Monte Carlo simulation of self-avoiding walks

Nathan Clisby
MASCOS, The University of Melbourne

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Introduction

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- enumeration of self-avoiding walks (SAW) and other lattice objects;
- Monte Carlo sampling of self-avoiding walks and polymers.
- In fact, key insight described here led initially to a bad enumeration algorithm, then a good Monte Carlo algorithm.

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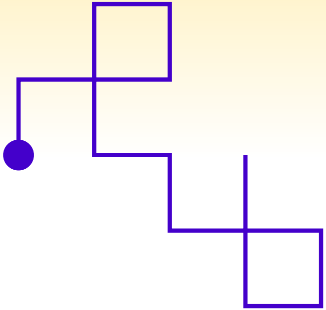
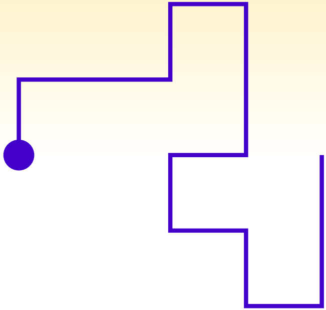
- Exactly captures universal properties such as critical exponents.



Simple random walk



Self-avoiding walk

Typical self-avoiding walks

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- μ is the connective constant; lattice dependent.

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- Polymer knotting, perhaps protein folding.
- Algorithms can be applied to realistic polymer systems, perhaps combining Monte Carlo with Molecular Dynamics.

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SAW have a natural one-dimensional order $\cdots$
$\cdots$ and segments of the walk which are well separated on the chain are (typically) well separated in space.

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  - large deformations are slow, but move rapidly around state space

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- More CPU time per move, but still dramatically more efficient.
- Made it possible to study dramatically longer SAW (from hundreds of steps to tens of thousands).

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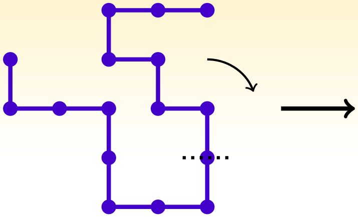
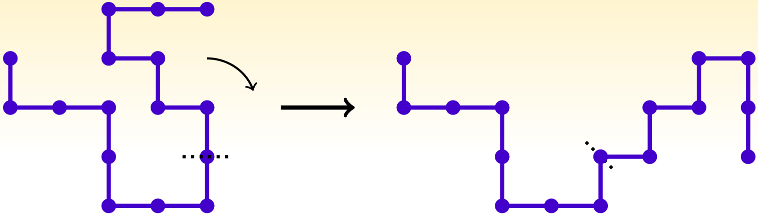
- "Global" because on average one quarter of the monomers are moved.



Example pivot move



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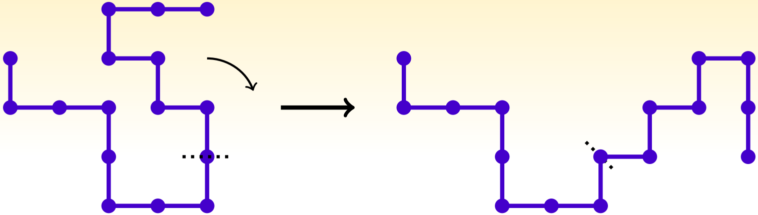

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- Integrated autocorrelation time for global observables $O(N^p)$, $p \approx 0.19$ for square lattice, $p \approx 0.11$ for cubic.
- Usual implementation: CPU time $O(N)$ for an "essentially new" configuration.

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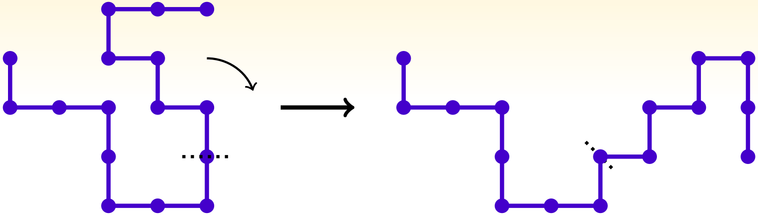

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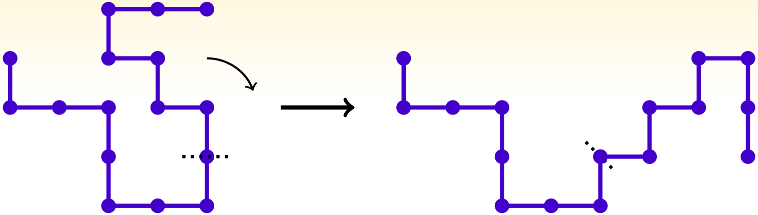

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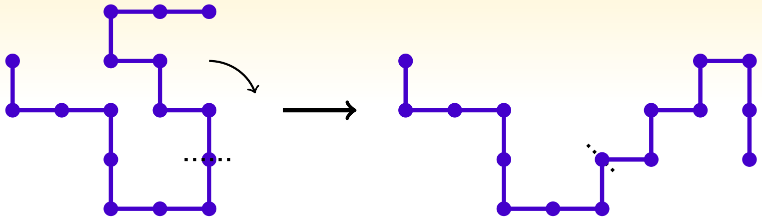

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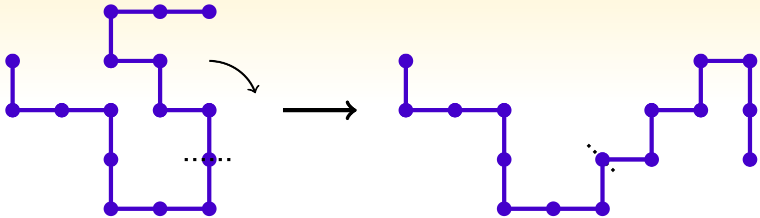

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With the right implementation, pivot move has *global effect* for the cost of a *local* move. Tricky part is checking that after subwalk is rotated the walk remains self-avoiding.

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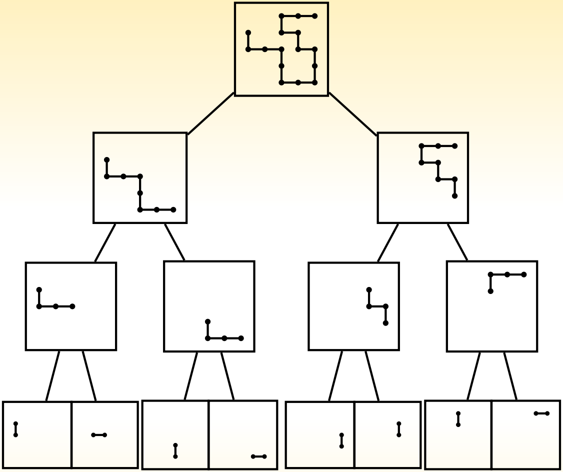
SAW can be decomposed into two (equal) subwalks, with a symmetry operation concatenating the two subwalks.
This results in a natural *binary tree* structure.



SAW-tree representation of a walk.

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- R_e^2, R_g^2, R_m^2 can all be calculated in this way.
- Problem of keeping track of changes after a pivot move is bookkeeping, can be done in time $O(\log N)$.

Intersection testing

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- Mean number of contacts between two *halves* of an N-step SAW is constant (Müller and Schäfer, 1998).

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- This idea captured by storing *bounding box* information in a binary tree.

