Fast Monte Carlo simulation of self-avoiding walks and related models of polymers

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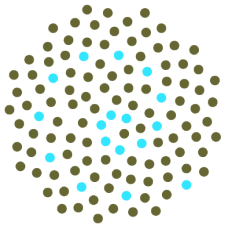
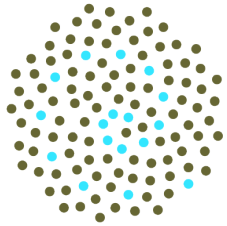


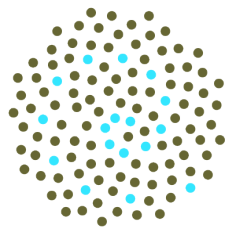
Polymers

- Widely important, e.g. in biology (DNA, proteins) and chemistry (plastics, rubber).
- Self-avoiding walks (SAWs) and related models are important in the theoretical understanding of critical phenomena.



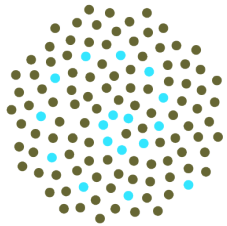
Why use Monte Carlo with non-local moves?

- Few exact results for $d \geq 3$.
- Monte Carlo simulation most effective means to estimate universal features such as critical exponents.
- Monte Carlo is also an effective tool to study properties of more realistic models (competes with MD).
- Effective non-local moves, with low rejection rates, are dramatically more efficient than local moves.
- Polymers: pivot, cut-and-paste.
- Autocorrelation time for global observables in CPU units:
  - Local moves $O(N^2)$ (e.g. reptation);
  - Pivot algorithm $O(N)$ (Madras & Sokal implementation).



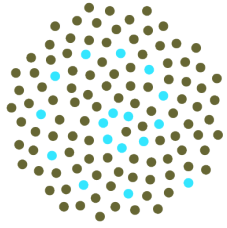
Pivot algorithm

- Invented in 1969 by Lal.
- The power of the method only realised since influential paper by Madras and Sokal in 1988 (over 500 citations).
- Large change in global observables with each successful pivot.

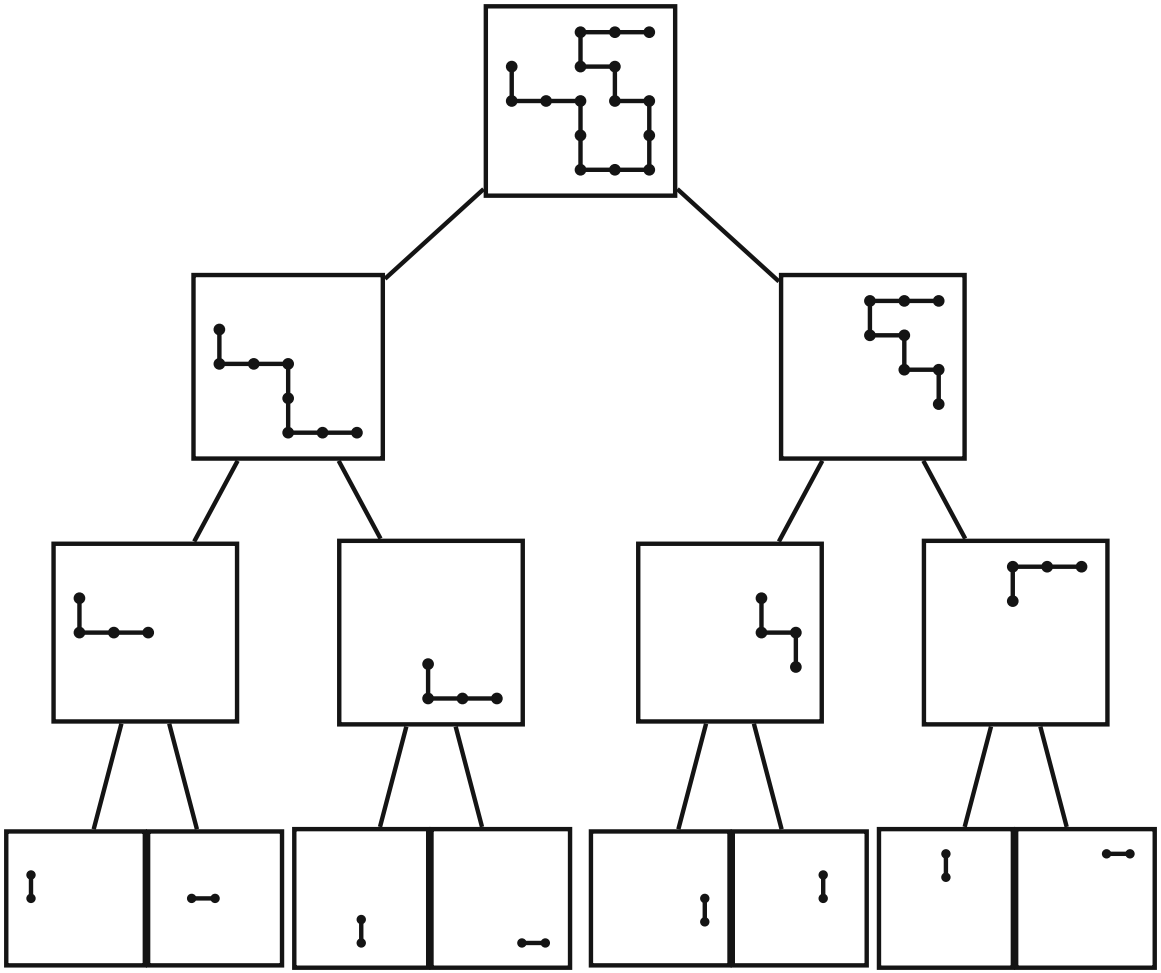


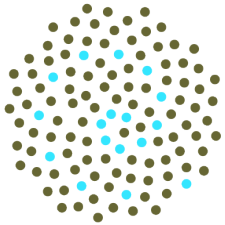
Implementing non-local moves efficiently

- Two problems to resolve:
  - Fast update of global observables when a move is made.
  - Fast calculation of *change* in interaction energy.
- Resolution:
  - Represent polymer as a binary tree.
  - Each monomer is a leaf in the tree.
  - Internal nodes store aggregate information about all monomer descendants, e.g. global observables and "bounding box" information.
  - Need to define tree-rotation operations so that structure of tree can be altered (splitting / merging).
  - Apply non-local moves to root of the tree only.



