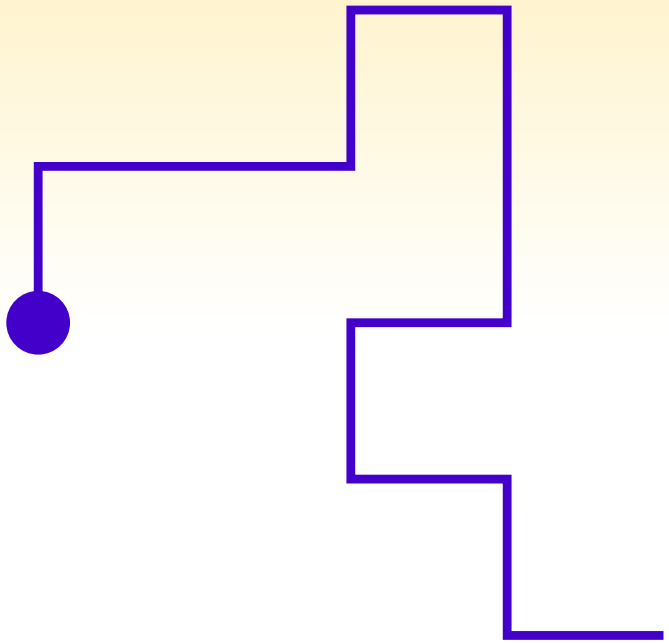

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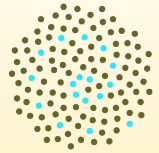

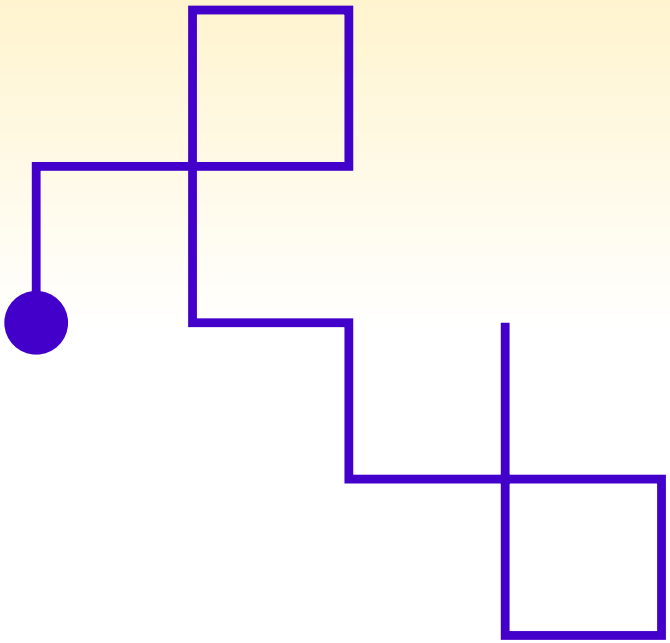

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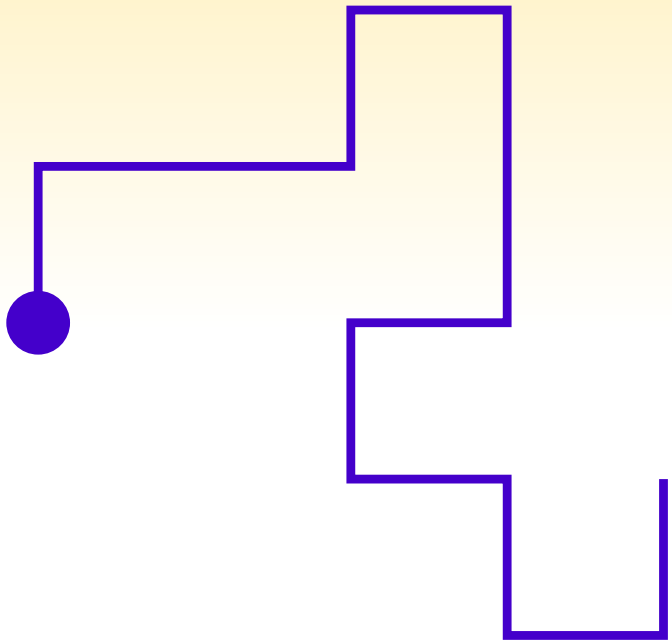