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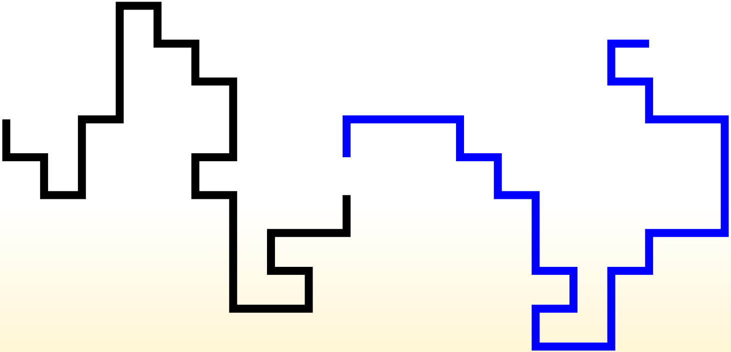
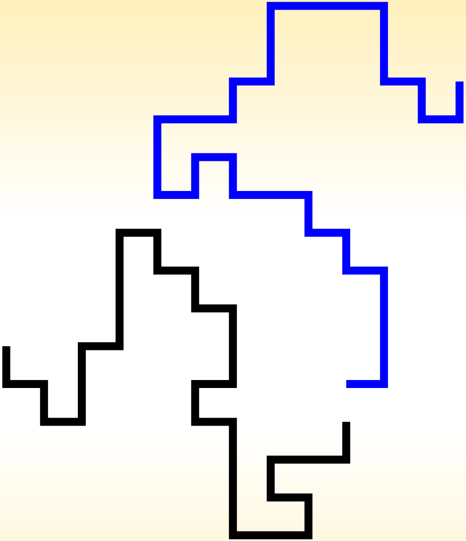
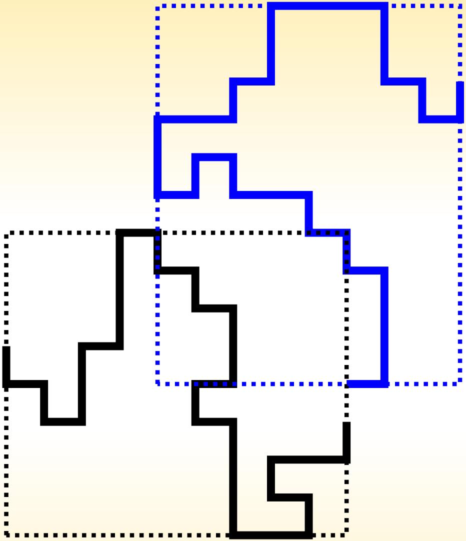
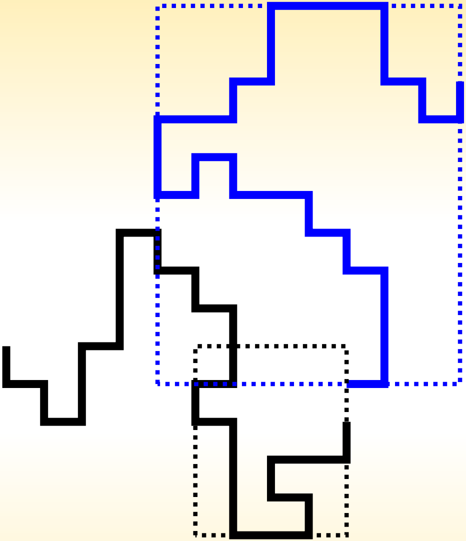
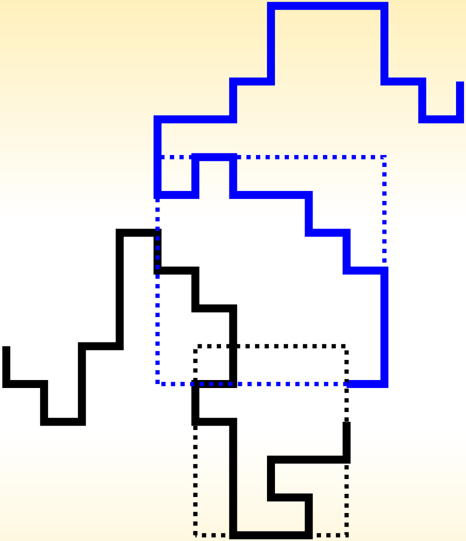
- Algorithm uses "depth-first search" in an attempt to find intersections, recursively applying the observation that when the bounding box of two subwalks do not intersect, then the subwalks themselves cannot intersect.
- $O(1)$ contacts $\Longrightarrow$ mean CPU time $O(\log N)$ to complete test.

