Efficient Monte Carlo simulation of polymers

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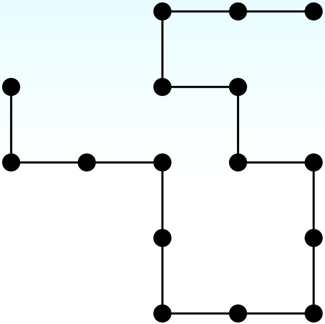
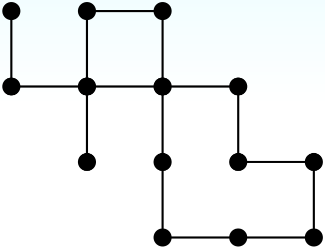


SAW



Not a SAW

Critical phenomena

- The number of SAWs of length N, c_N, tells us about how many conformations are available to SAWs of a particular length:

$$c_N \sim A\ N^{\gamma-1}\mu^N\,[1 + \mathrm{corrections}]$$

- Mean square end to end distance tells us about the size of a typical SAW:

$$\langle R_{\mathrm{e}}^2\rangle_N \sim D_e N^{2\nu}\,[1 + \mathrm{corrections}]$$

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Monte Carlo

- Scheme: top-level method for sampling polymer configurations. Examples include: Markov chain Monte Carlo, umbrella sampling, Wang-Landau, PERM.
- Move set: operations which are used to generate new configurations from old ones.
- Implementation: polymer data structure.
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- Sample from a probability distribution.
- Generate a new configuration from current one.
- Ensure that chain samples uniformly from whole set of configurations.
- Efficiency for calculating observable A determined by degree of correlation in the time series A_i. In particular, the integrated autocorrelation time τ_{int} of the chain.
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Moves

- A move is a transformation of the SAW which may result in a new SAW.
- Local moves include one bead flips and the reptation or slithering snake move.
- Non-local moves include pivots and cut-and-permute moves.
- Many popular local and non-local moves can be defined in terms of "cut-and-paste" moves.

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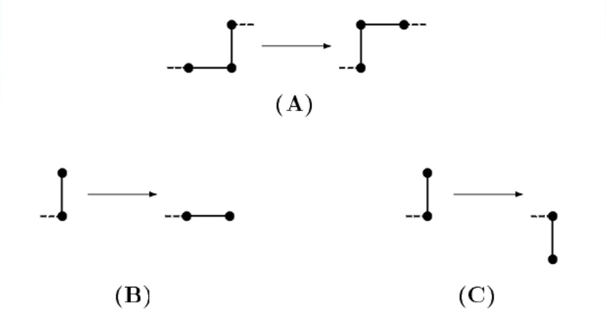
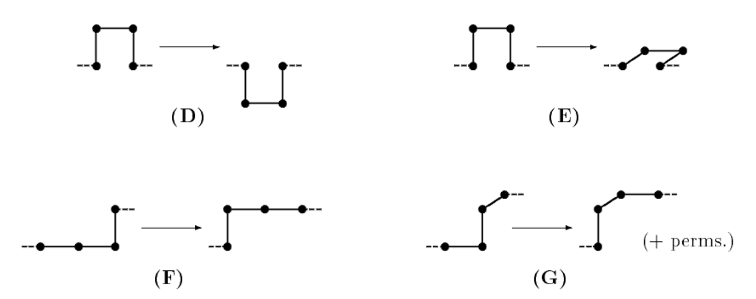


One bead moves (from Sokal, 1994 [Sok94])



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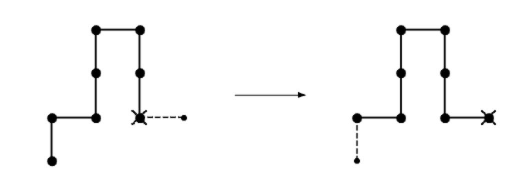
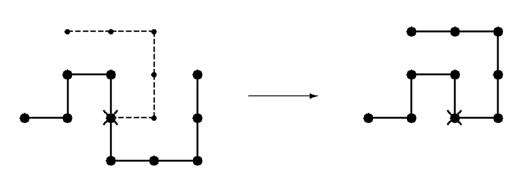
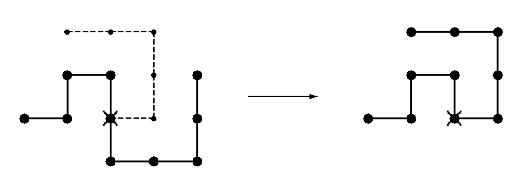


Slithering snake / reptation move (from Sokal, 1994 [Sok94])



Pivot move (from Sokal, 1994 [Sok94])

Non-local move (unless close to end)



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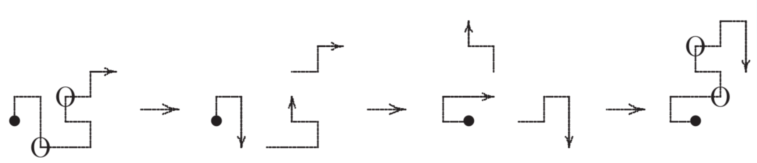
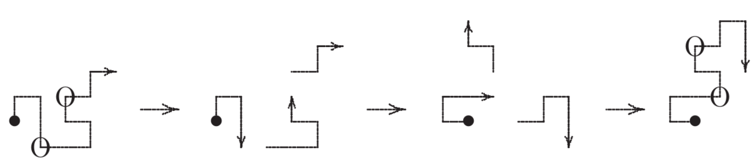


Cut-and-paste move, arbitrary symmetry, may permute sub-walks
(from Janse van Rensburg, 2009 [JvR09])

Scale of move depends on size of sub-walks – any length scale possible. Pivots are a special case of cut-and-paste moves.



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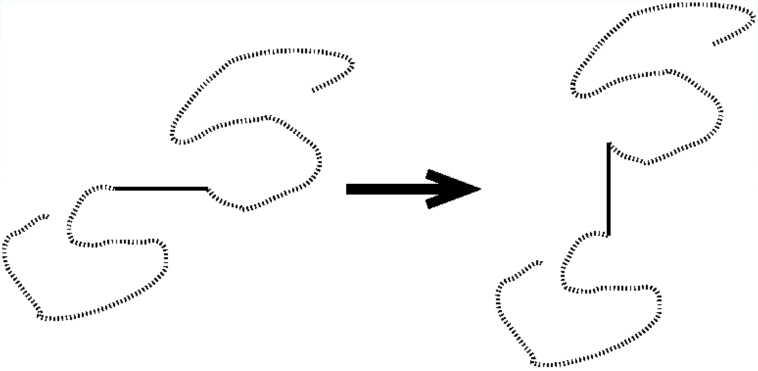

Rotating a single bond in the middle of a SAW, $O(N)$ monomers move distance $O(1)$. Cut-and-paste moves generalise what are usually regarded as “local” moves.

Pivot algorithm

- Invented in 1969 by Lal.
- The power of the method only realised since influential paper by Madras and Sokal in 1988 (over 500 citations).
- Monte Carlo method of choice for studying SAWs and similar models when the length of the walk is fixed.
- Markov chain, pivot operations generate new SAWs. When resulting configuration is not a SAW, move is rejected.
- Will now show a sequence of *successful* pivots applied to an $n = 65536$ site SAW on the square lattice.

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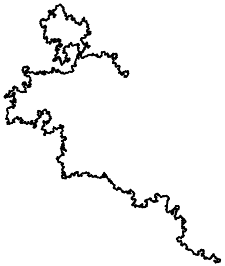