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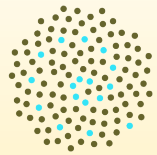

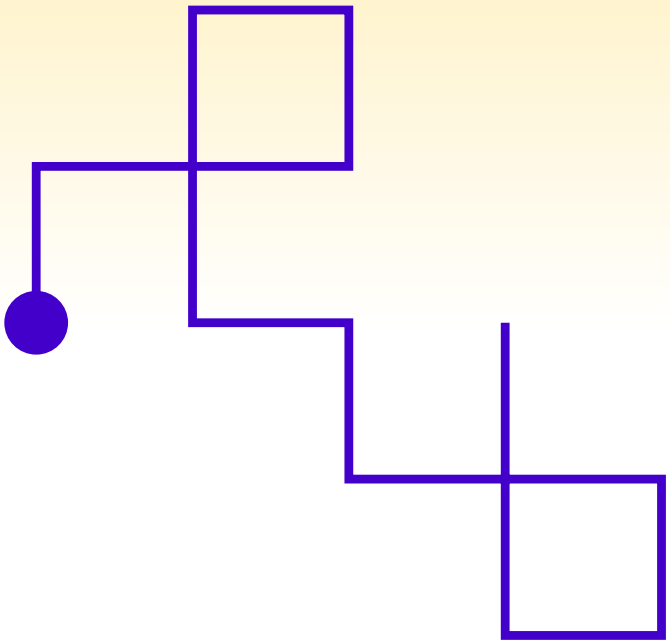

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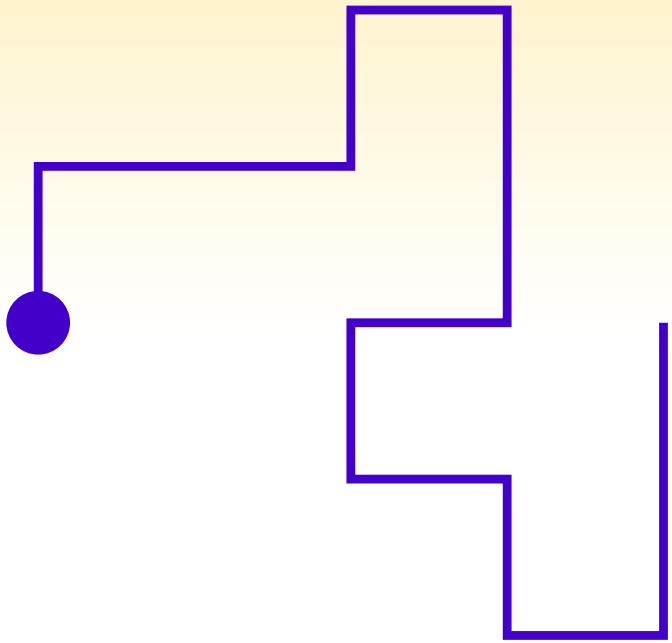