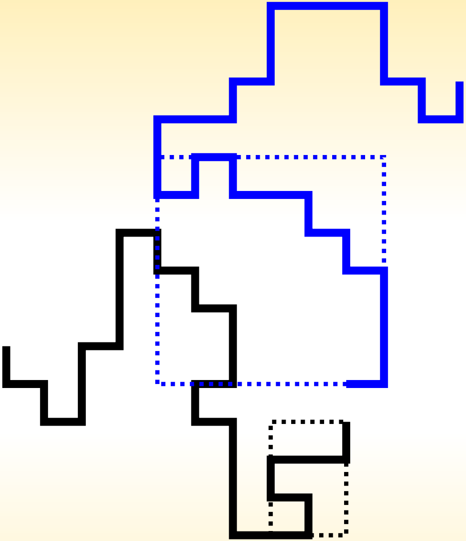


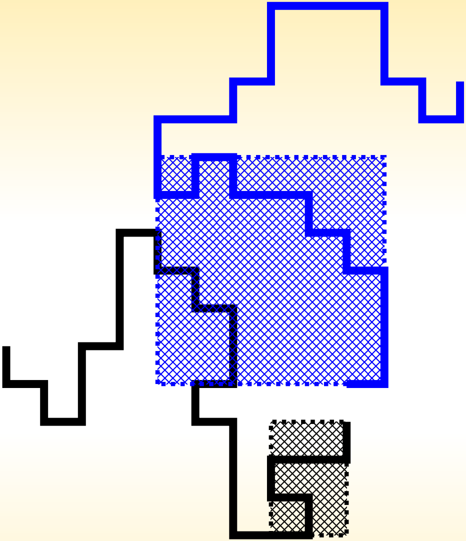


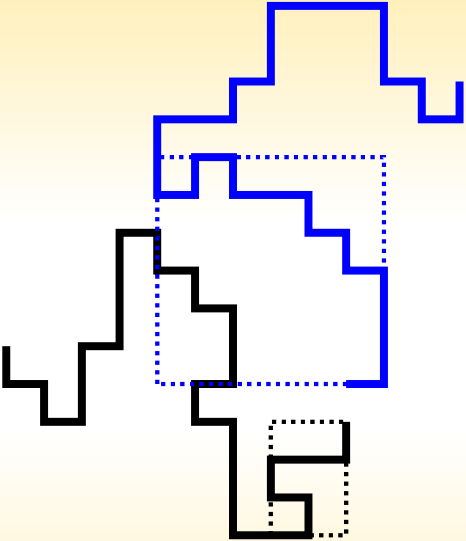


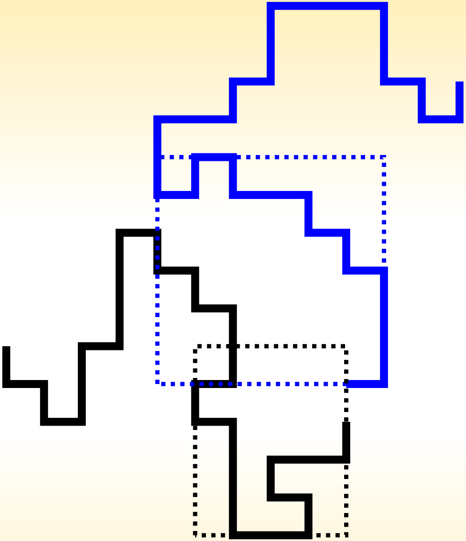


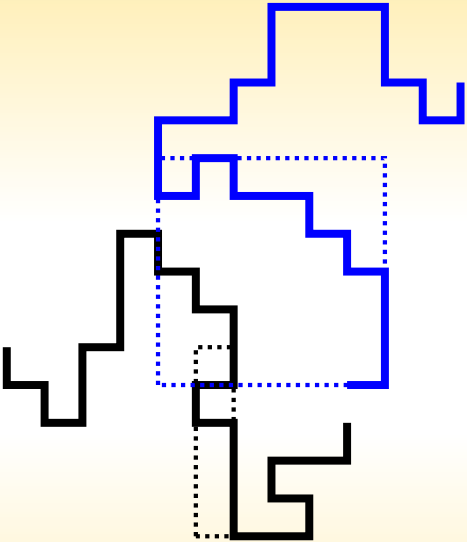


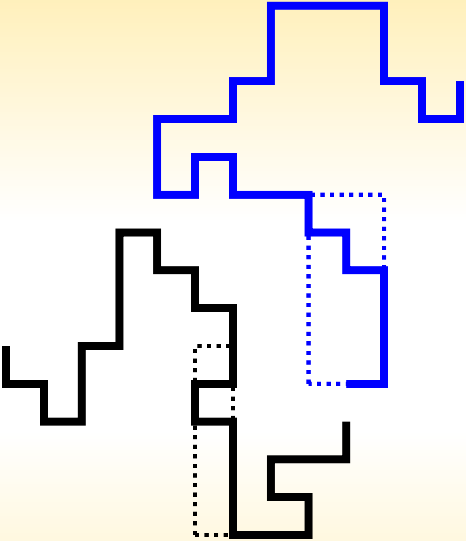


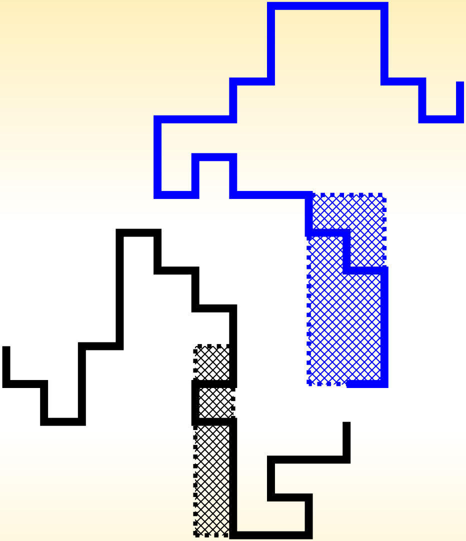


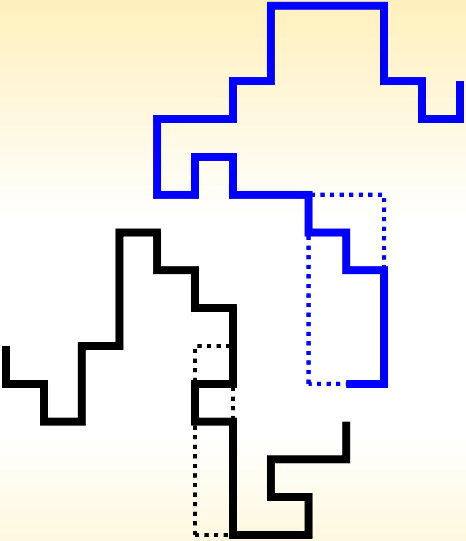


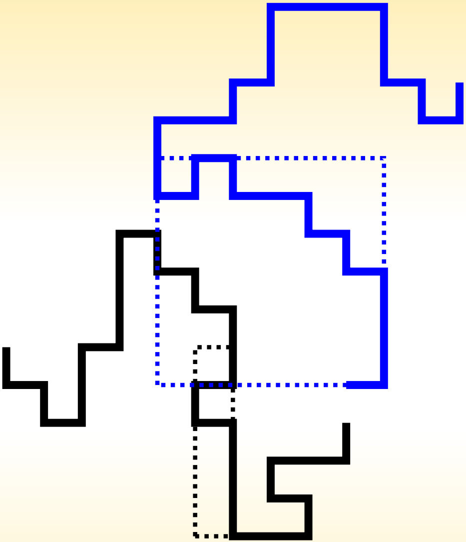


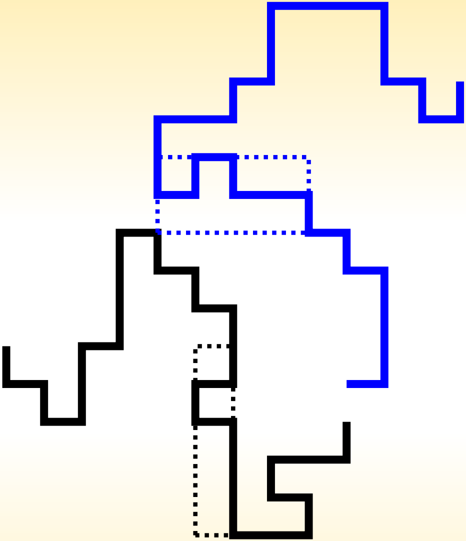


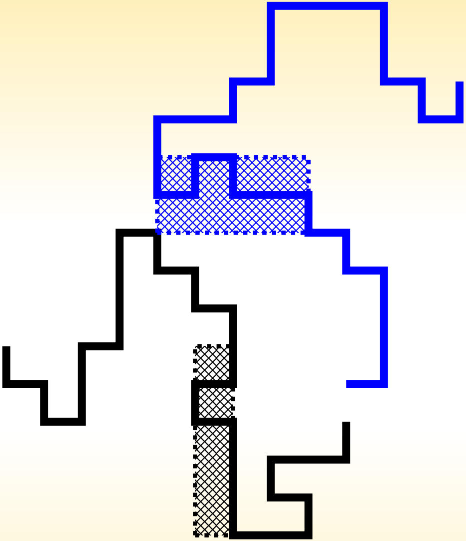


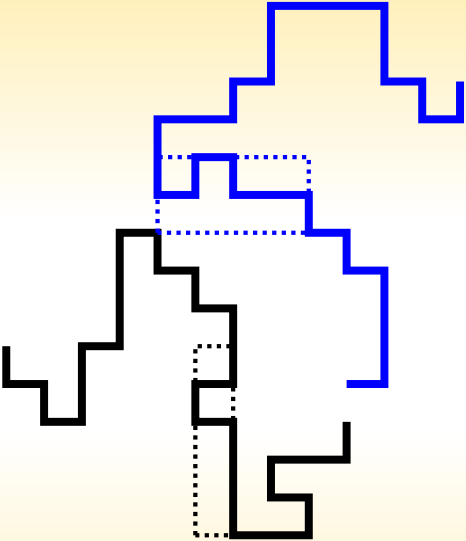


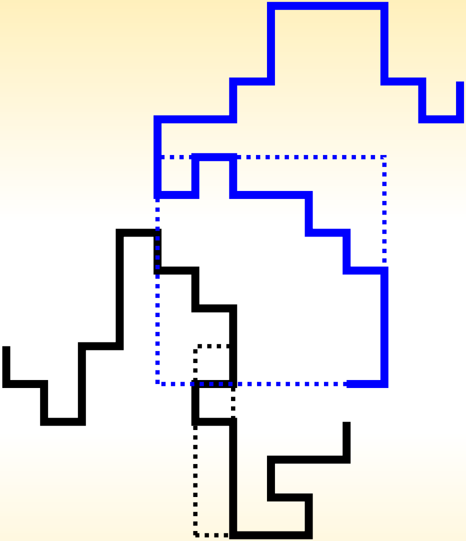


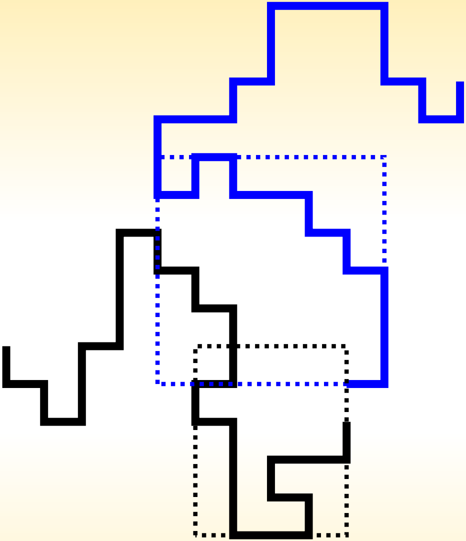


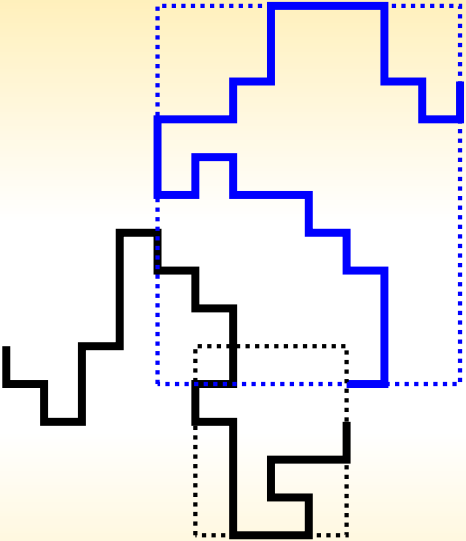


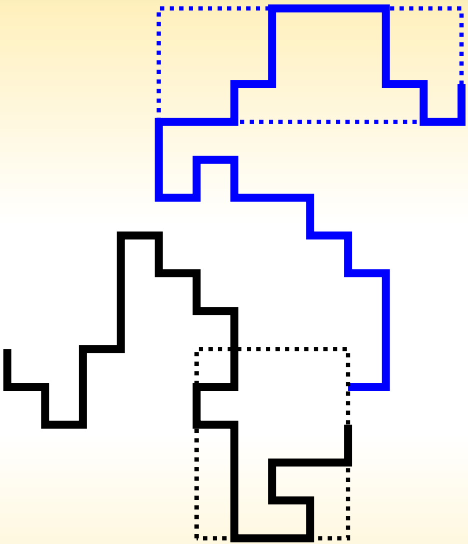


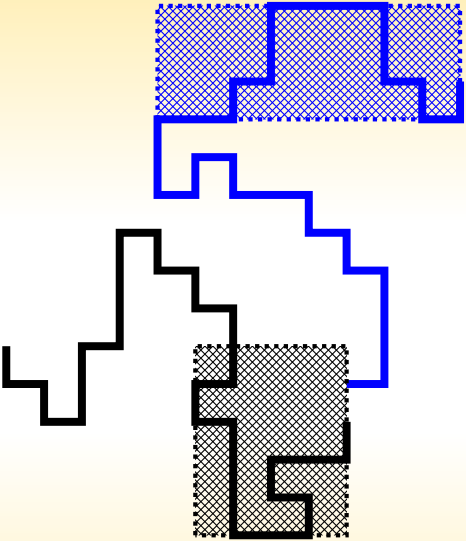


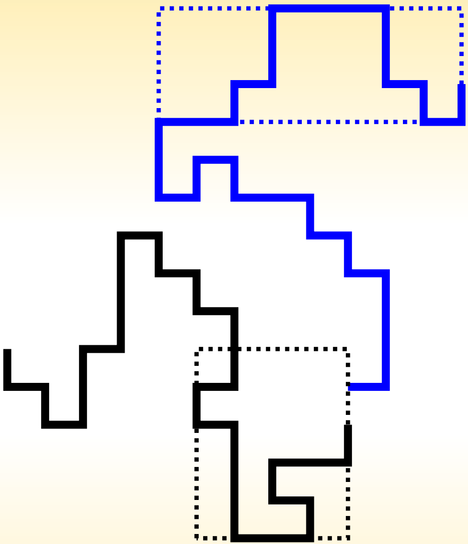


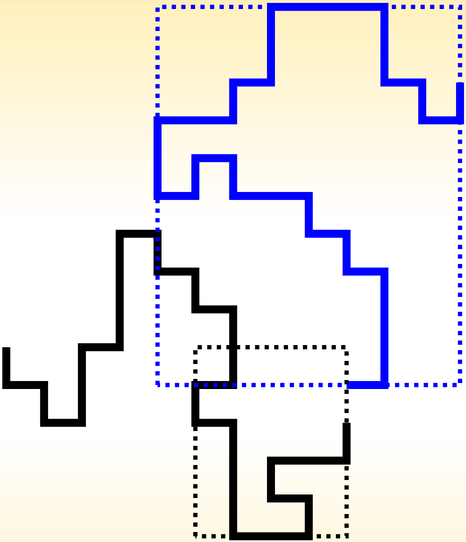


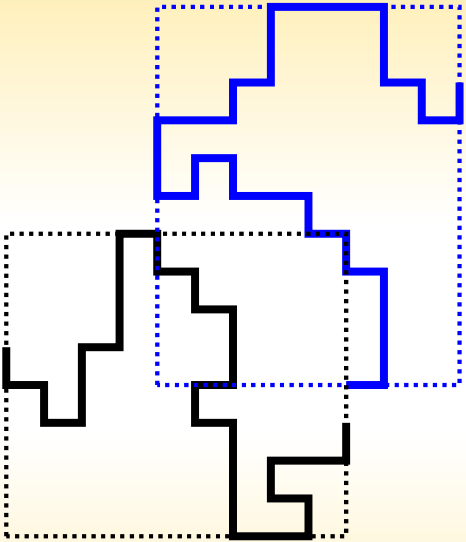


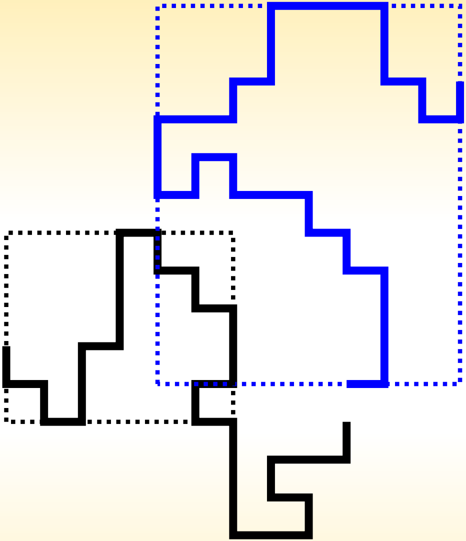