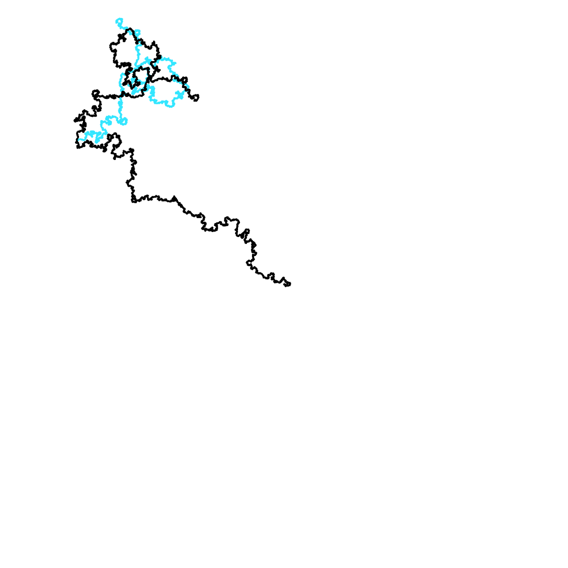

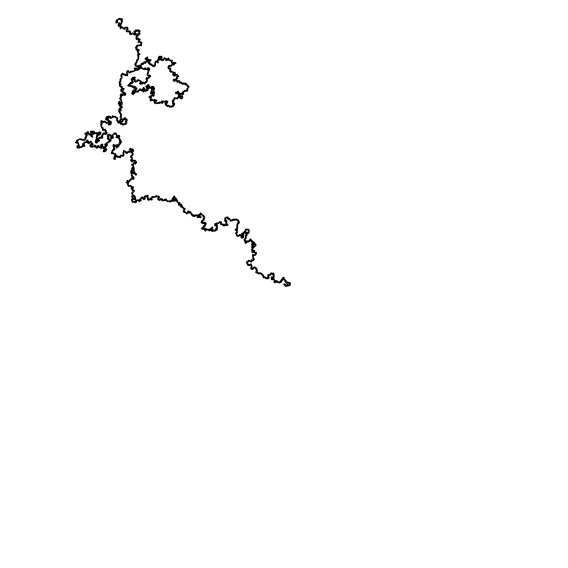

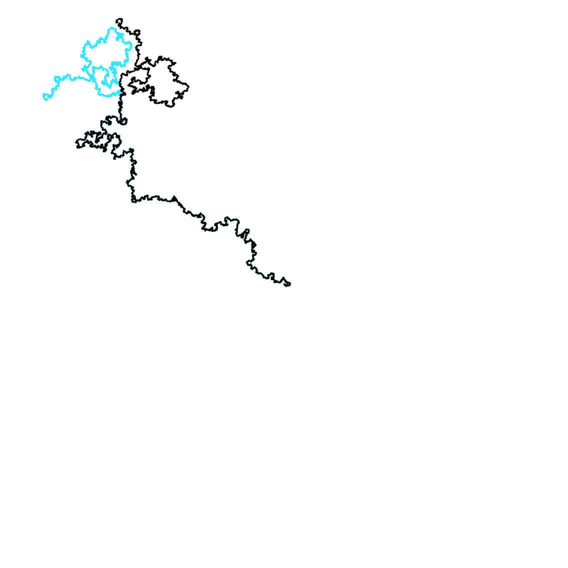

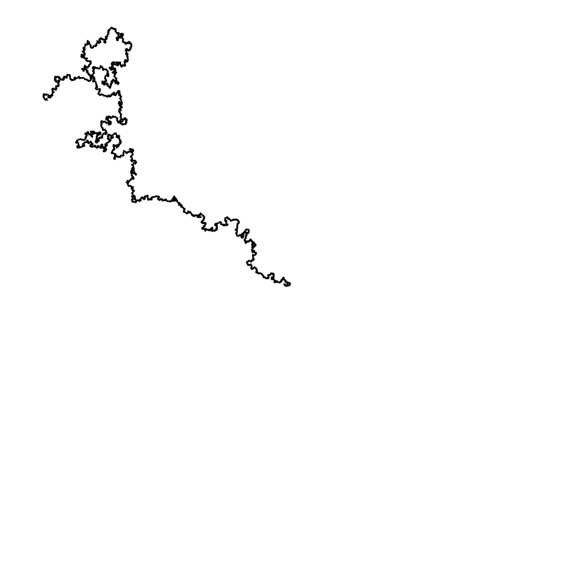

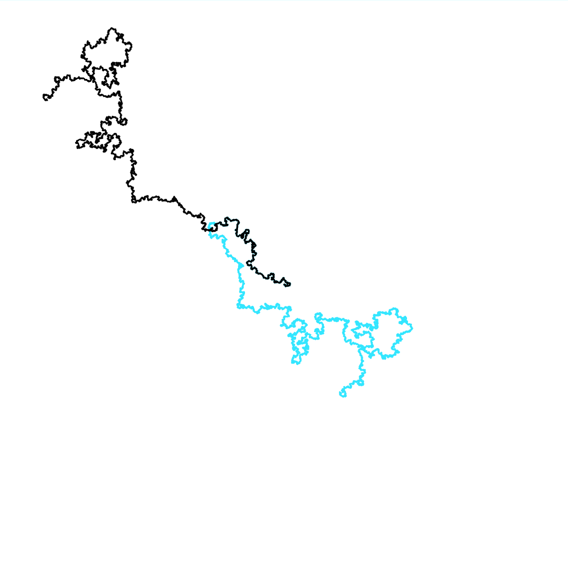

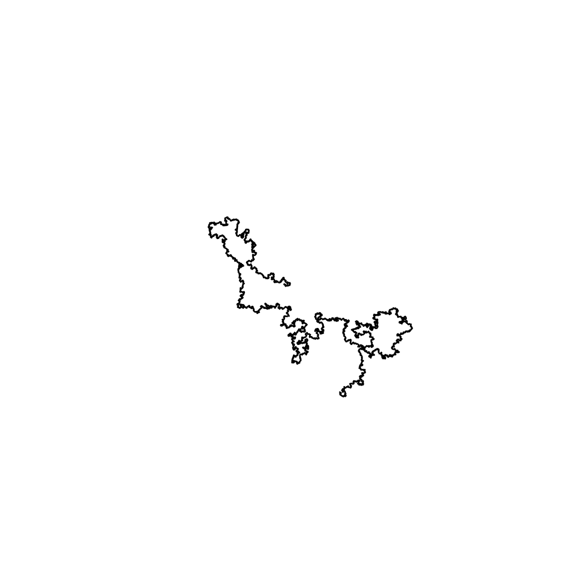

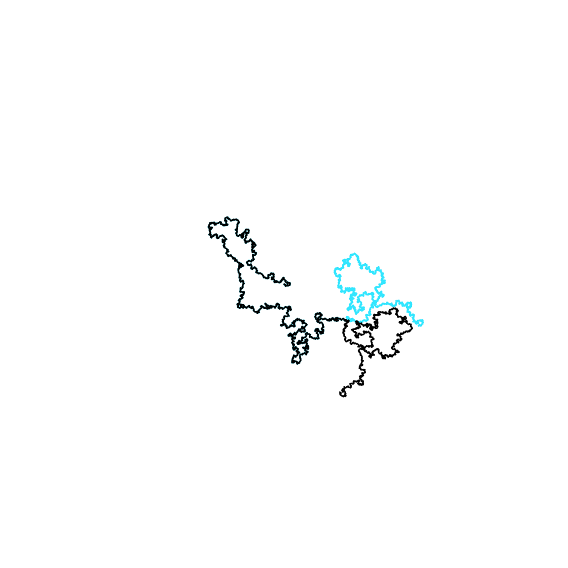

SAW-tree

- How do we implement pivot algorithm efficiently?
  - Represent SAW as a binary tree.
- Each node of tree contains global information about sub-walk, including bounding box and global observables.
- Ensures *all* cut-and-paste moves can be performed in time $O(\log N)$ via tree-rotations, as height of binary tree $O(\log N)$.
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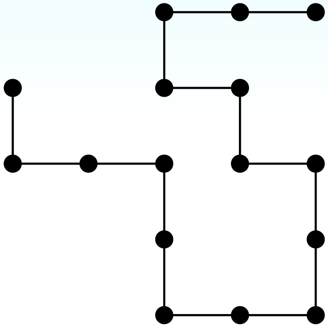

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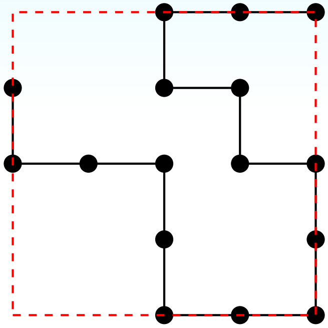

Bounding box

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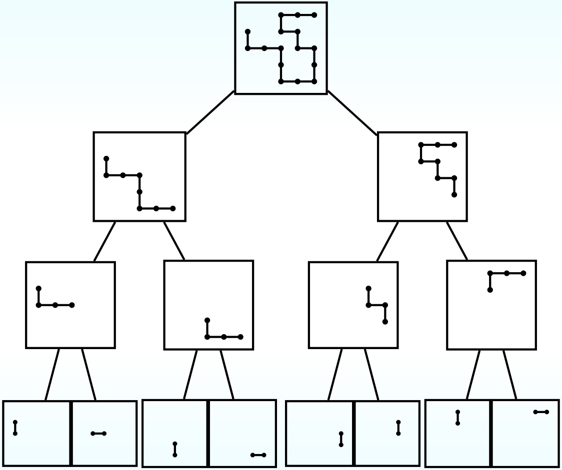

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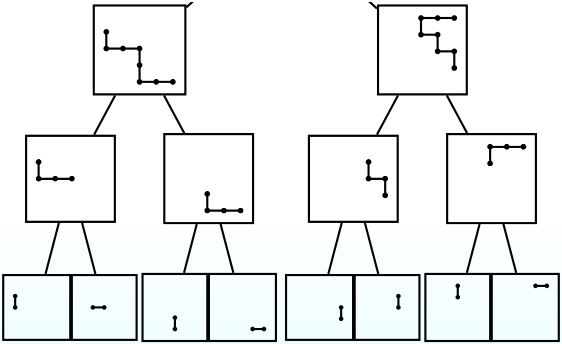