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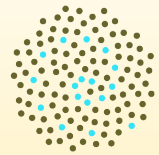
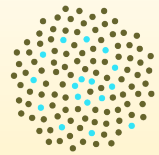
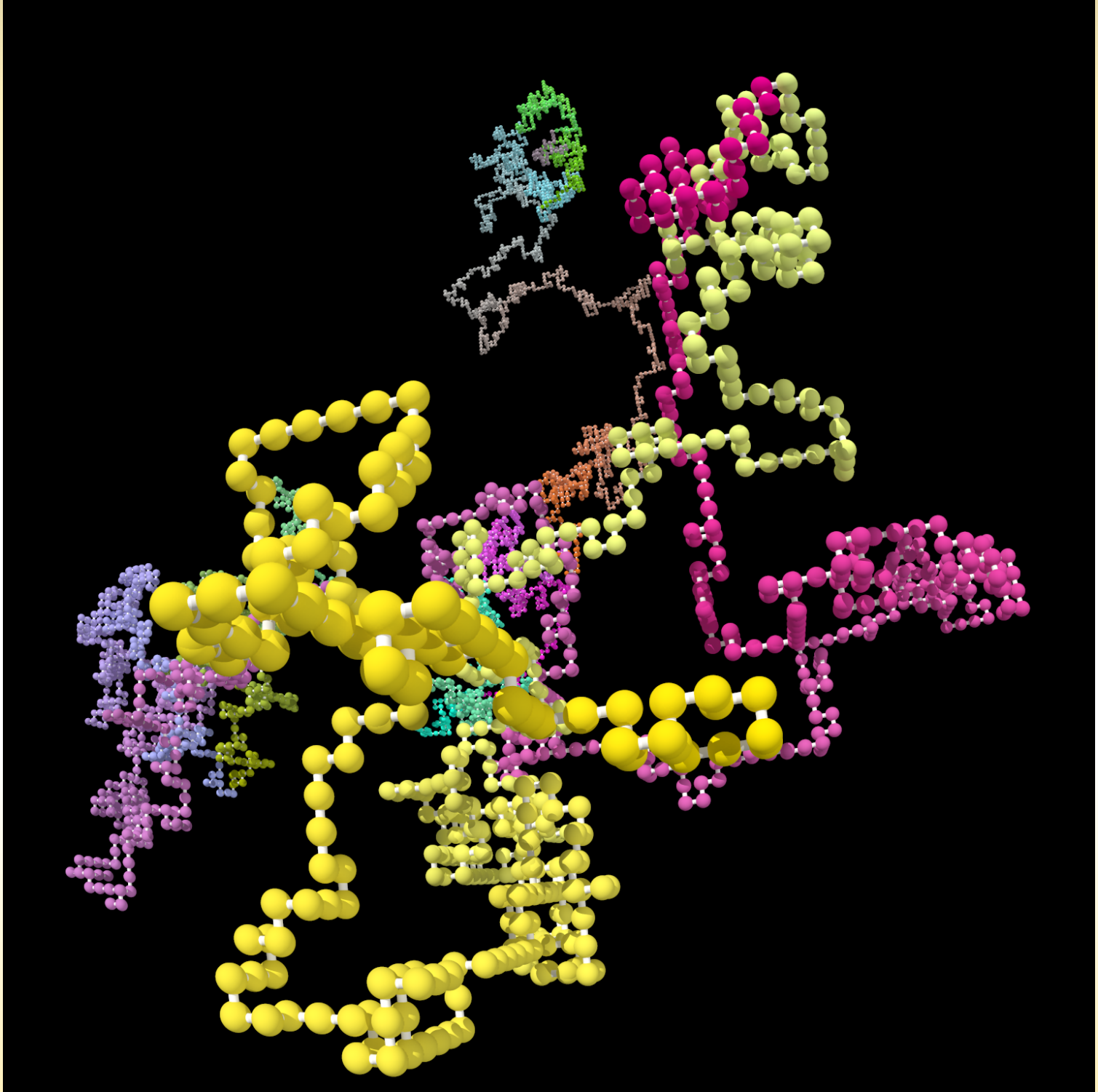
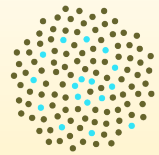


A typical SAW of 5000 steps on the simple cubic lattice:





- Polymers can't have two monomers in the same place.



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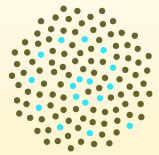

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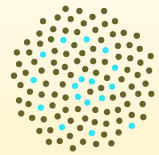

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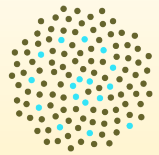
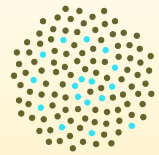
- E.g. growth in size of a polymer grows as number of monomers increases.