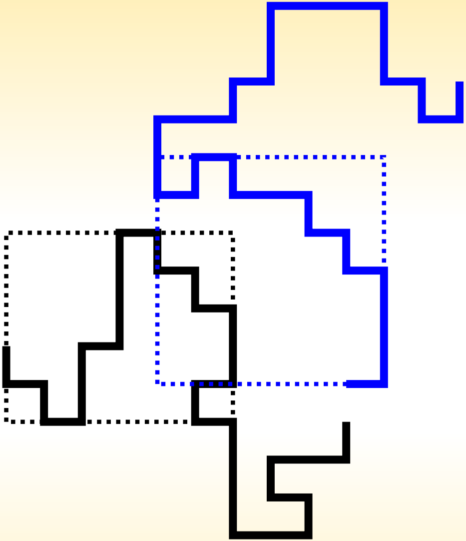


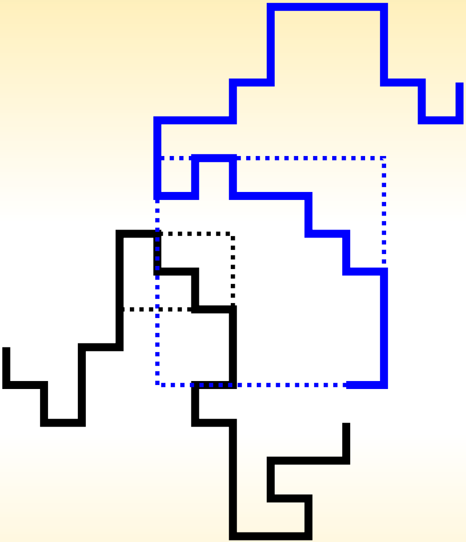


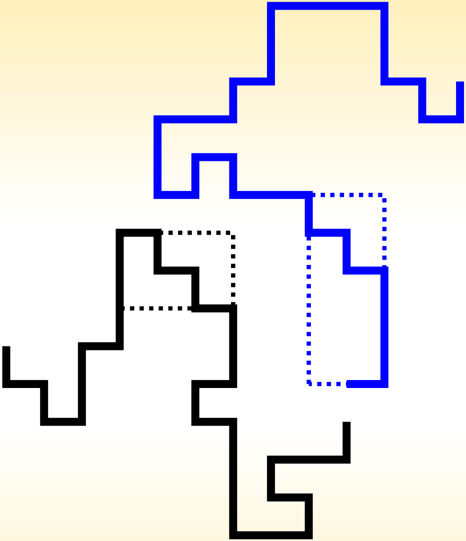


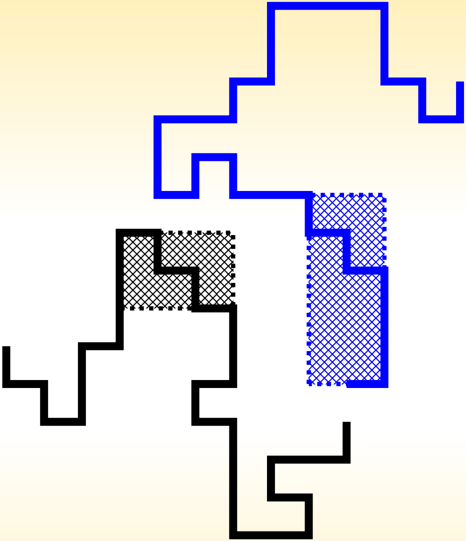


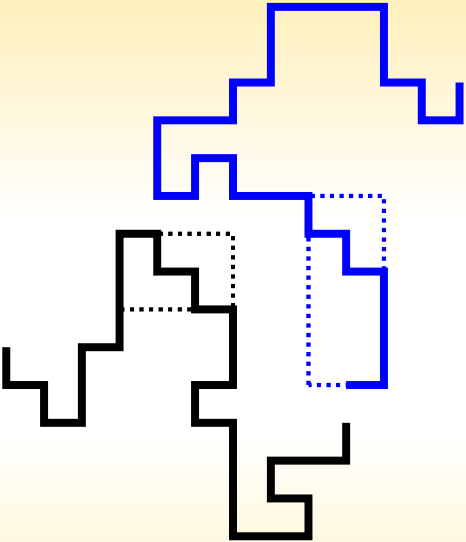


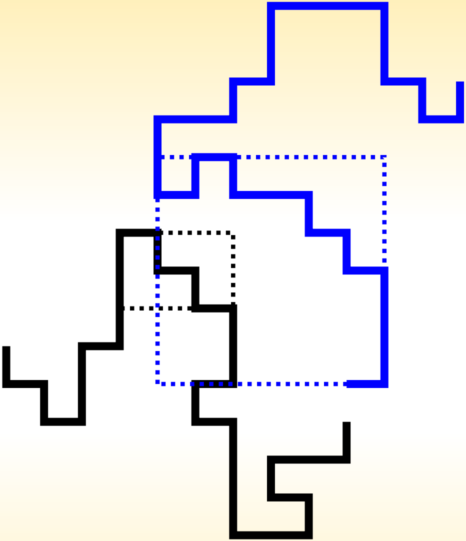


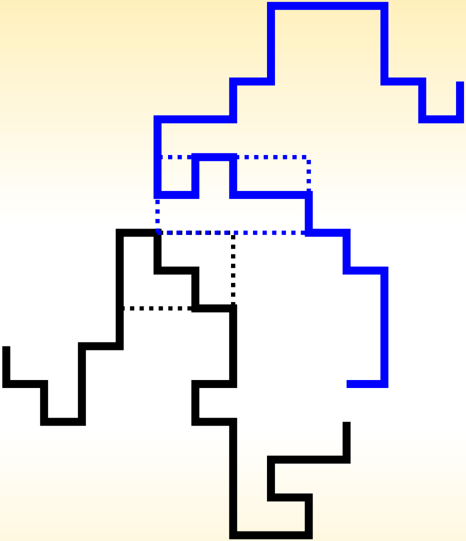


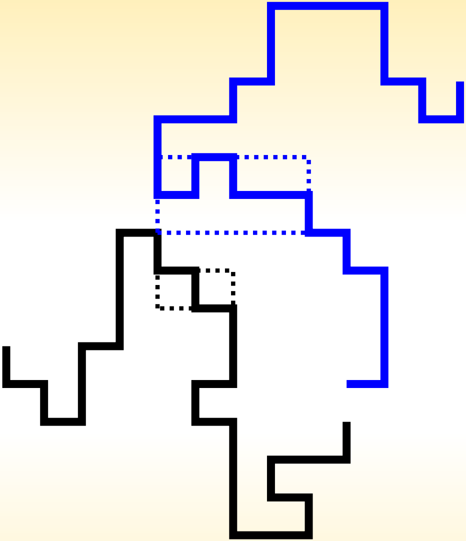


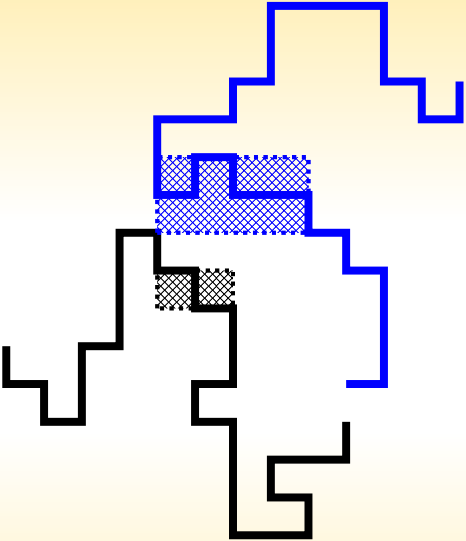


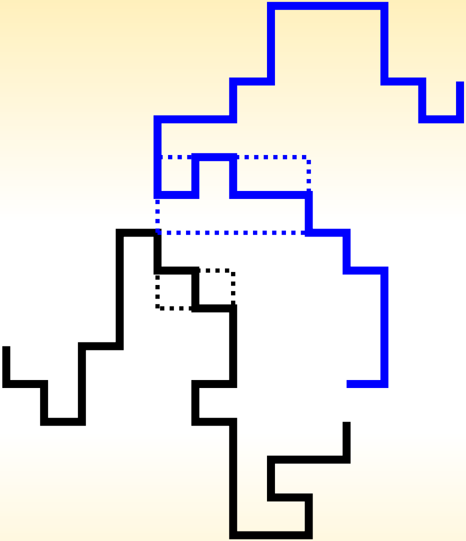


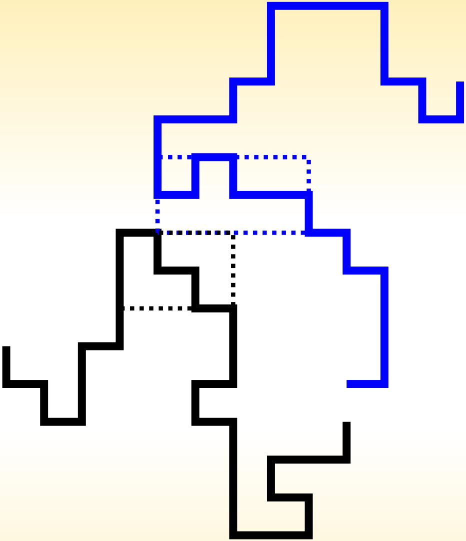


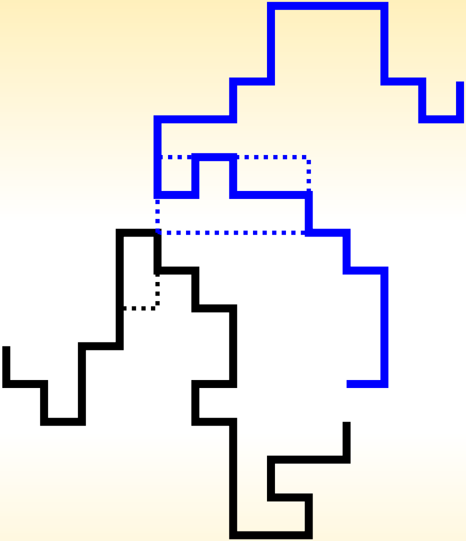


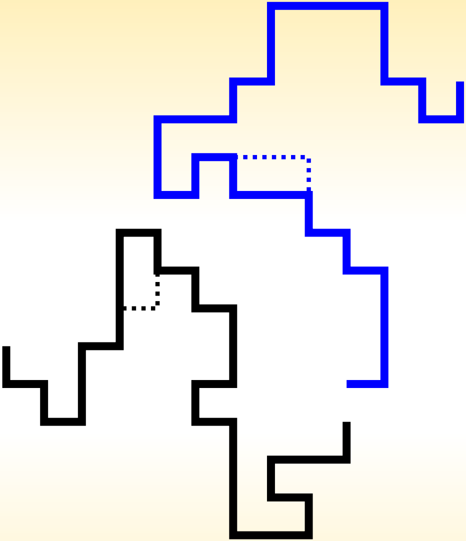


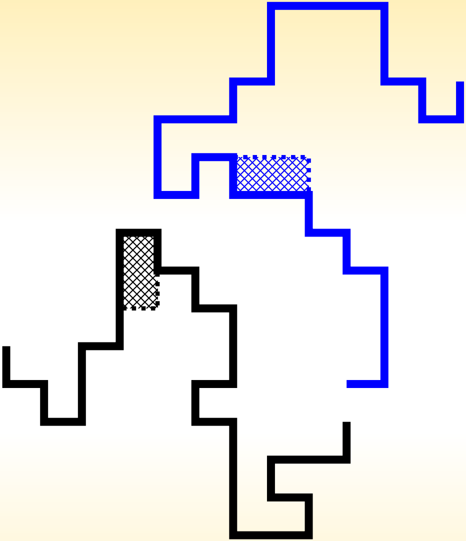


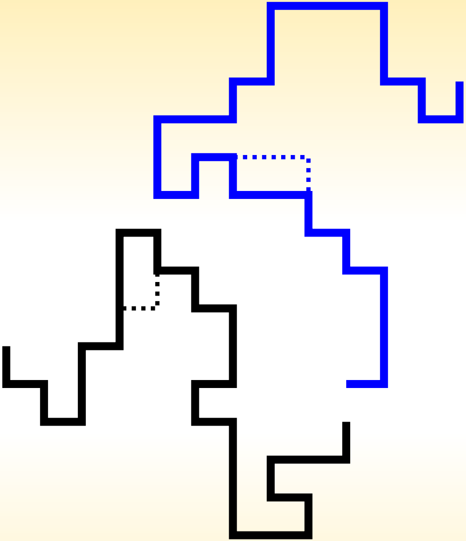


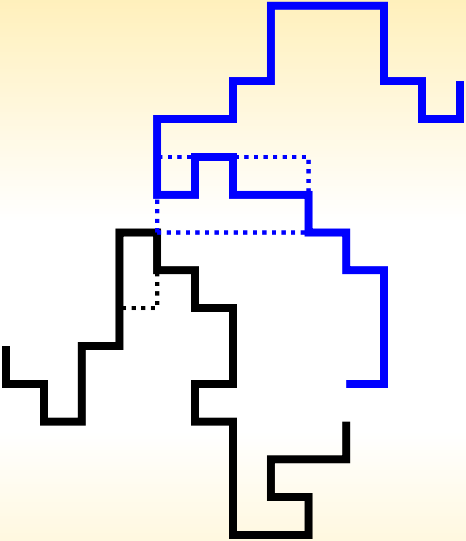


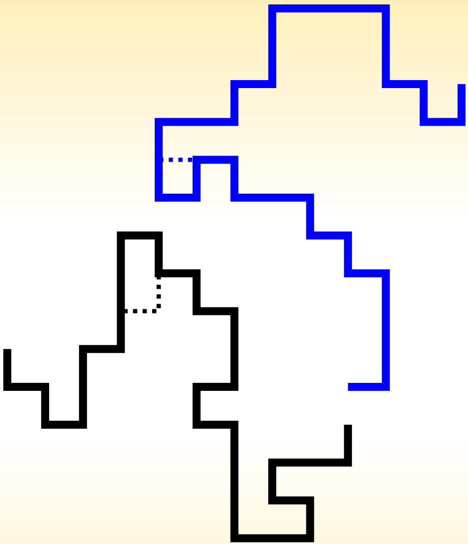


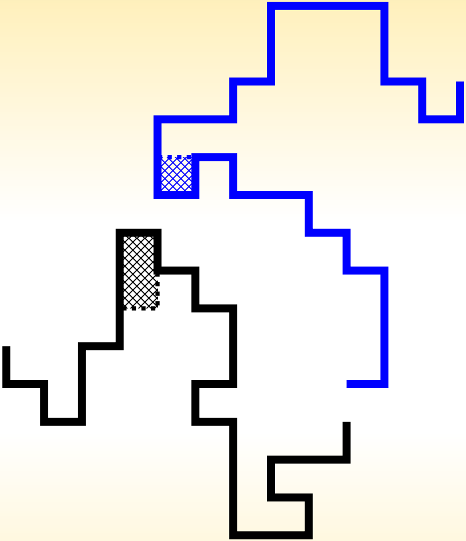


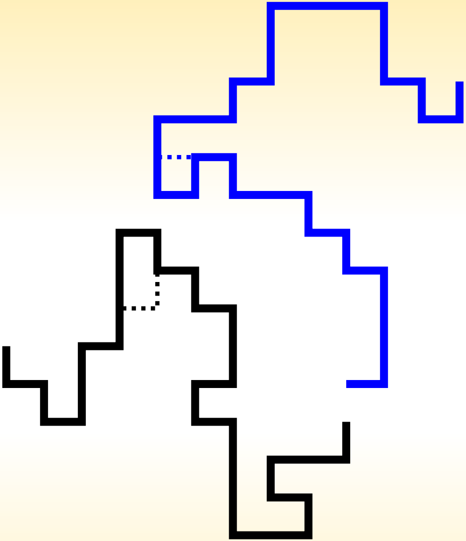


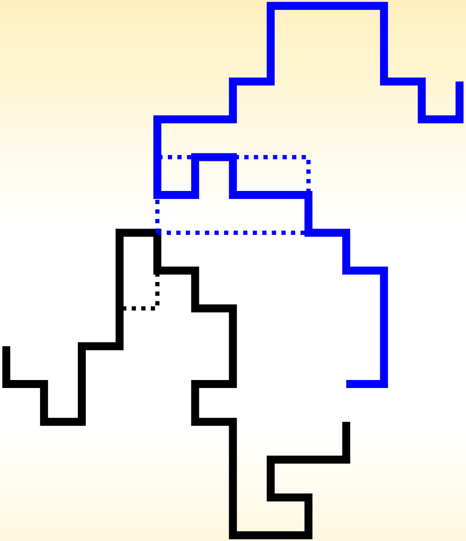


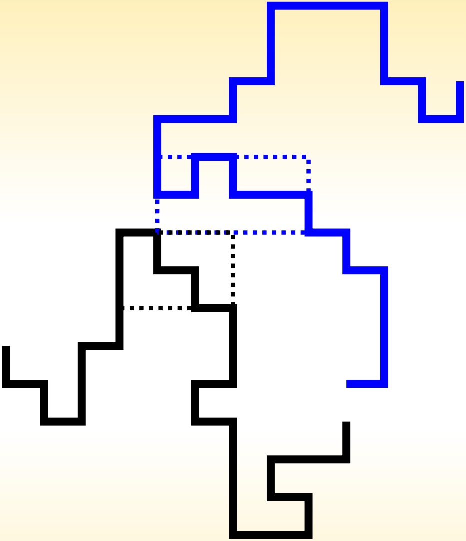