Pivot algorithm

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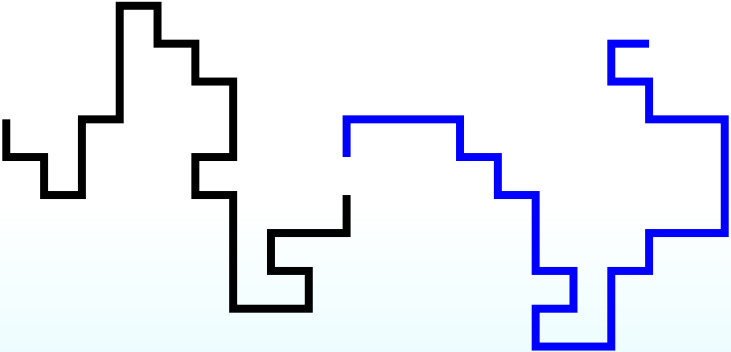

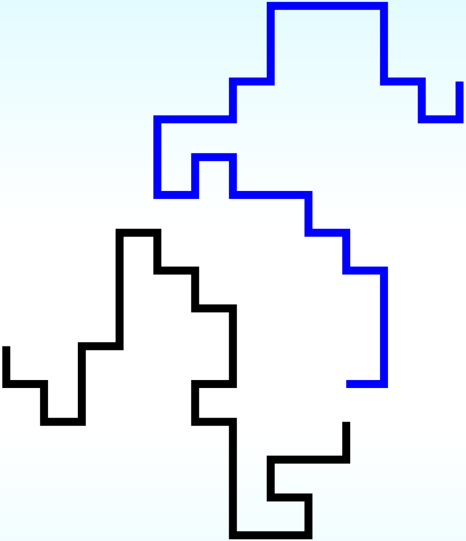

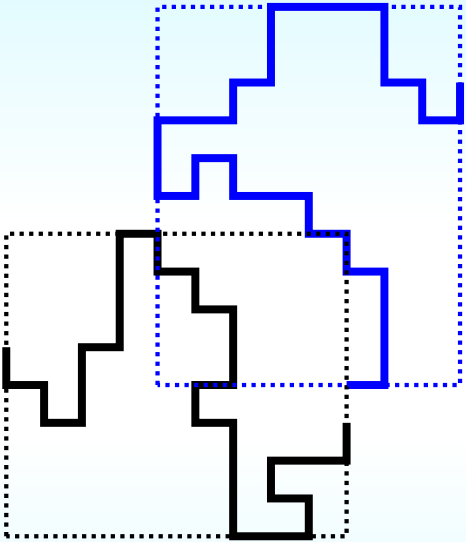

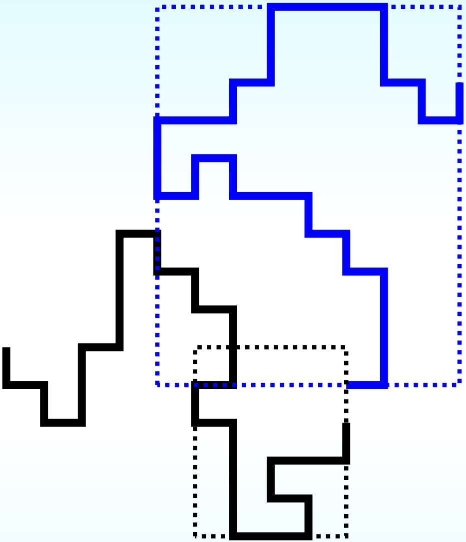

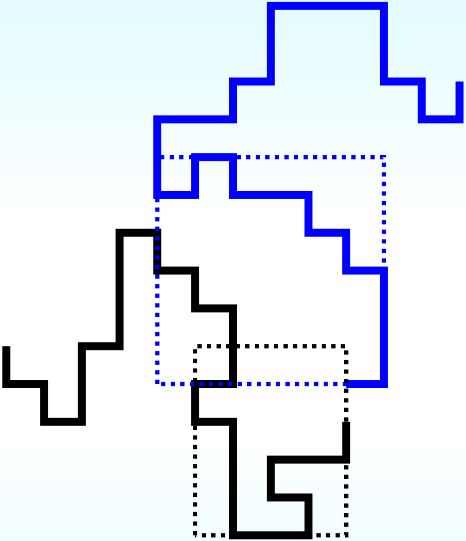

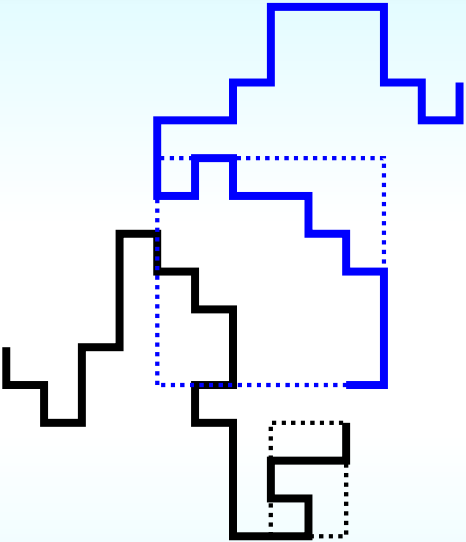

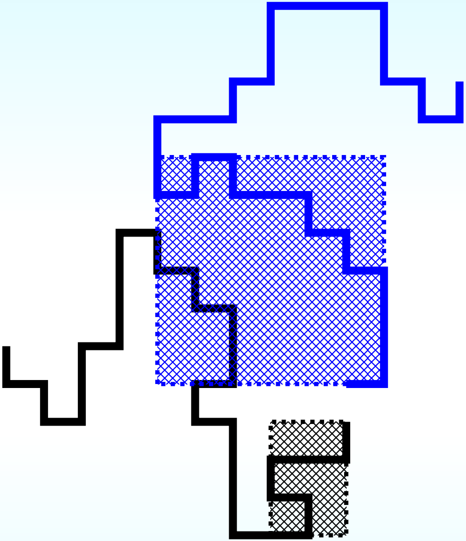

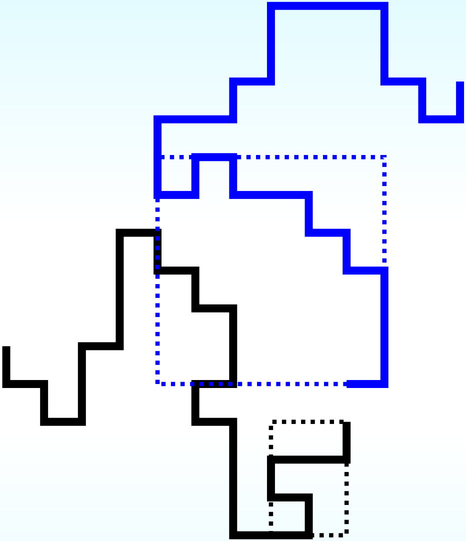

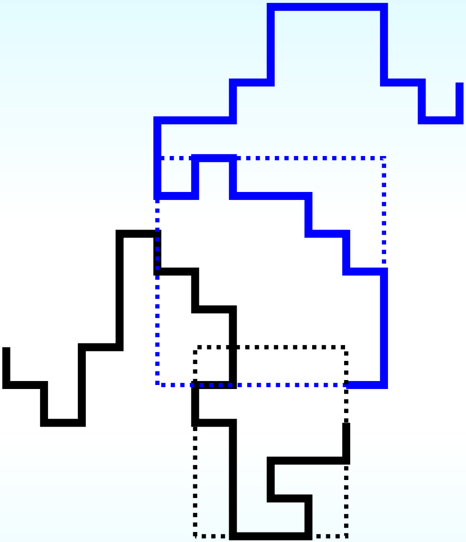

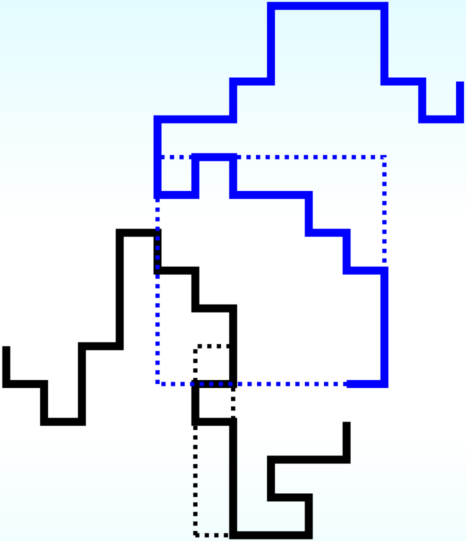

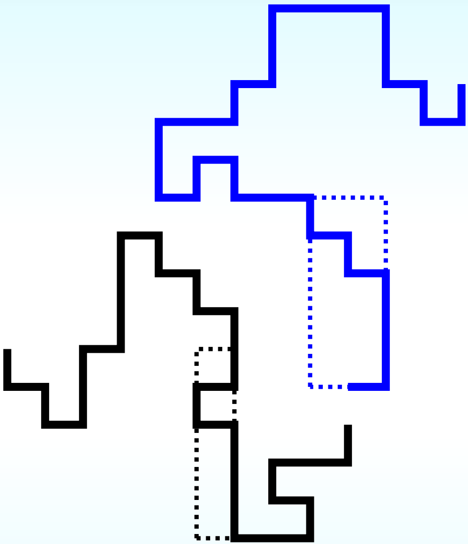

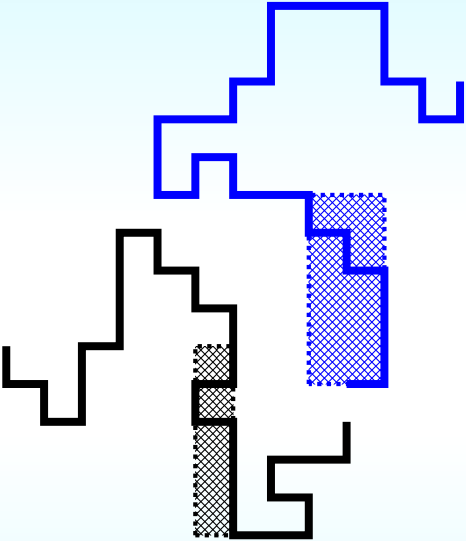

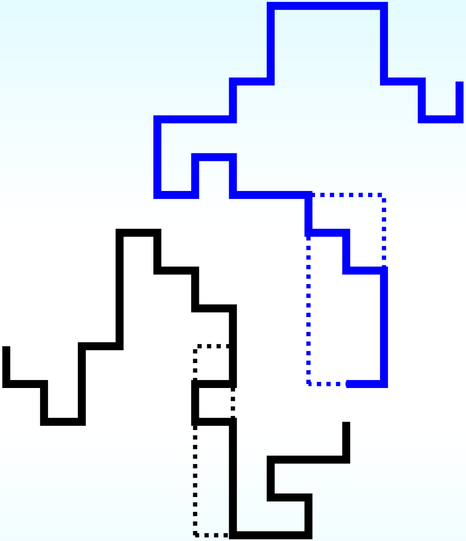

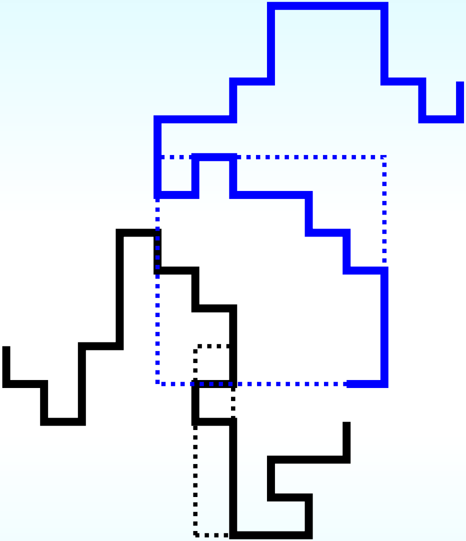

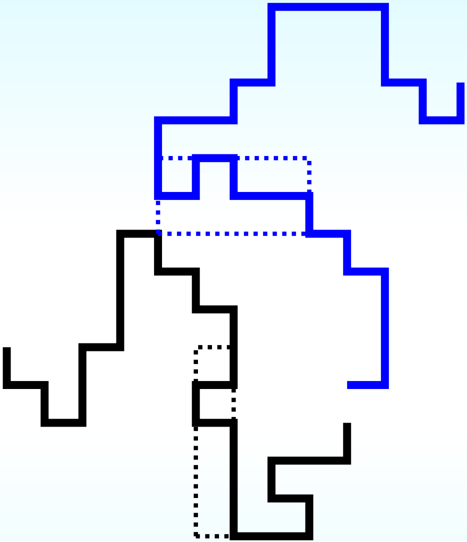

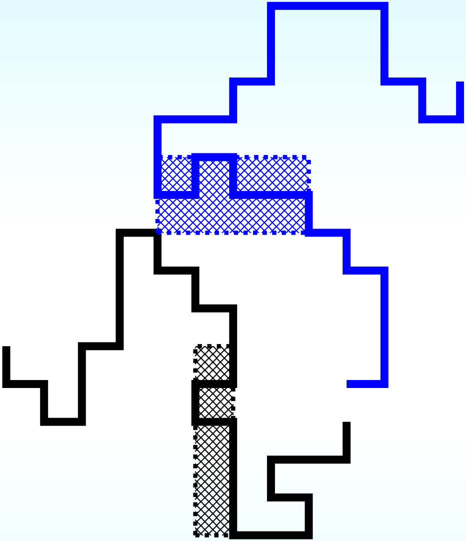

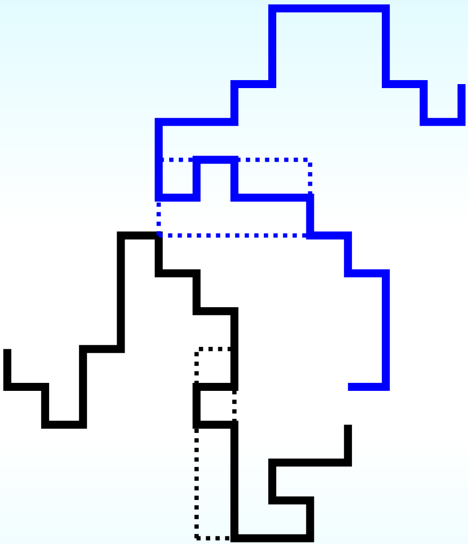

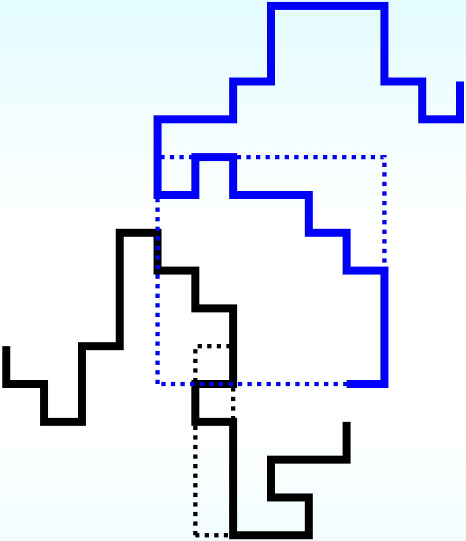

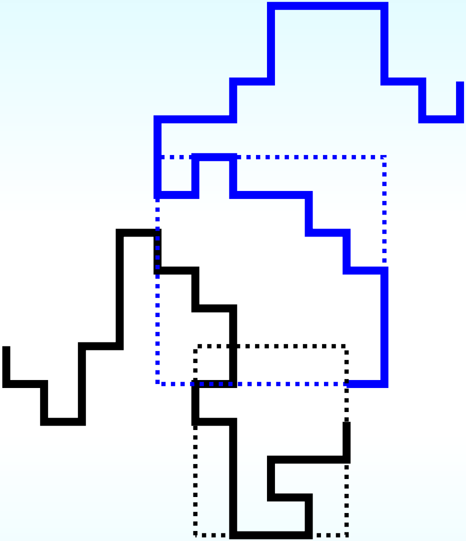

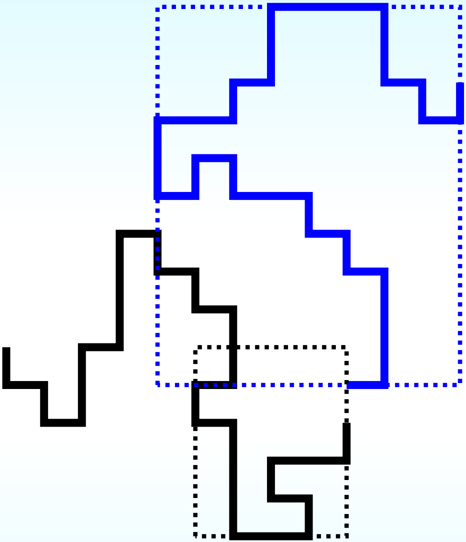

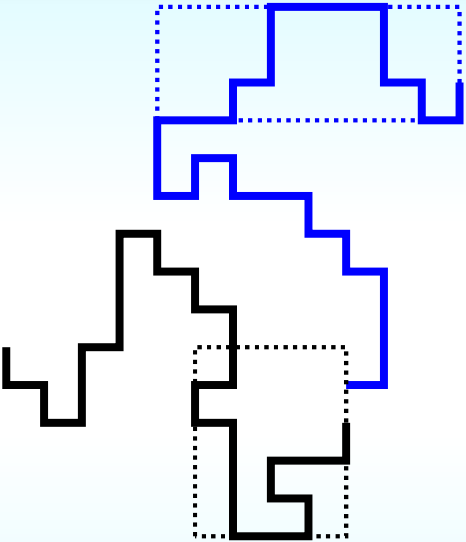

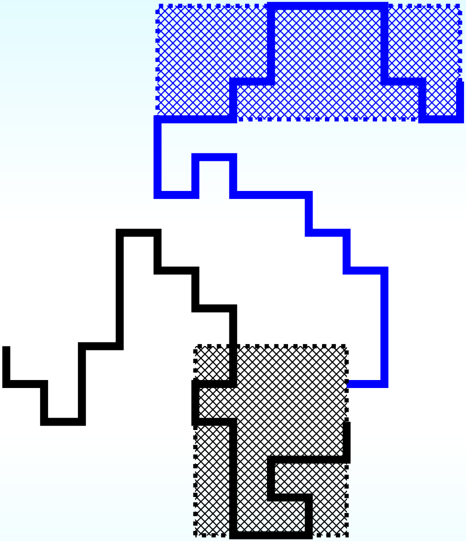

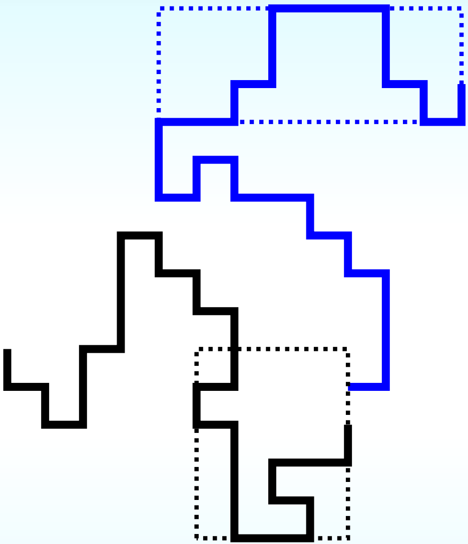