SAW-tree





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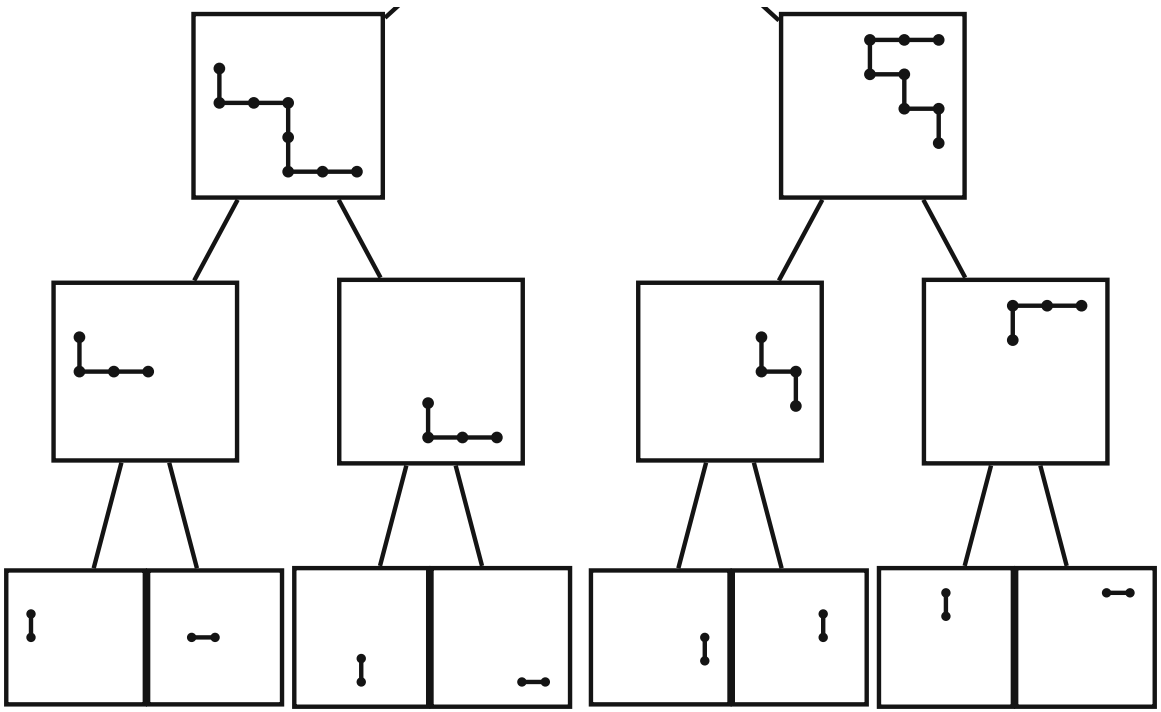
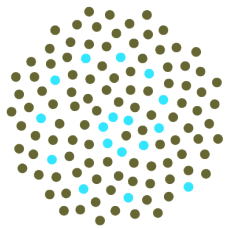
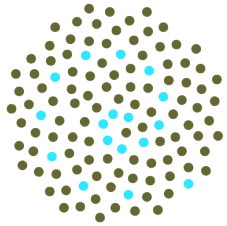
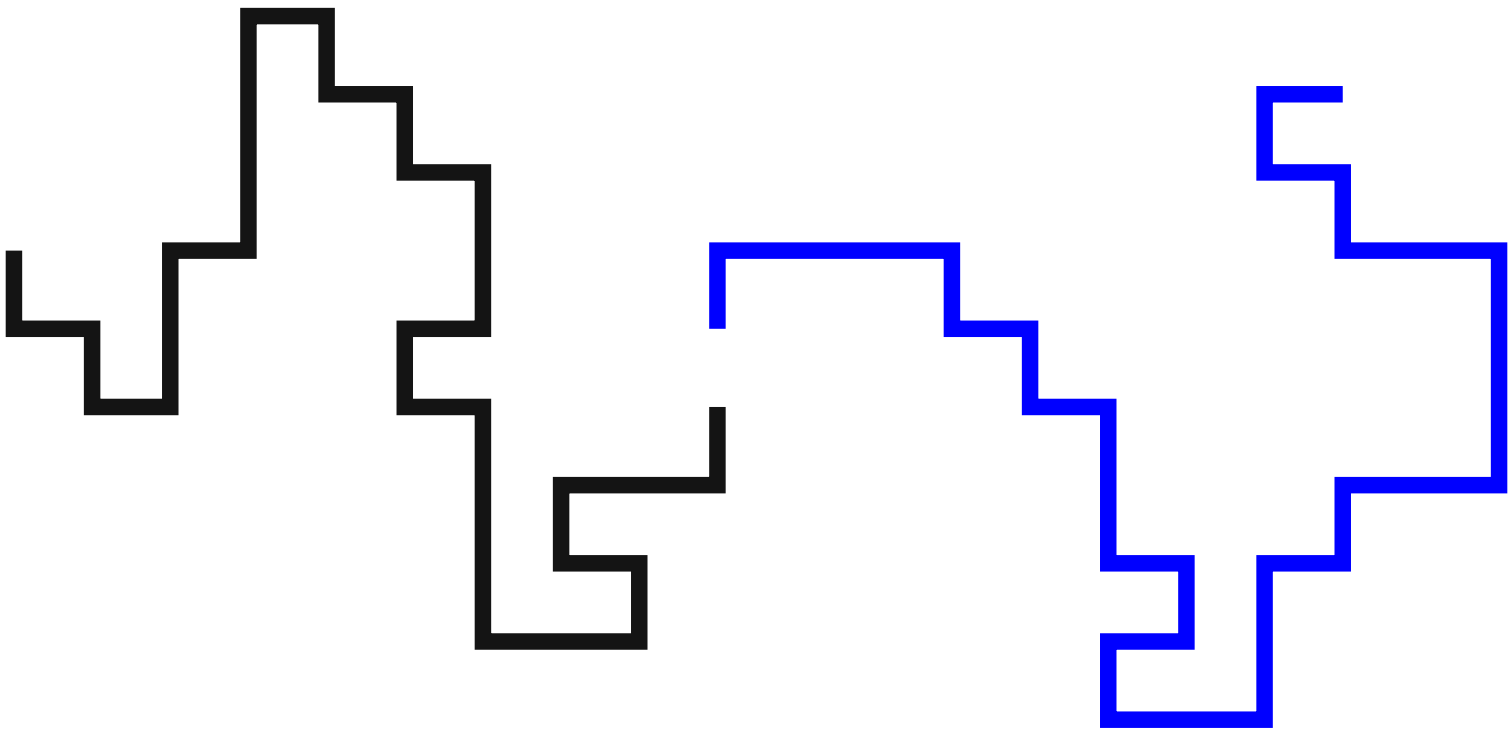