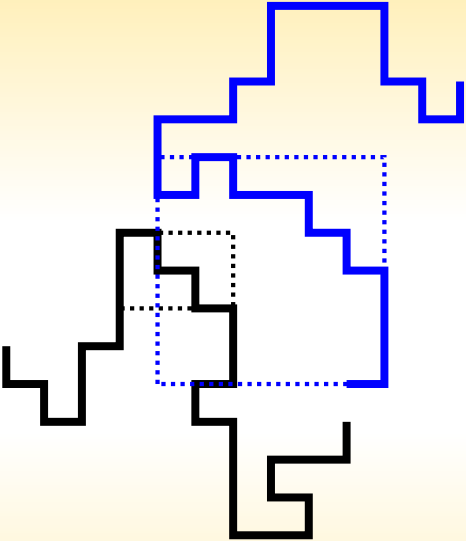


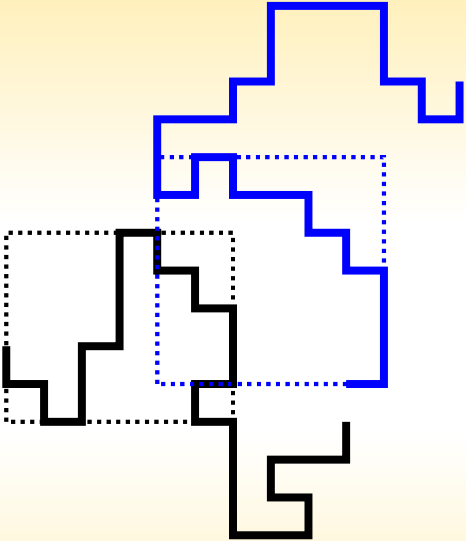


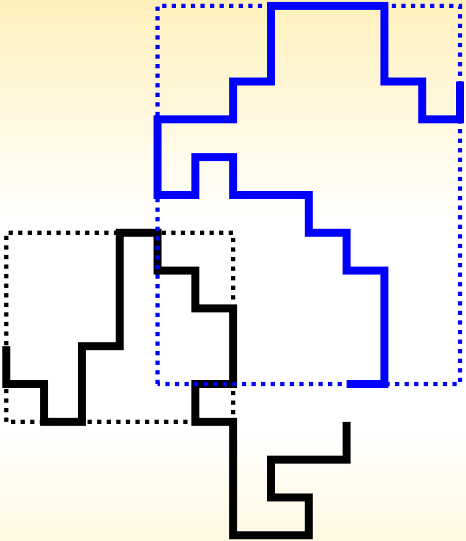


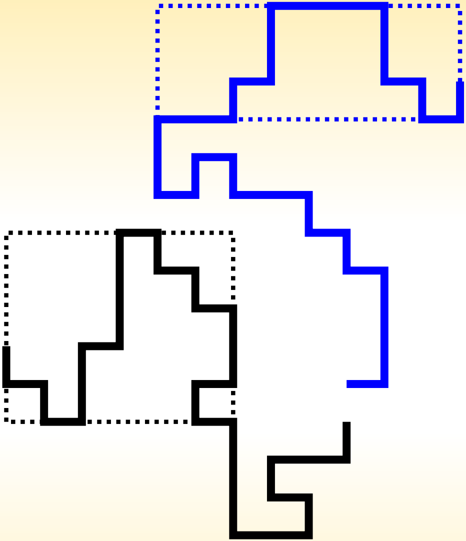


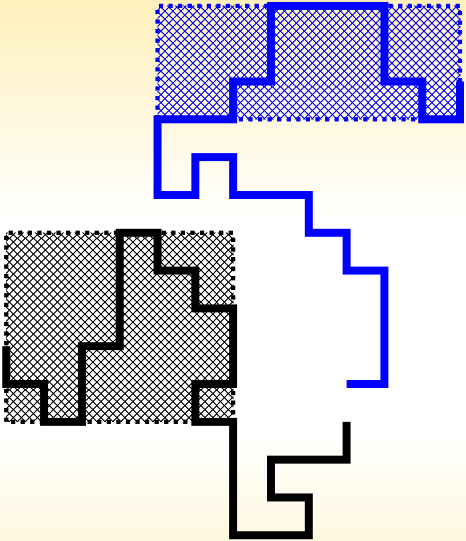


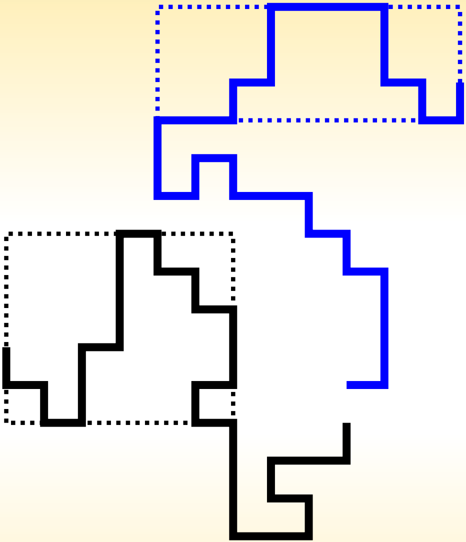


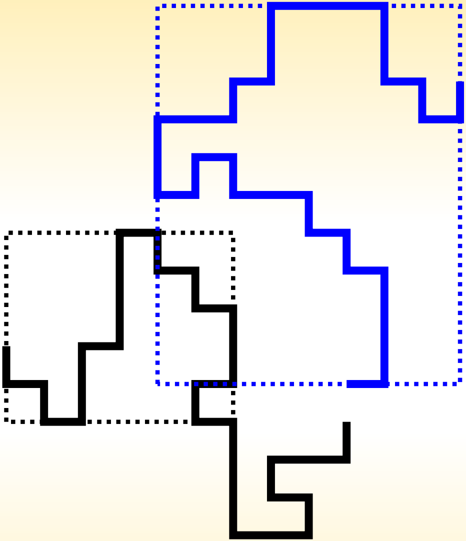


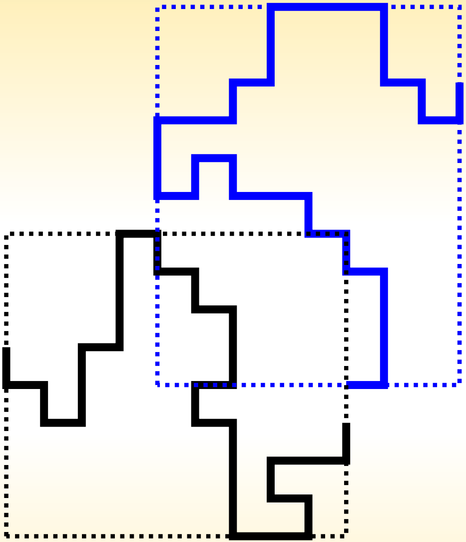


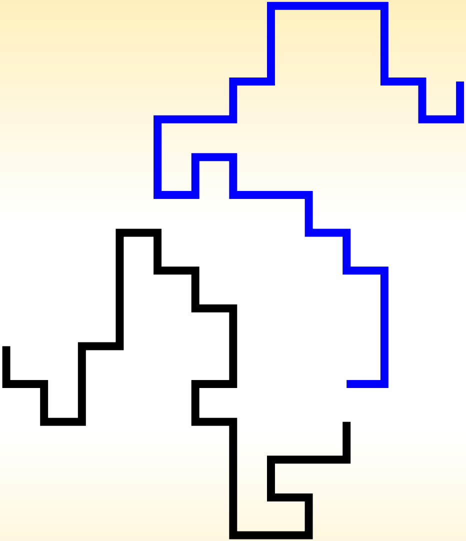












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CPU time per attempted pivot, for SAW of length N:

Lattice	Madras and Sokal	Kennedy	SAW-tree
Square	$O(N^{0.81})$	$O(N^{0.38})$	$o(\log N)$
Cubic	$O(N^{0.89})$	$O(N^{0.74})$	$O(\log N)$

Polymer knotting

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  - 1 million from efficiently implementing the pivot algorithm (Kennedy in 2002, C. in 2010)

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+	+	-	-	+	-
-	-	+	-	-	+
-	+	+	+	-	-