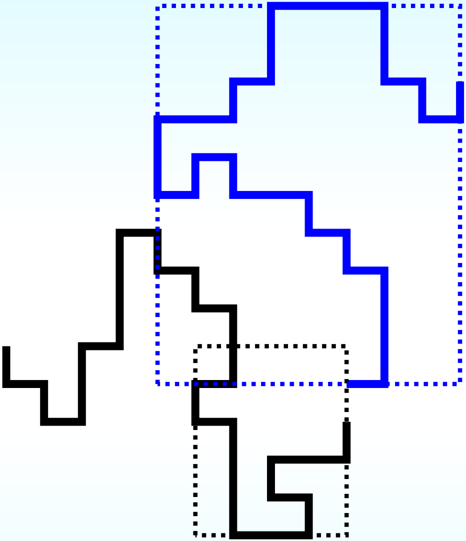

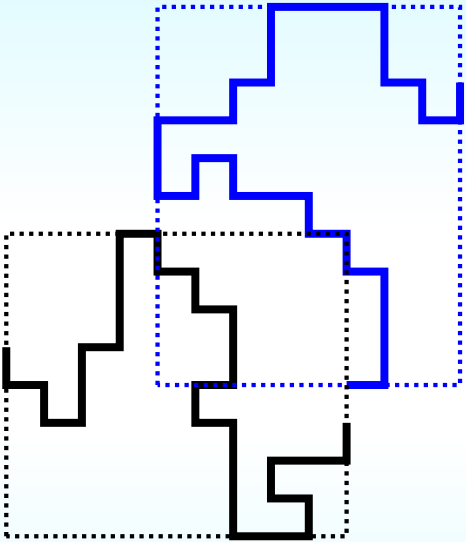

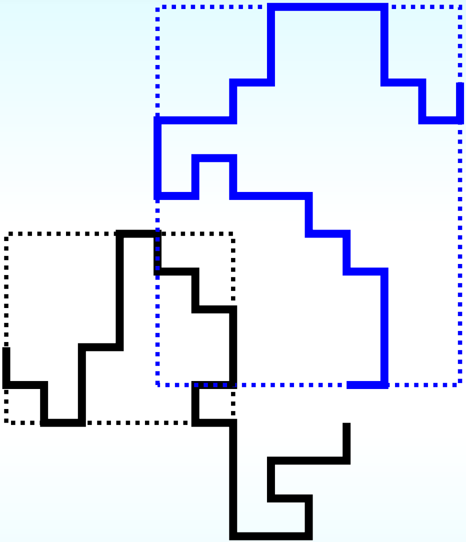

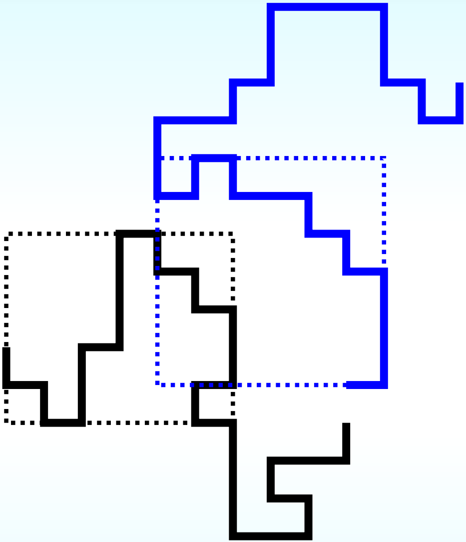

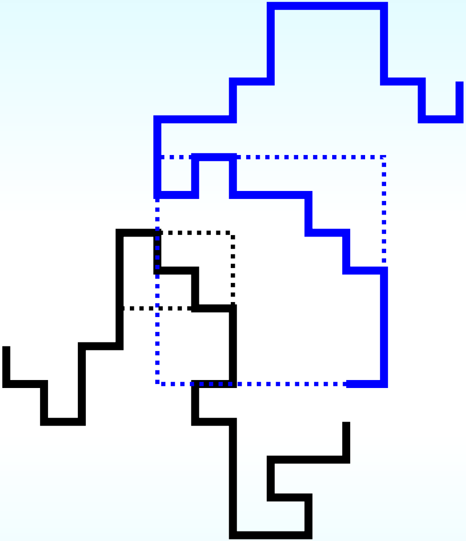

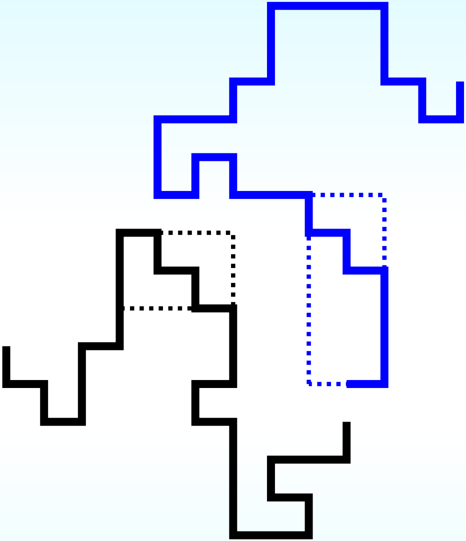

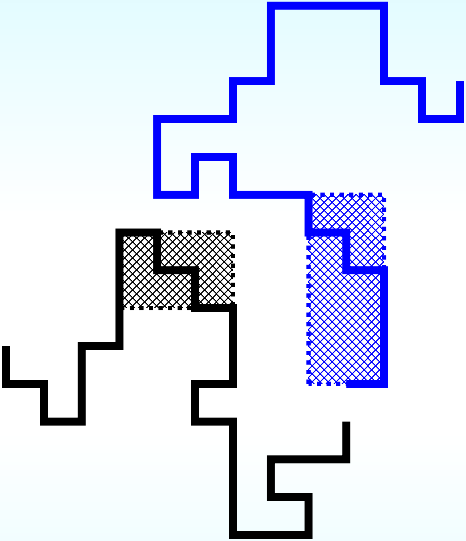

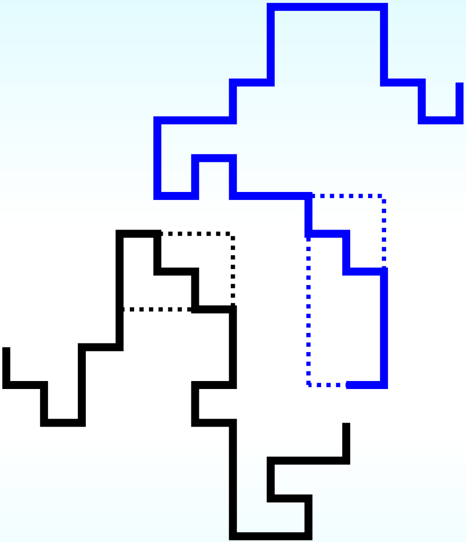

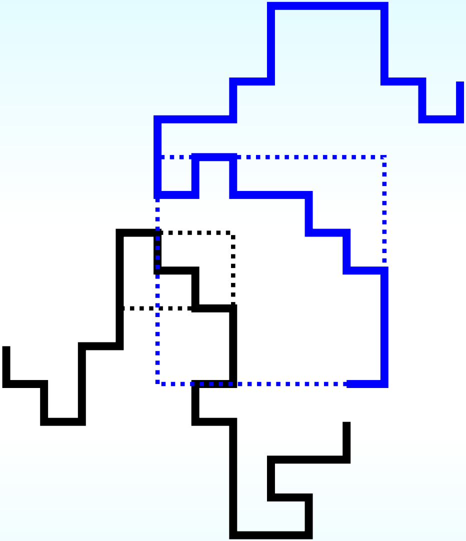

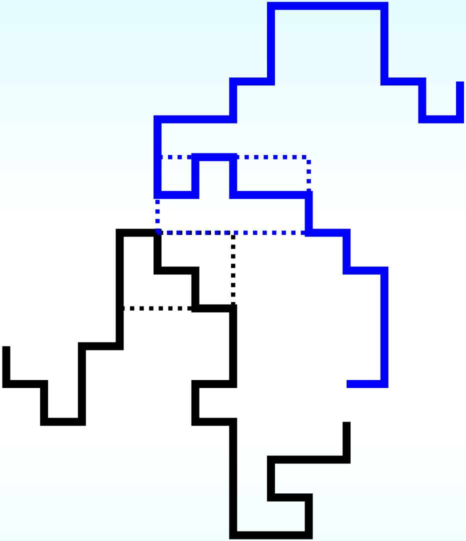

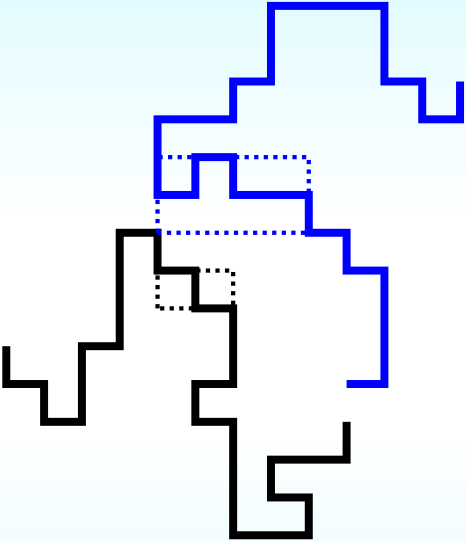

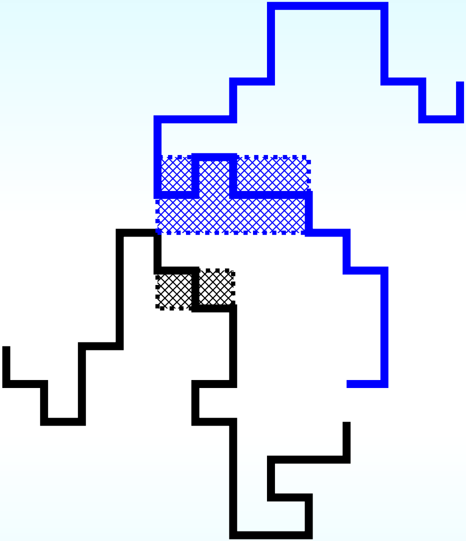

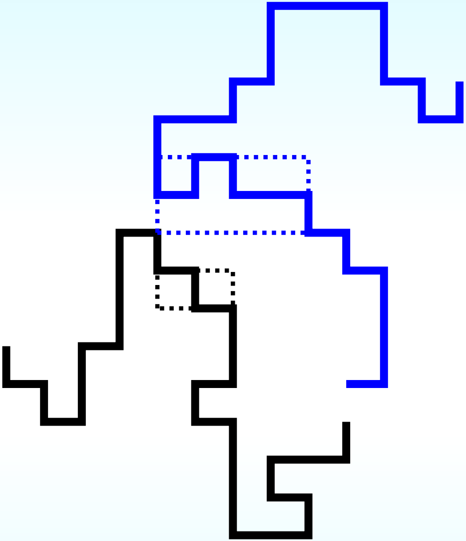

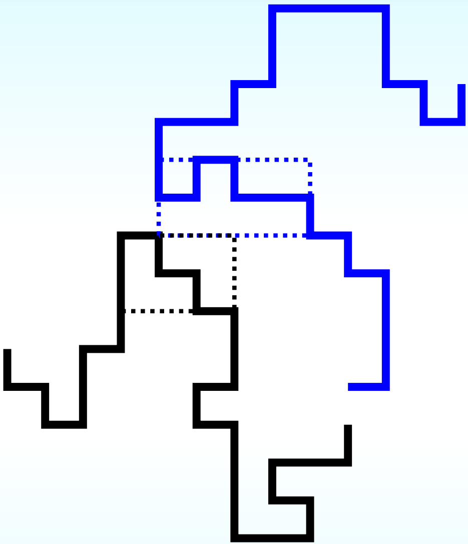

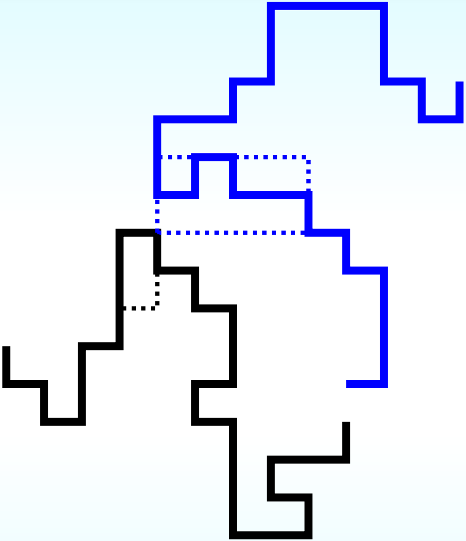

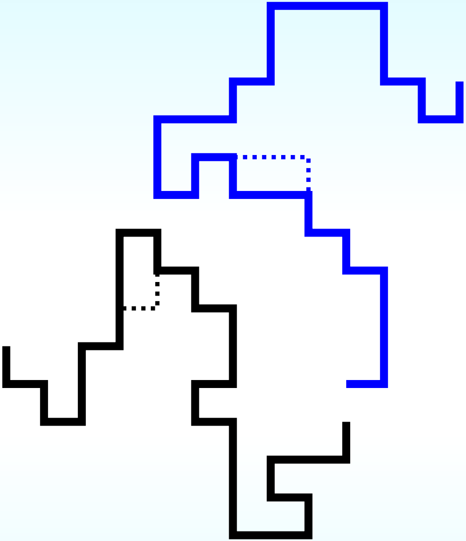

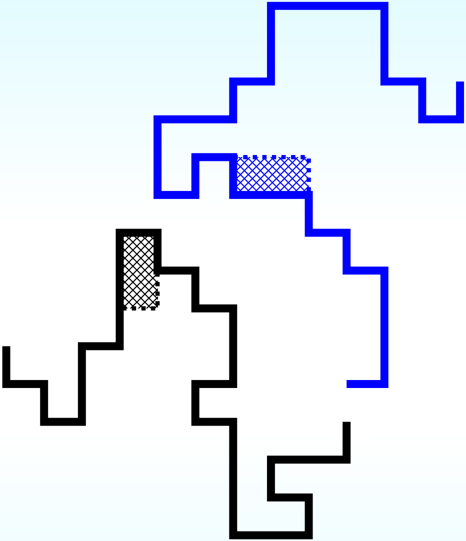

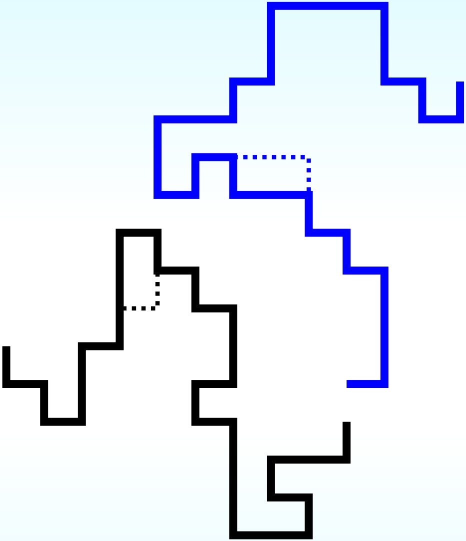

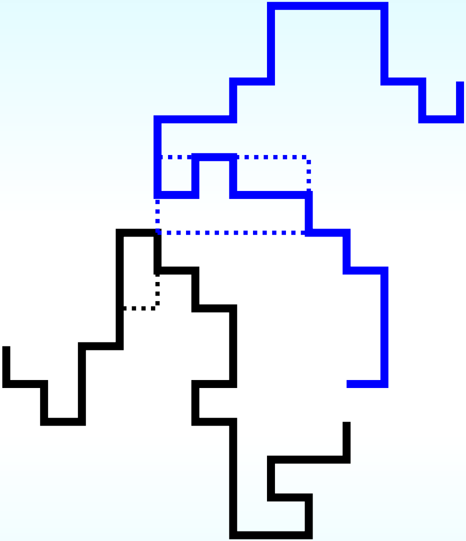

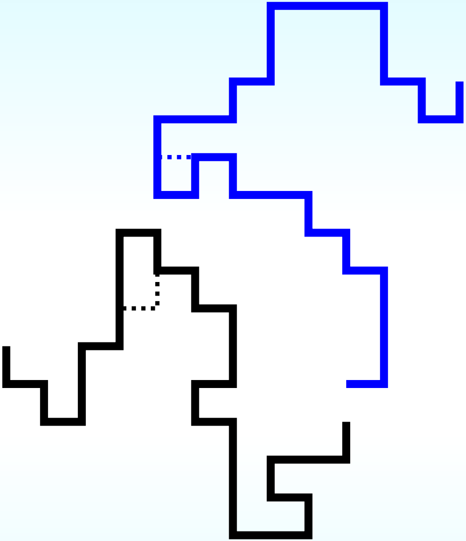

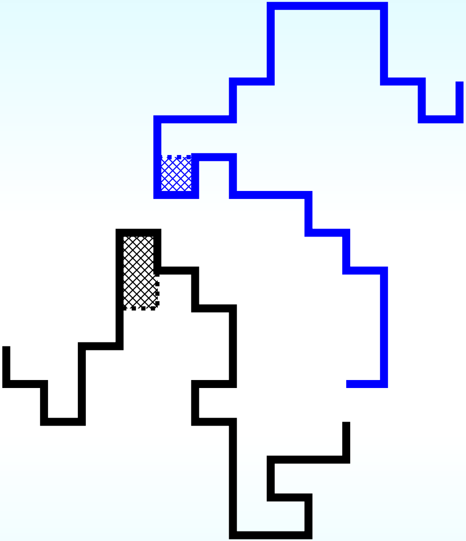

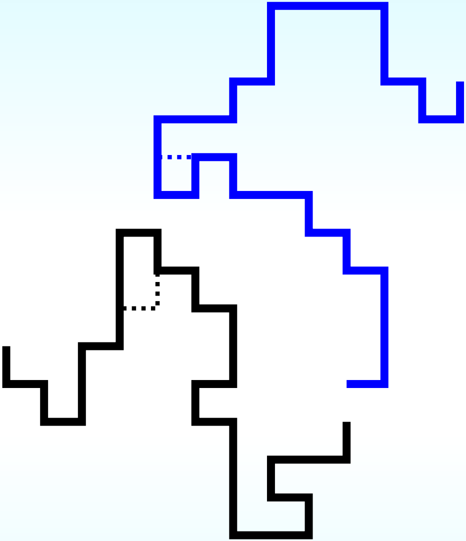

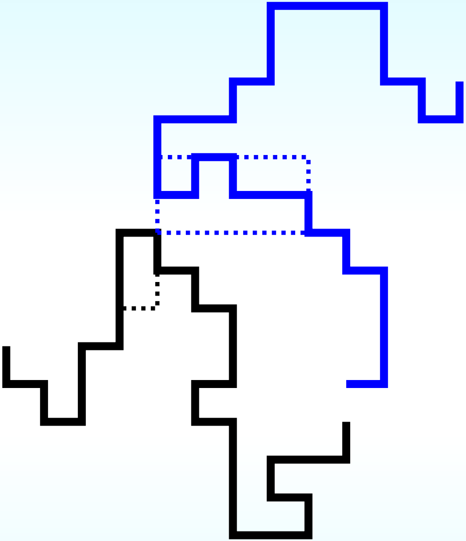

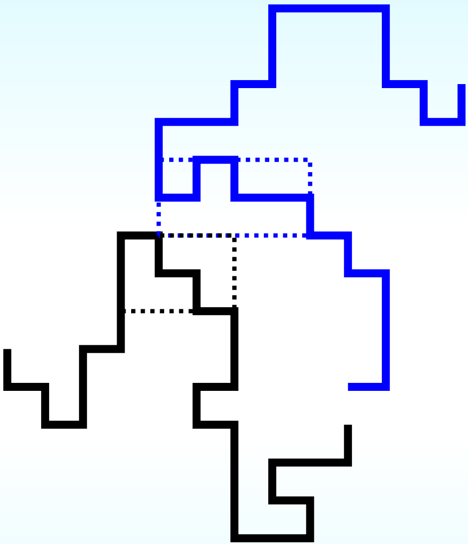

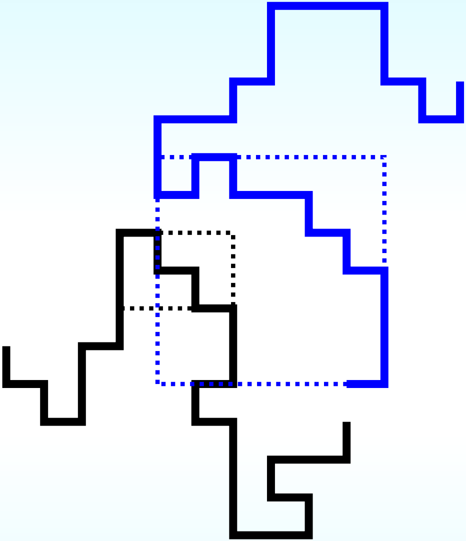