- Typical size of a SAW / polymer grows with the number of monomers, N, as:

$$\mathbf{R} = DN^{\nu}$$



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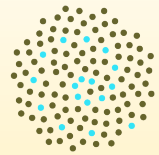

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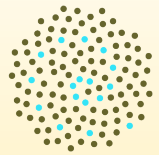

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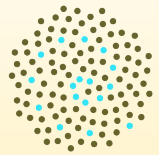

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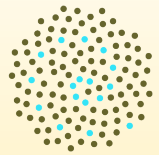

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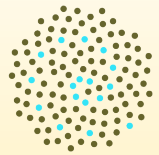

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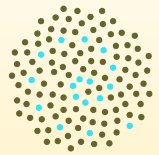
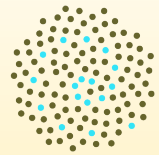


Pivot algorithm

- Markov chain Monte Carlo (MCMC) sampling very powerful for SAW, especially for $d = 3$.



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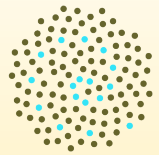
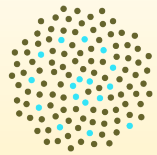


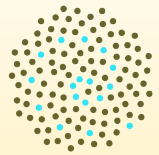
Pivot algorithm

- Markov chain Monte Carlo (MCMC) sampling very powerful for SAW, especially for $d = 3$.
- Estimate physical properties of system by sampling from all possible configurations (state space).
- Basic idea: generate new configurations by deforming current configuration via a "move".



Pivot algorithm

- How can we sample self-avoiding walks?



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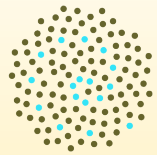
- How can we sample self-avoiding walks?
- Local moves make a small deformation, e.g. adding or removing a monomer, $O(N^2)$ moves to get an "essentially new" configuration.



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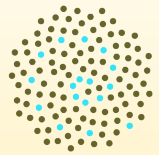

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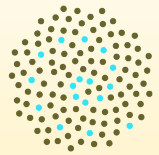
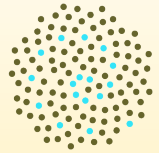
- Global moves can do much better.
- Pivot move: $O(1)$ successful moves for an essentially new configuration.



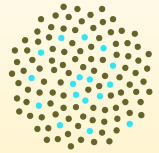
Pivot algorithm

- Procedure:



Pivot algorithm

- Procedure:
  - Choose a pivot site at random



Pivot algorithm

- Procedure:
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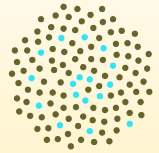

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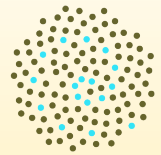

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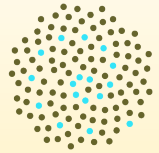