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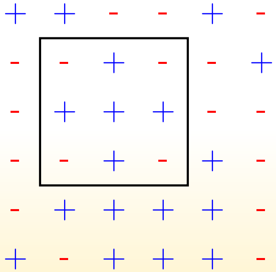

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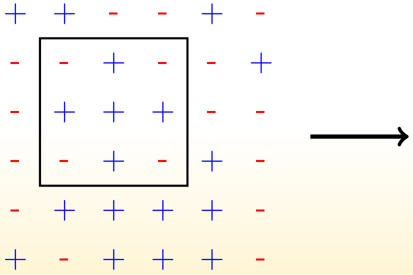

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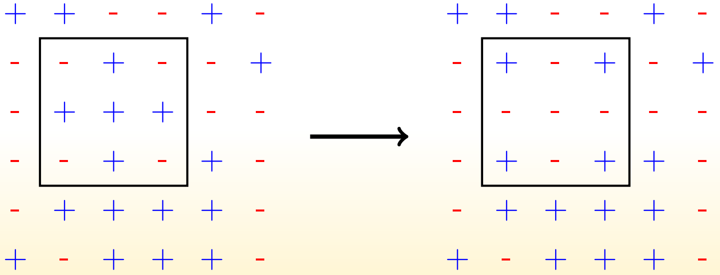

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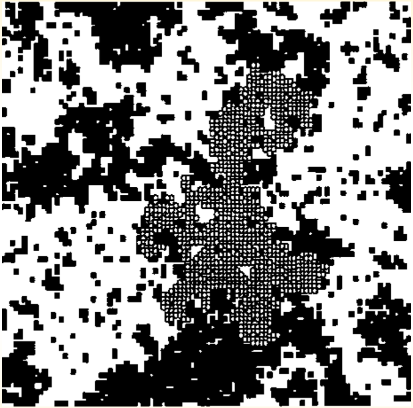
$$\begin{matrix} + & + & - & - & + & - \\ - & - & + & - & - & + \\ - & + & + & + & - & - \\ - & - & + & - & + & - \\ - & + & + & + & + & - \\ + & - & + & + & + & - \end{matrix} \quad \longrightarrow \quad \begin{matrix} + & + & - & - & + & - \\ - & + & - & + & - & + \\ - & - & - & - & - & - \\ - & + & - & + & + & - \\ - & + & + & + & + & - \\ + & - & + & + & + & - \end{matrix}$$

Whereas these are the kinds of clusters the system "wants" to flip at criticality:



(Image of a Wolff algorithm update due to Wolfhard Janke)