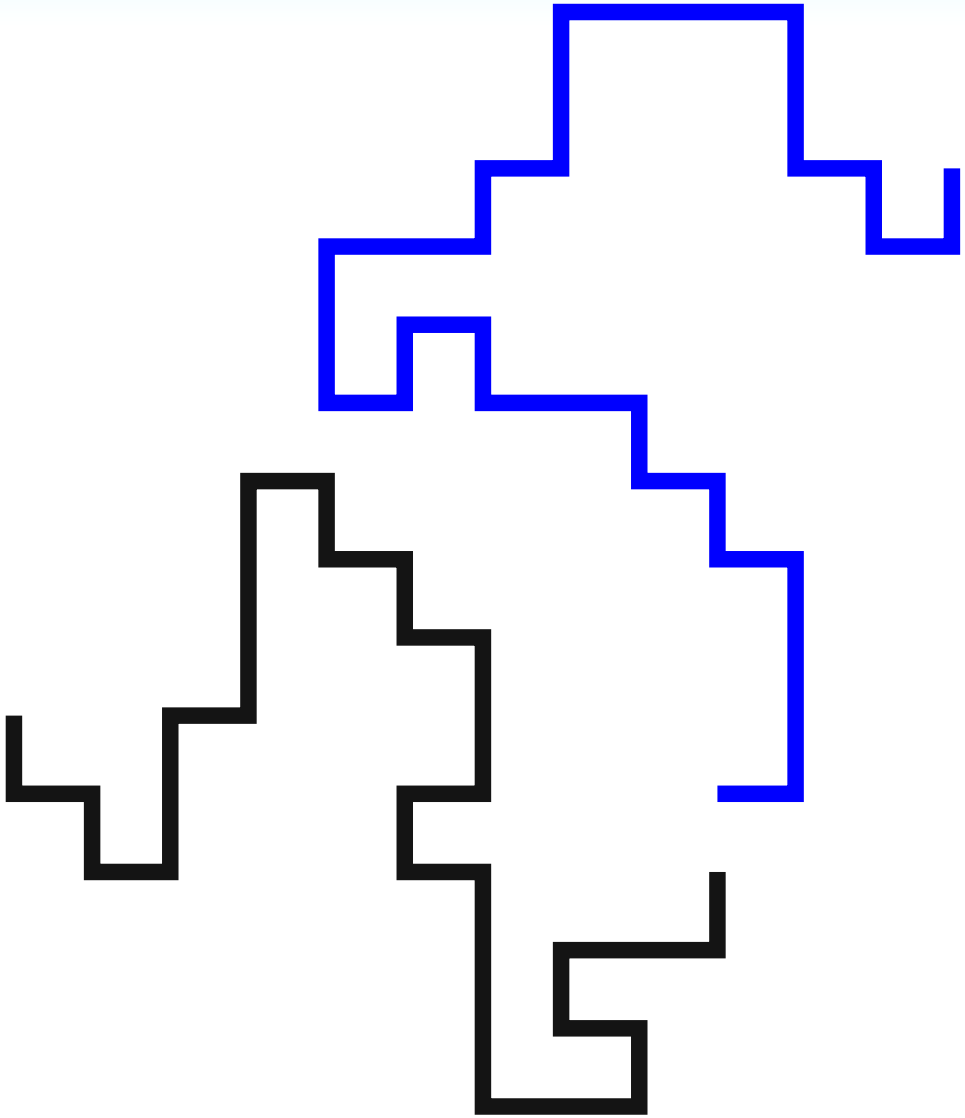


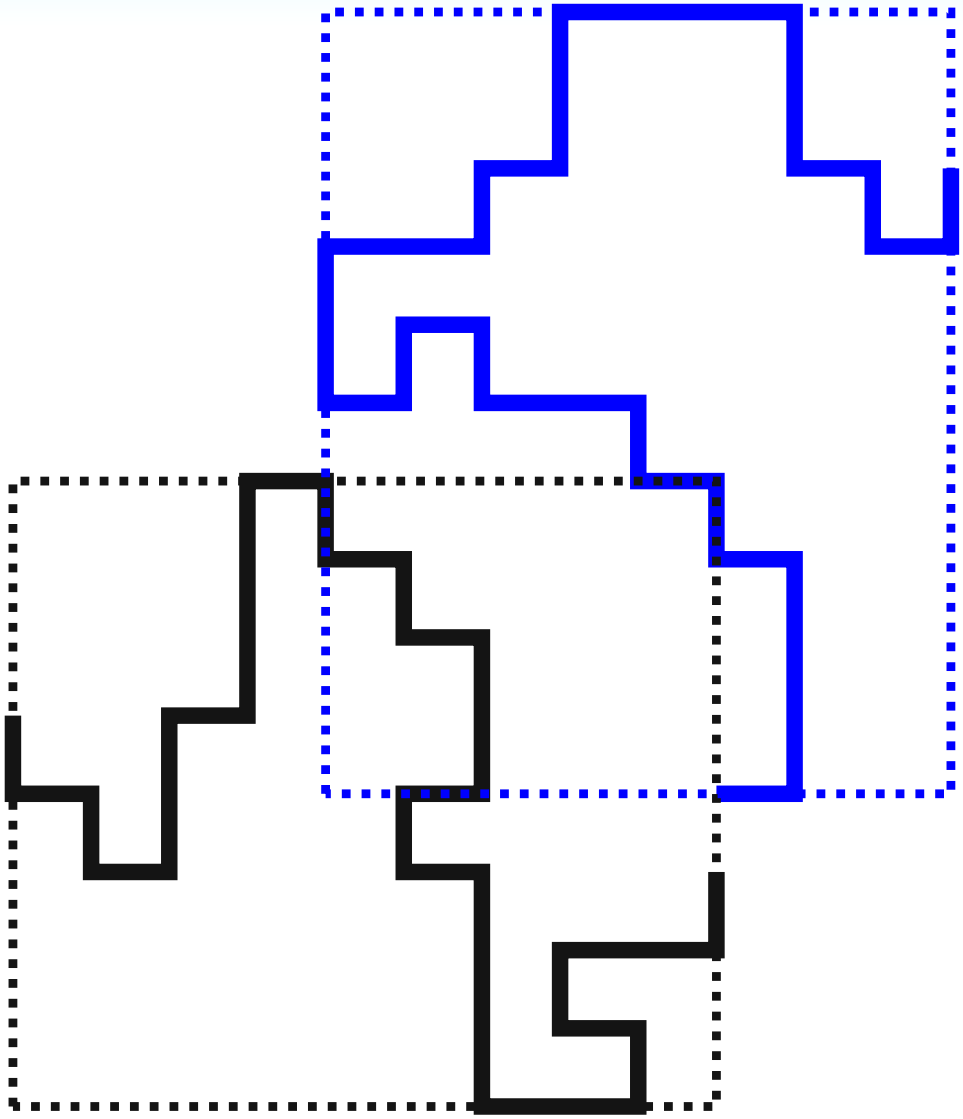
Pivot algorithm

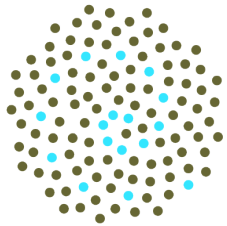
- After applying pivot to a SAW with 64 sites, will show algorithm to determine whether new configuration is self-avoiding.
- Can be easily adapted to calculating interaction energy for monomers with short-range interaction, e.g. ISAW.
- Will now show how the algorithm determines that a walk is self-avoiding after a pivot. The 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.