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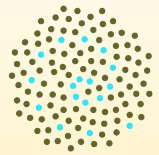
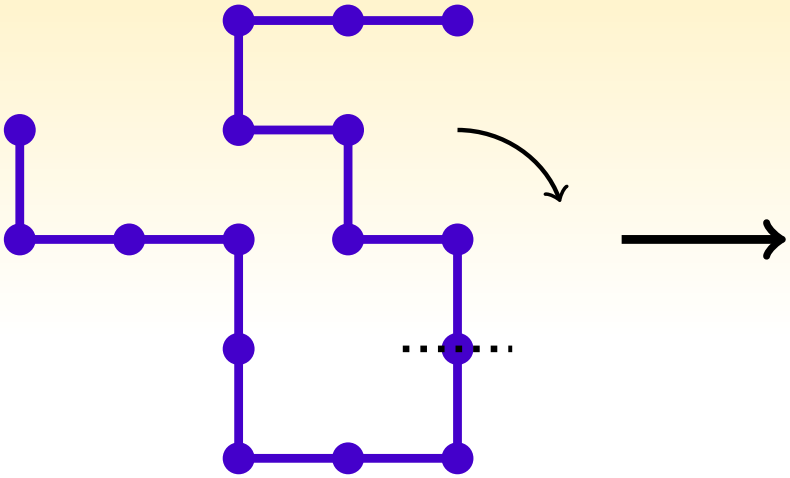
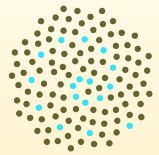
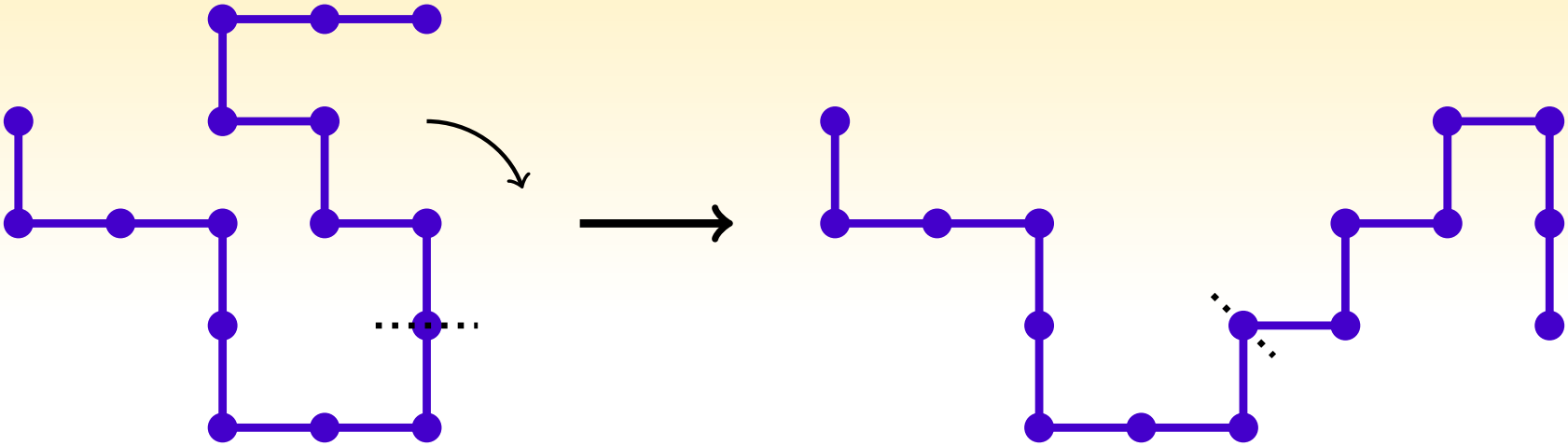
- Ergodic, samples SAWs uniformly at random.





Example pivot move





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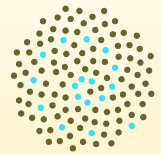
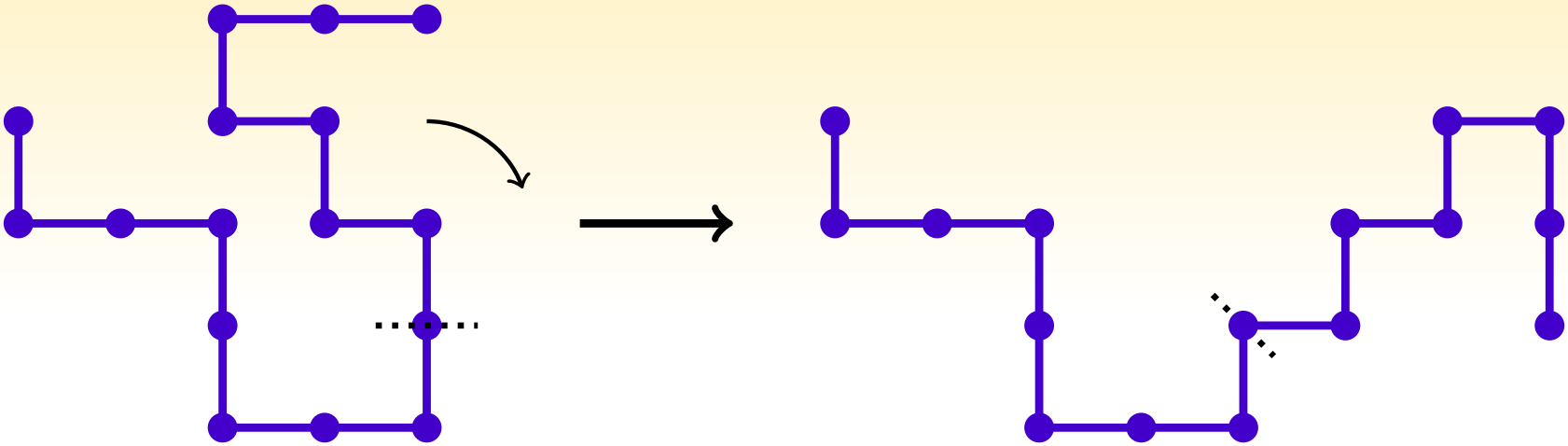
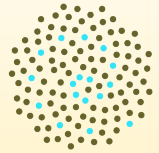