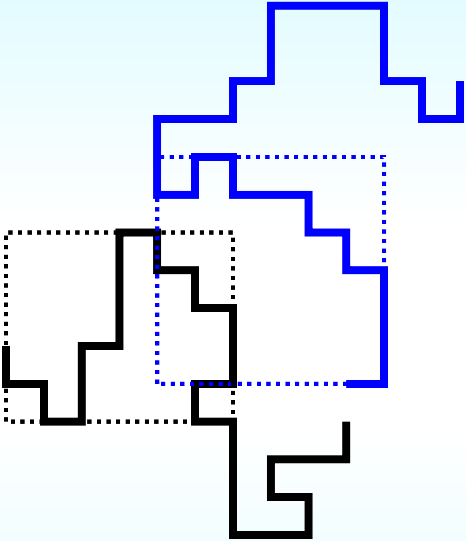

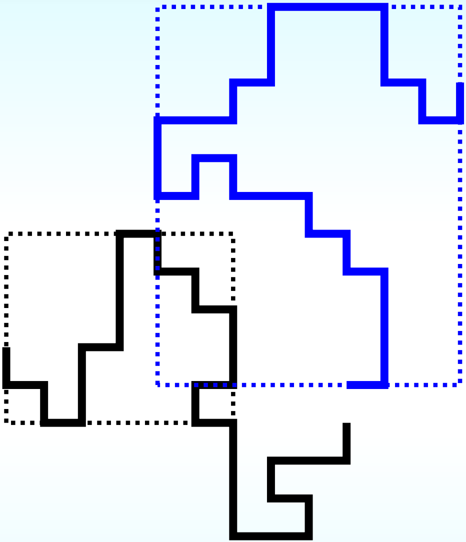

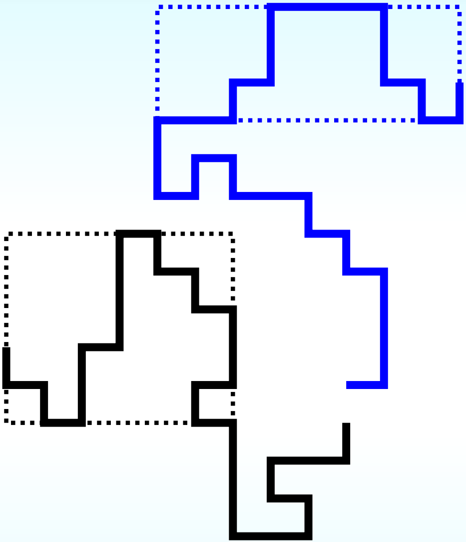

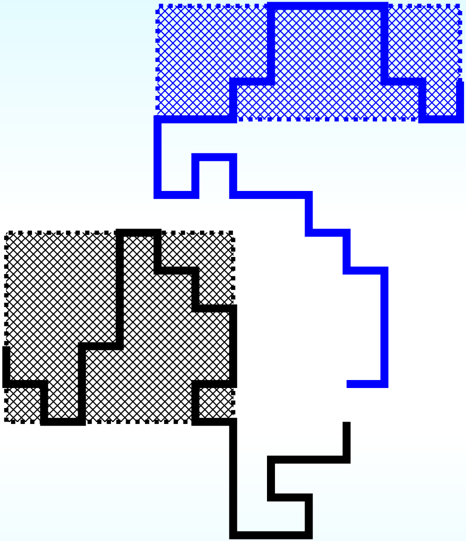

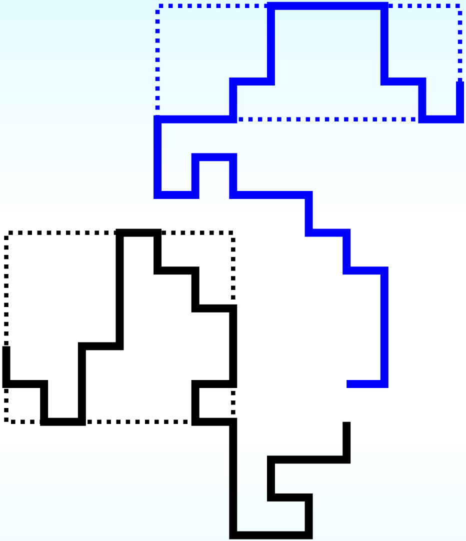

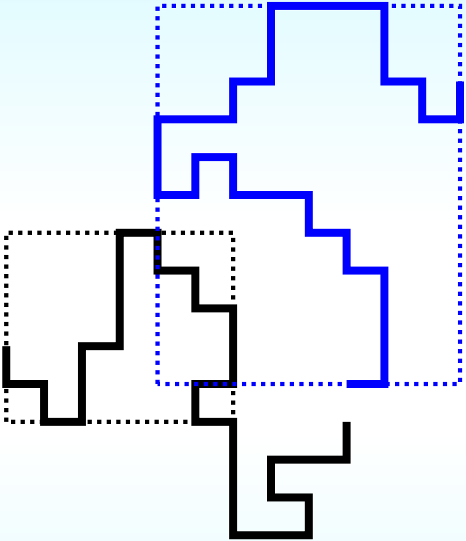

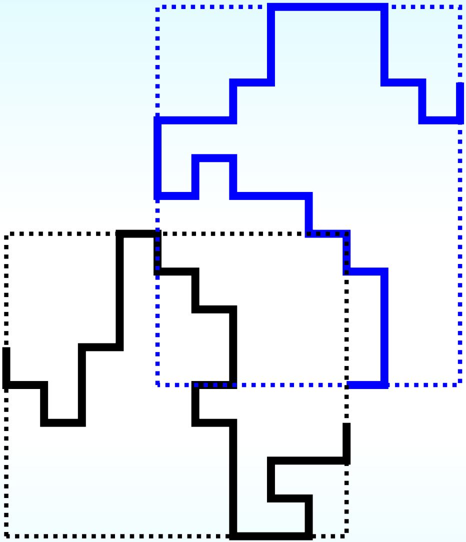

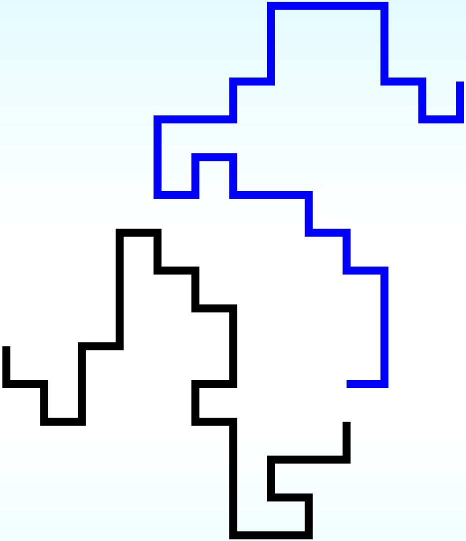

Implementing cut-and-paste moves via the SAW-tree:

- Split polymer into pieces, $O(\log N)$.
- Apply move(s) to sub-walk(s), $O(1)$.
- Calculate change in interaction energy between sub-walks. For SAWs, $O(\log N)$.
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- Kennedy (2002): implementation which is approximately $O(N^{0.74})$.
- SAW-tree implementation of the pivot algorithm, average case $O(\log N)$ for N-step SAWs [Cli10a]. Enables simulation of much longer SAWs, so far up to 265 million steps.
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CPU time per attempted pivot, for SAWs of length N:

	$\mathbb{Z}^2$			$\mathbb{Z}^3$		
N	S-t (μs)	M&S/S-t	K/S-t	S-t (μs)	M&S/S-t	K/S-t