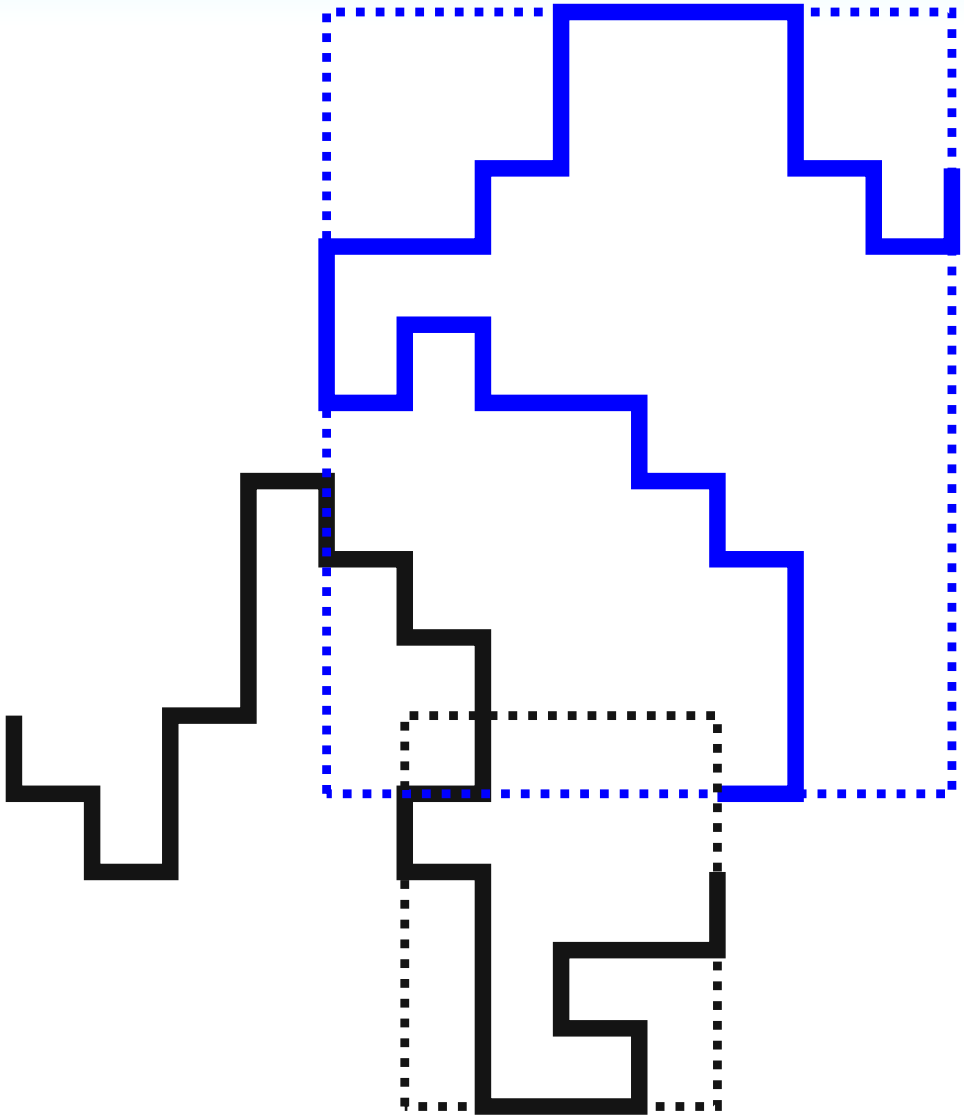


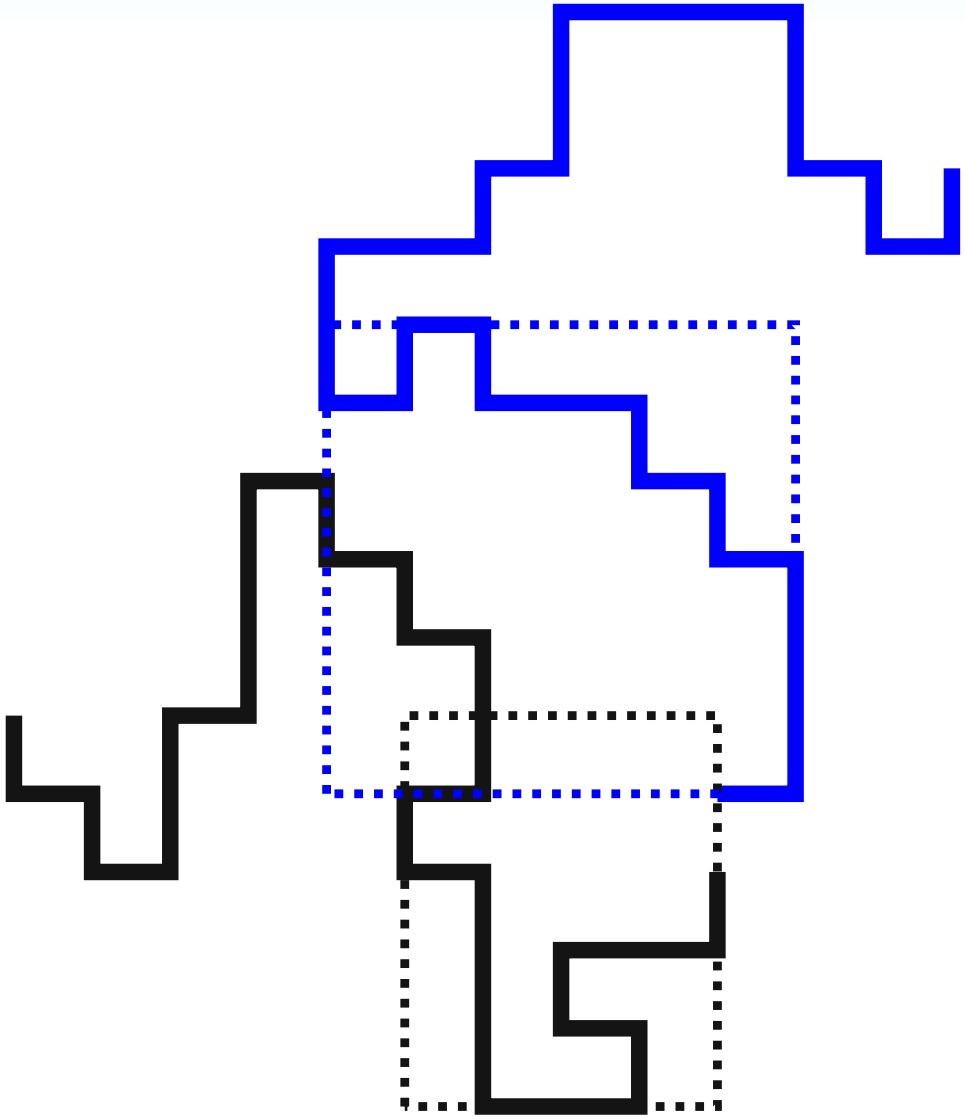


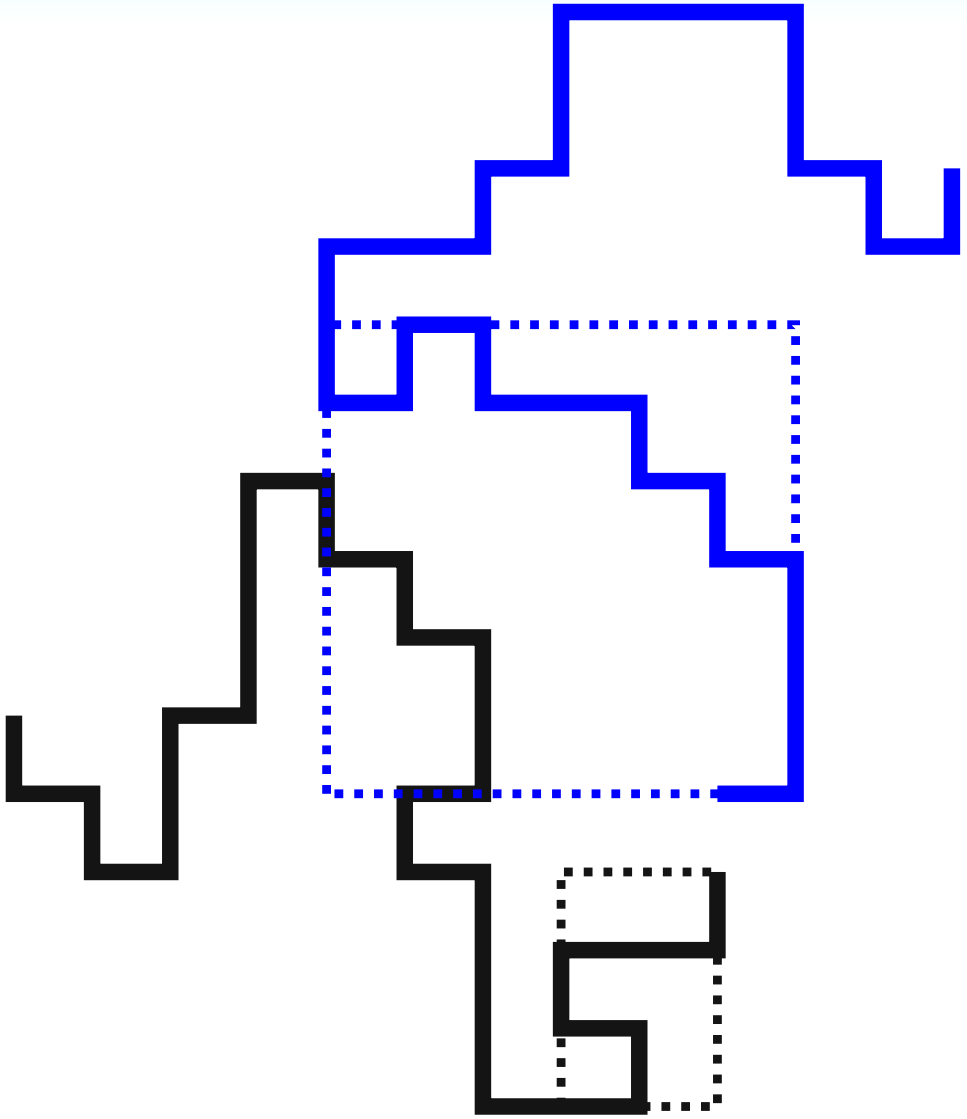