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- Does improve things, but no algorithm as spectacularly as successful as the pivot algorithm is available.

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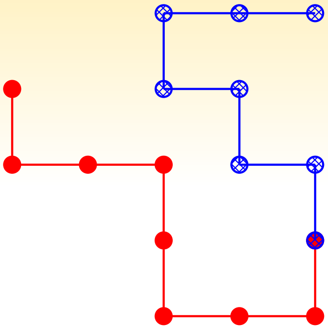
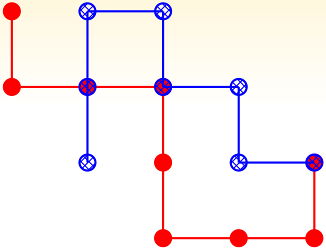
- Indicator function for successful concatenation is our observable, and

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



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



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- Iterate to obtain estimates for c_N for longer walks.

$$\begin{aligned} c_N &= \frac{c_N}{c_{N/2}^2} \cdot \frac{c_{N/2}^2}{c_{N/4}^4} \cdots \frac{c_{2k}^{N/2k}}{c_k^{N/k}} c_k^{N/k} \\ &= \langle B_{N/2,N/2} \rangle \langle B_{N/4,N/4} \rangle^2 \cdots \langle B_{k,k} \rangle^{N/2k} c_k^{N/k} \end{aligned}$$

where c_k is known.

- Can then use $c_N \sim A\mu^N N^{\gamma-1}$ to estimate μ:

$$
\begin{aligned}
\log \mu_N &\equiv \frac{1}{N} \log c_N \\
&= \frac{1}{k} \log c_k + \frac{1}{2k} \log\langle B_{k,k}\rangle + \frac{1}{4k} \log\langle B_{2k,2k}\rangle + \cdots \\
&\qquad \cdots + \frac{1}{N} \log\langle B_{N/2,N/2}\rangle \\
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- Corrections vanish with increasing N! In limit of large N systematic error of estimator $\to 0$.

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- best previous estimate via "PERM" algorithm: $\mu = 4.6840386(11)$ (Grassberger, 2005).

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- Linear order and spatial separation seems to make SAW a special case.
- Challenge: find efficient algorithms and computer implementations for other systems. (Very active research area, e.g. cluster algorithms, Wang-Landau method, PERM, worm algorithms.)