31	0.41	0.894	1.06	0.59	0.981	1.37
1023	0.87	5.15	1.90	1.71	6.31	3.75
32767	1.27	68.6	4.92	3.36	79.2	21.5
1048575	2.91	2510	32.2	7.53	3830	385
33554431	4.57	35200	134	12.58	61700	7130

Dimerization

- Most straightforward method to calculate γ: dimerization, i.e. concatenating two SAWs to see if they form a longer SAW.
- Indicator function for successful concatenation is our observable, and

$$B(\omega_1, \omega_2) = \begin{cases} 0 & \text{if } \omega_1 \circ \omega_2 \text{ not self-avoiding} \\ 1 & \text{if } \omega_1 \circ \omega_2 \text{ self-avoiding} \end{cases}$$

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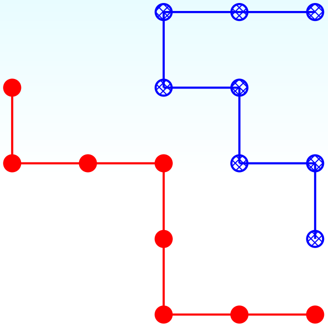
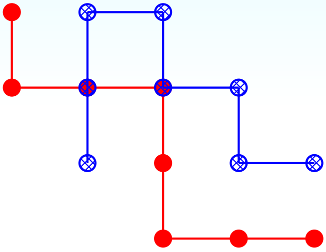


$B(\omega_1, \omega_2) = 1$



$B(\omega_1, \omega_2) = 0$

Dimerization

- $$\langle B \rangle = \frac{\text{Number of } 2N-1 \text{ step SAWs}}{\text{Number of pairs of } N-1 \text{ step SAWs}}$$
  $$= \frac{c_{2N-1}}{c_{N-1}^2}$$
  $$\sim \frac{A\mu^{2N-1}(2N-1)^{\gamma-1}}{A^2\mu^{2N-2}(N-1)^{2\gamma-2}}$$