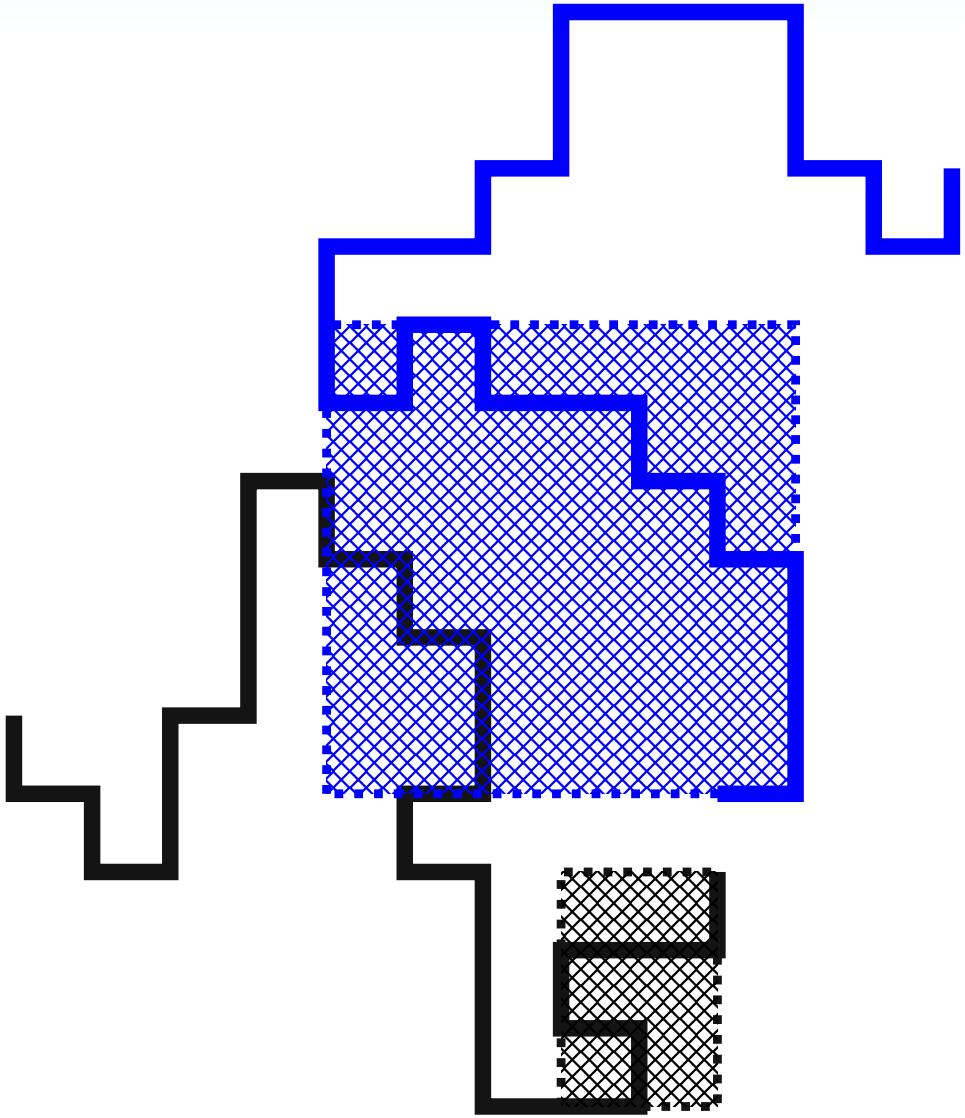


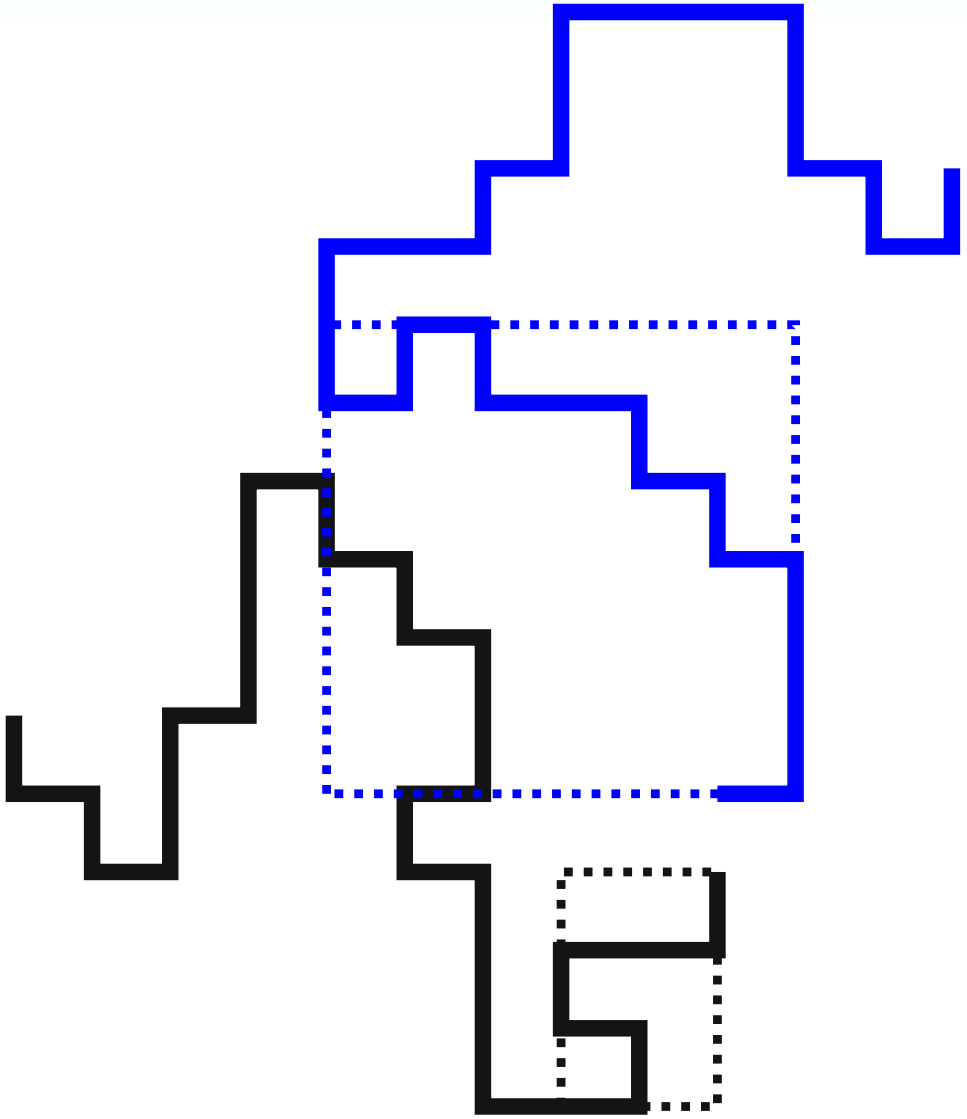


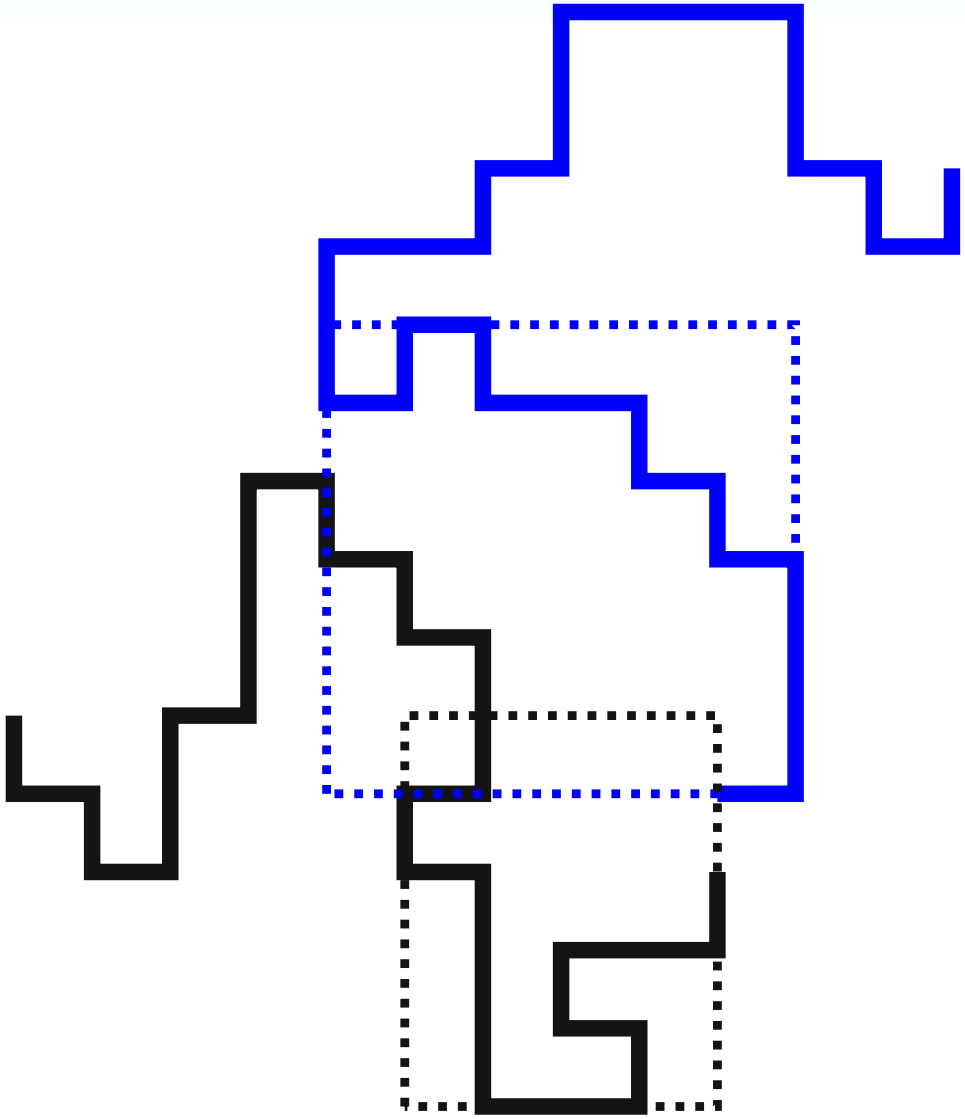