Example pivot move

Run simulation



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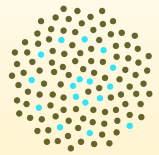

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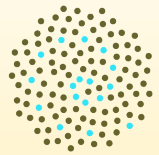

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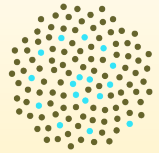
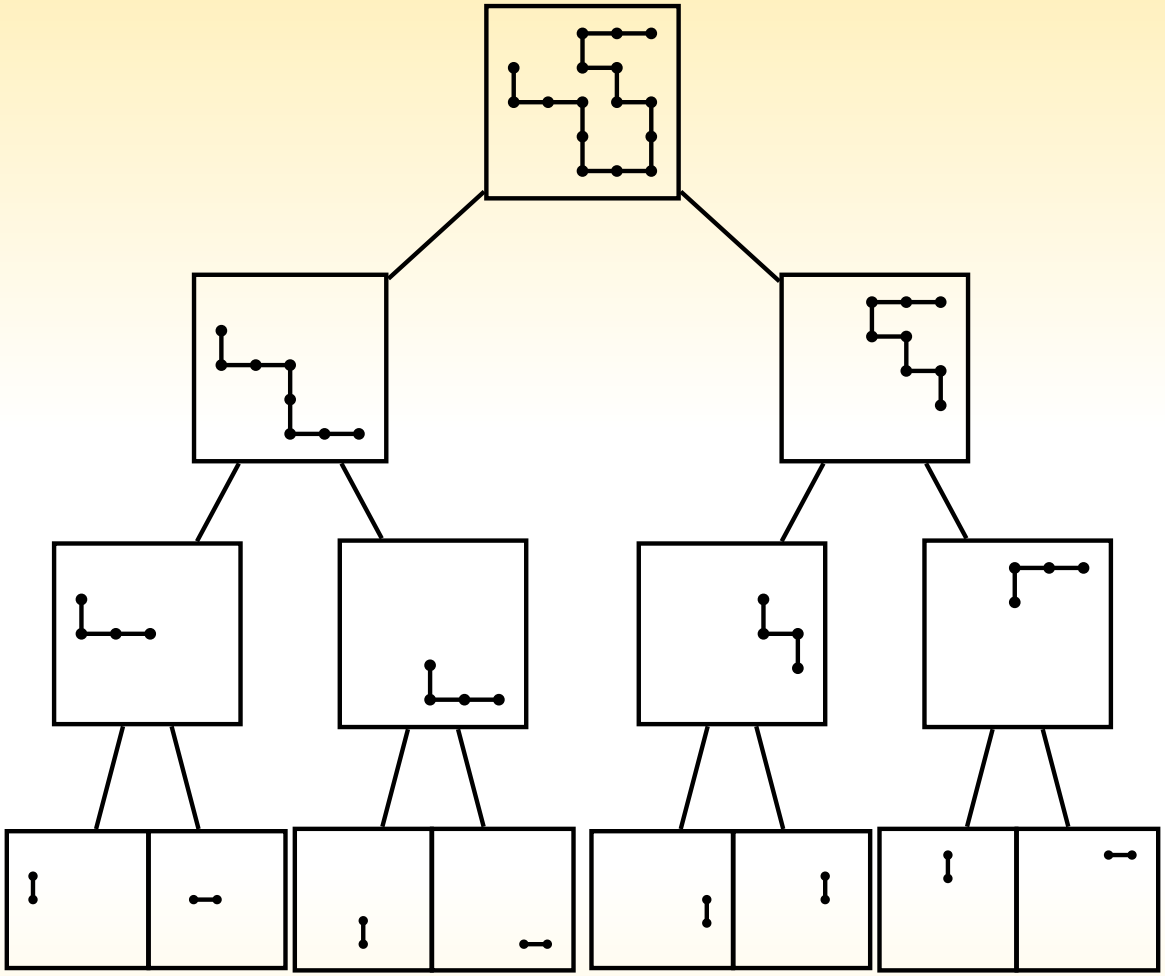
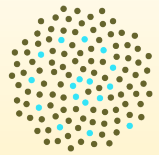
- Bookkeeping can be handled efficiently in binary tree structure.