  $$\sim \frac{2^{\gamma-1}\mu}{A} N^{1-\gamma}\,[1 + \text{corrections}]$$
- Generate two Markov chains of $N-1$ step SAWs using pivot algorithm.
- Sample $B(\omega_1, \omega_2)$ for every time step.

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- How many pivots must be completed before two walks are essentially new configurations with respect to observable B?
- Shape of walks close to the joint clearly important.
- Simple argument suggests mean distance from joint where first intersection occurs is $O(N^{2-\gamma})$.
- For uniform sampling, probability that pivot site is before $O(N^{2-\gamma})$ is $O(N^{1-\gamma})$. Is $\tau_{\mathrm{int}} = O(N^{\gamma-1})$?
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- Choose pivot sites preferentially close to the joint.
- Natural to choose using a power law.
- Robust choice: $\Pr(d) \propto \frac{1}{d}$, d is distance from joint.
- Sites chosen at all length scales with equal probability. Probability that $i \in [L, 2L]$ is $O(1/\log N)$; "scale-free" pivot moves.
- Lower bound for τ_{int}: the time necessary to achieve a pivot before the first intersection.
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- Robust choice: $\Pr(d) \propto \frac{1}{d}$, d is distance from joint.
- Sites chosen at all length scales with equal probability. Probability that $i \in [L, 2L]$ is $O(1/\log N)$; “scale-free” pivot moves.
- Lower bound for τ_{int}: the time necessary to achieve a pivot before the first intersection.
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Confined polymers

- Length scales introduced by putting polymer in a confined region, e.g. between two parallel plates, or in a tube.
- Perform cut-and-paste moves on polymer.
- If we select endpoints of sub-walks uniformly from log(distance), we guarantee that all length scales will be accounted for.
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Other systems with intermediate length scales

- Polymer knotting (knots are localized on self-avoiding polygons).
- Polymers near θ (collapse) transition.
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