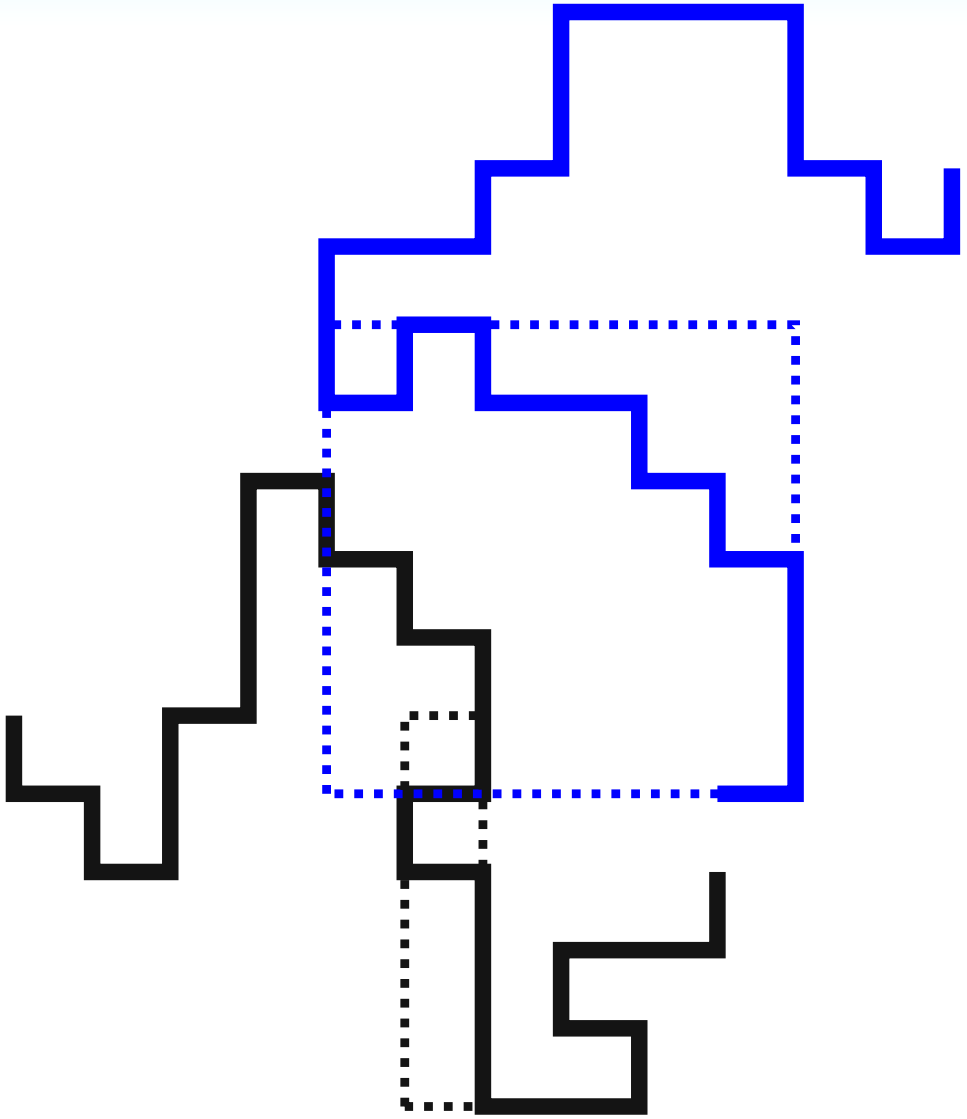


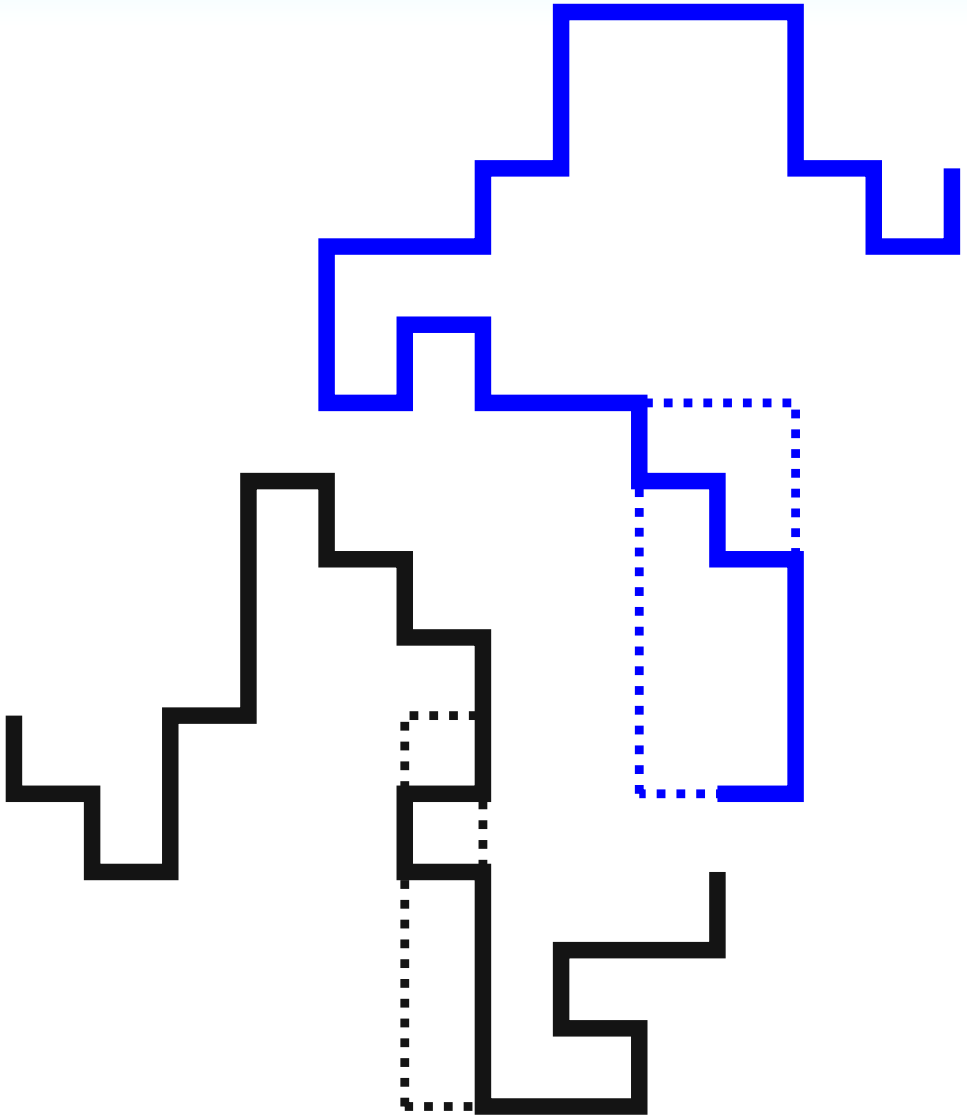


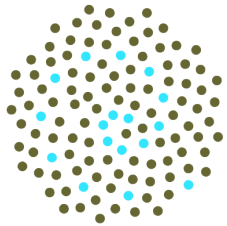