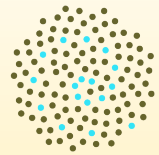




SAW-tree representation of a walk.



- With a binary tree implementation, pivot move has *global effect* for *local cost*.



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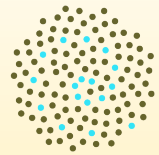

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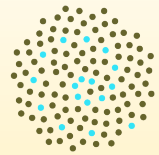

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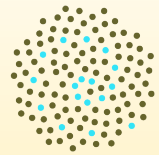

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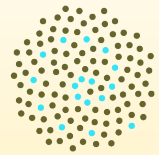

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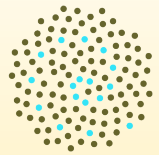

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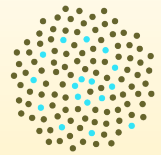

Hydrodynamic radius

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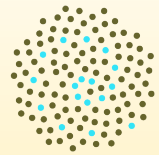

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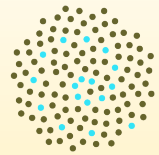

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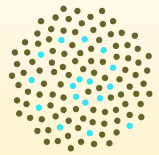

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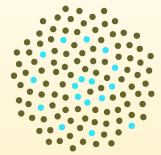

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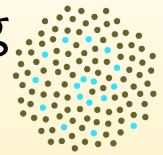

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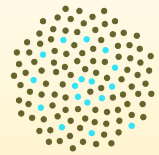

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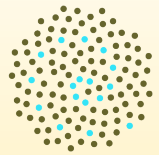

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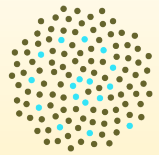

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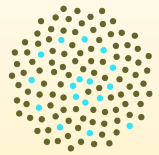

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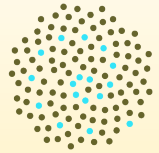

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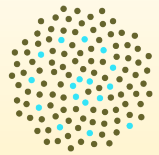

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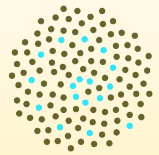
- Our estimator is a weighted version of $1/r_{ij}$, monomers i and j chosen at random.



Results

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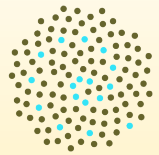

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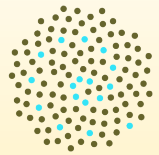

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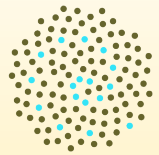

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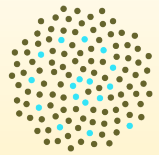

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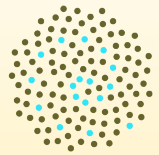

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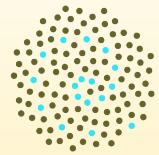

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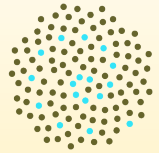

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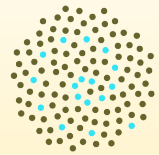

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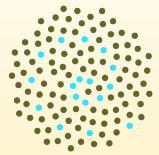

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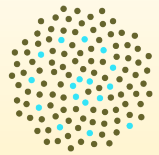

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