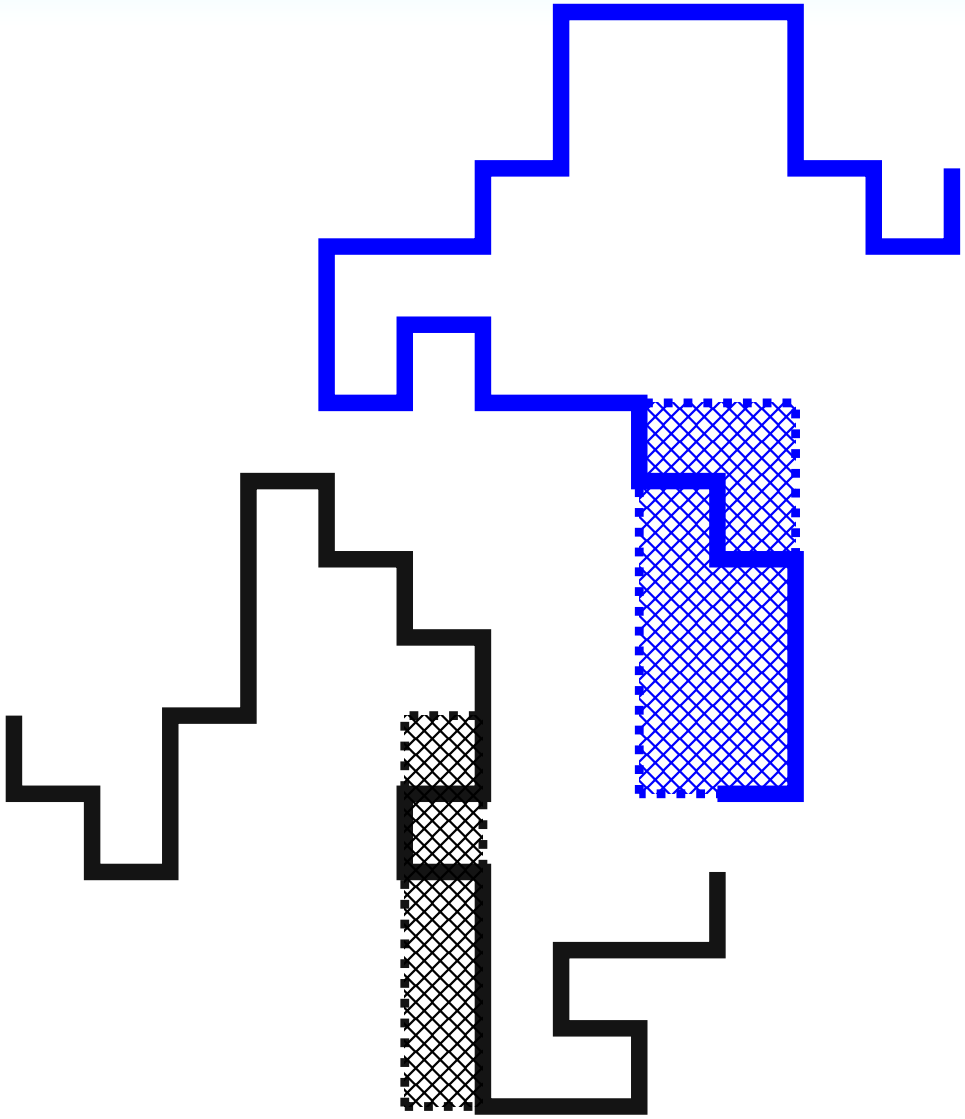


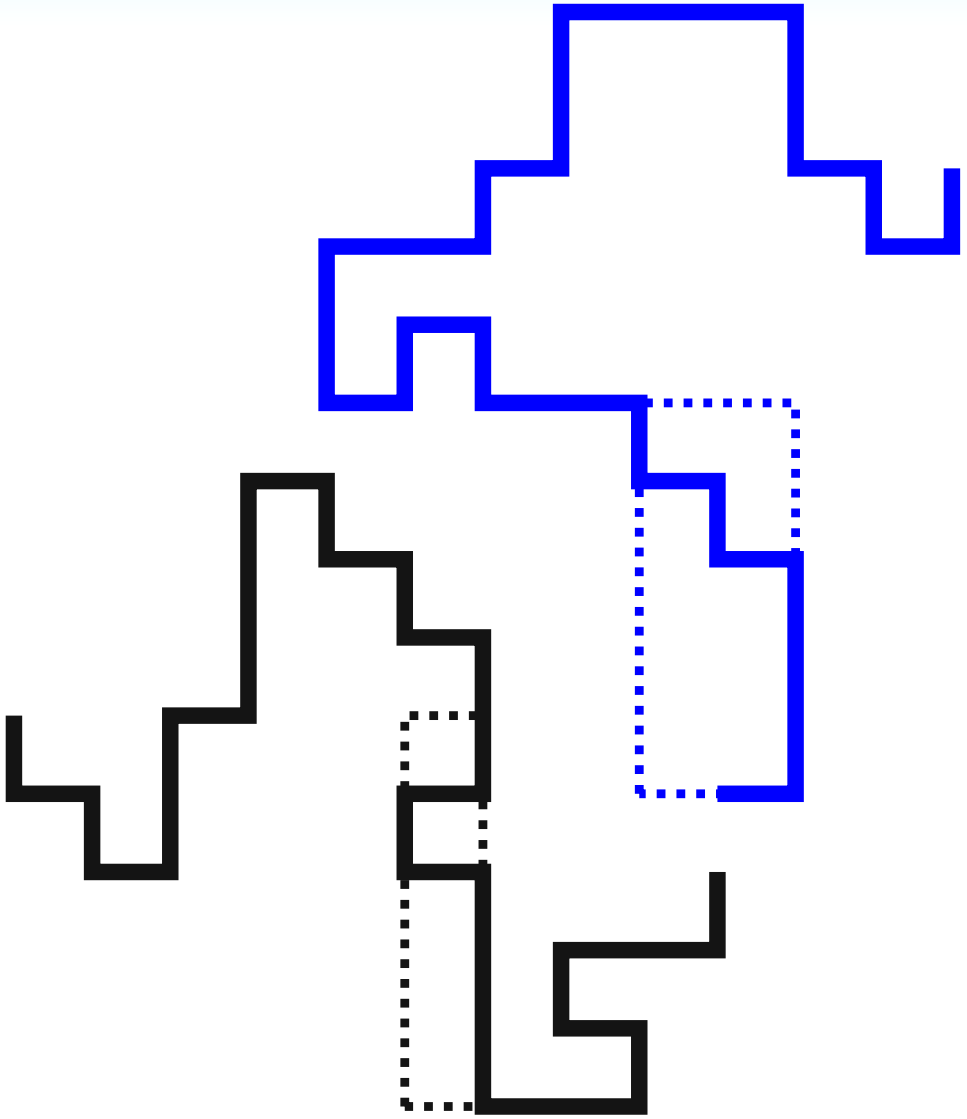


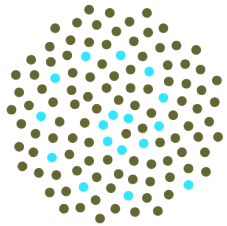


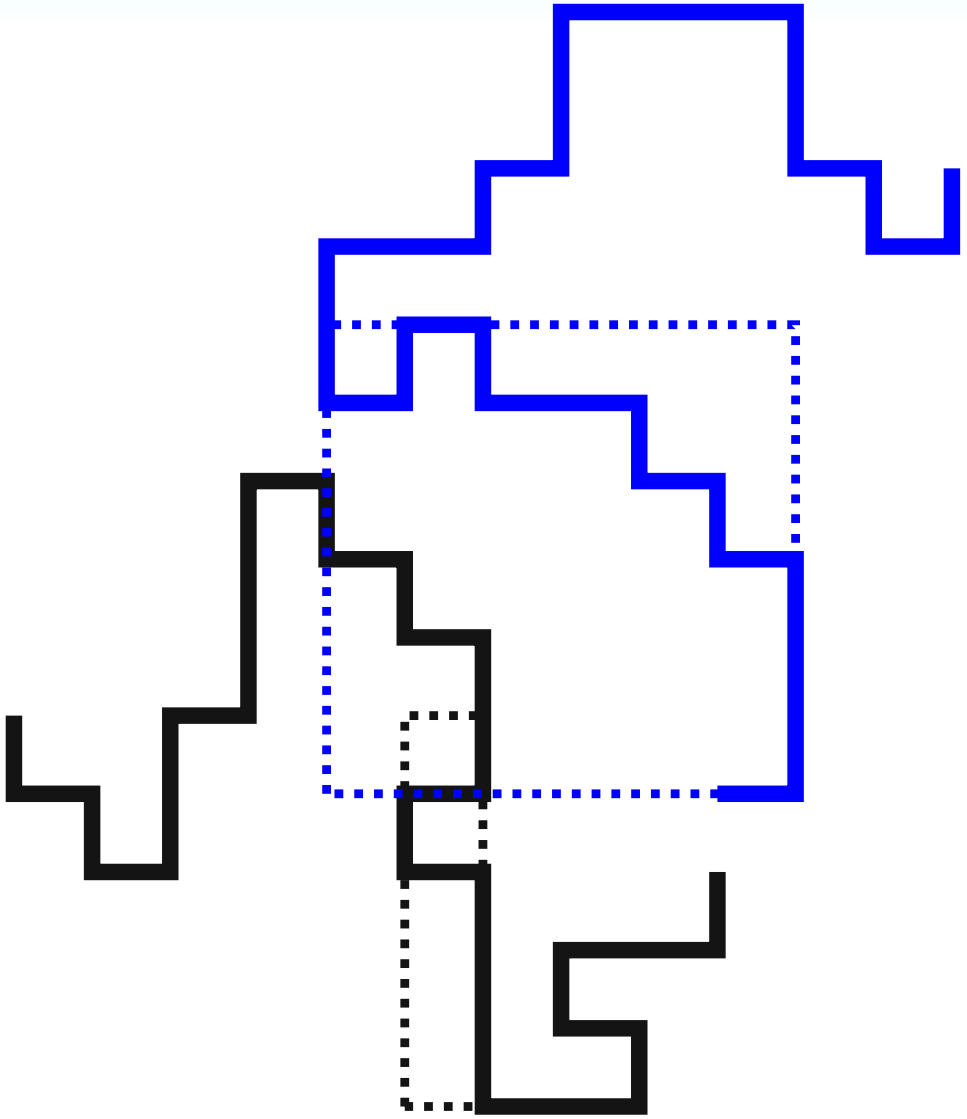


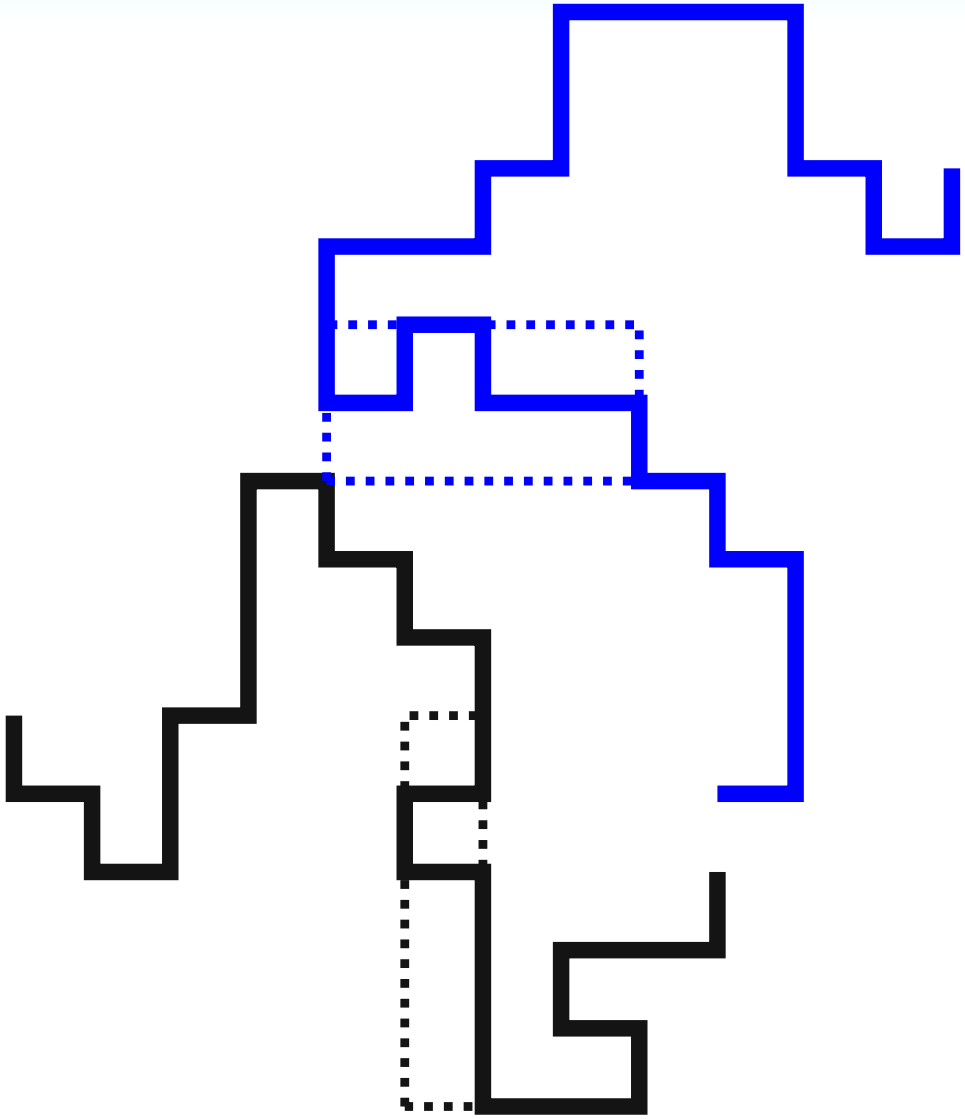


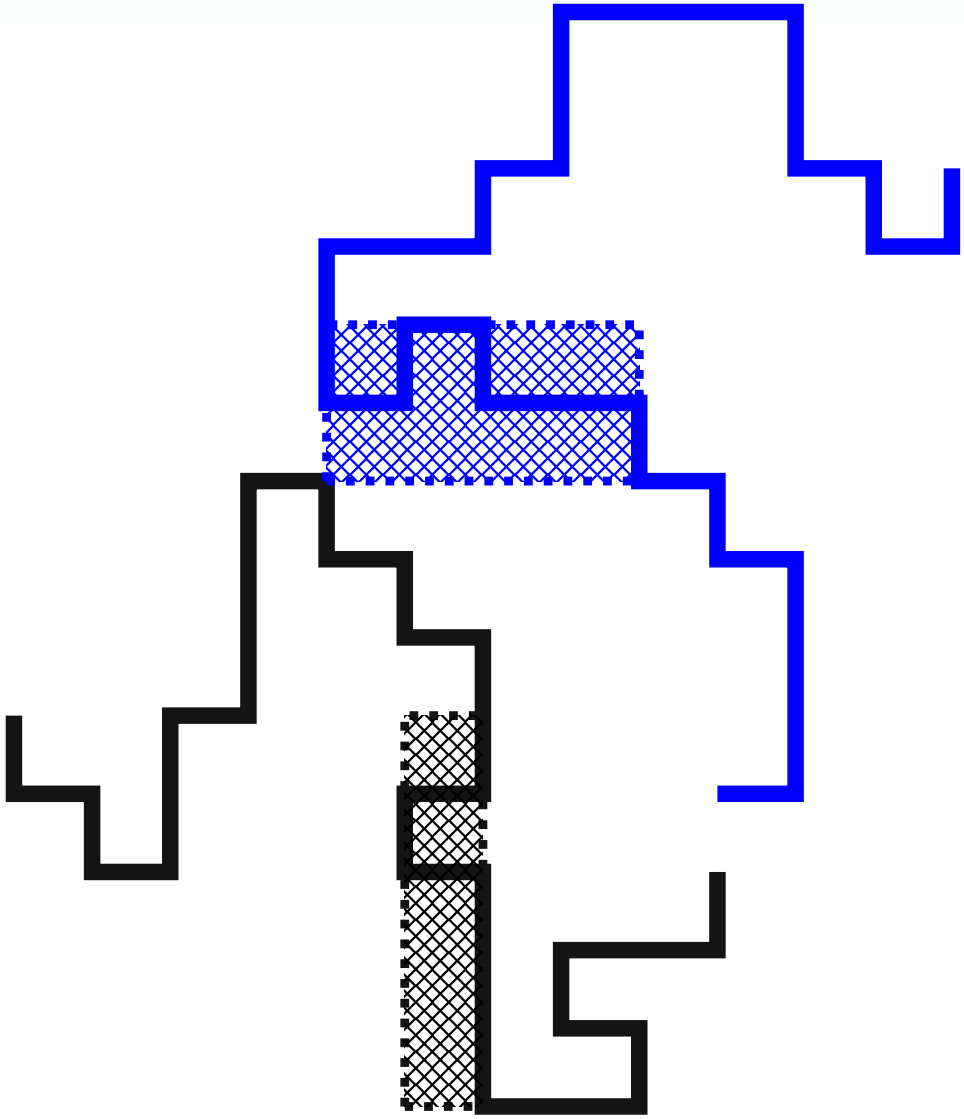


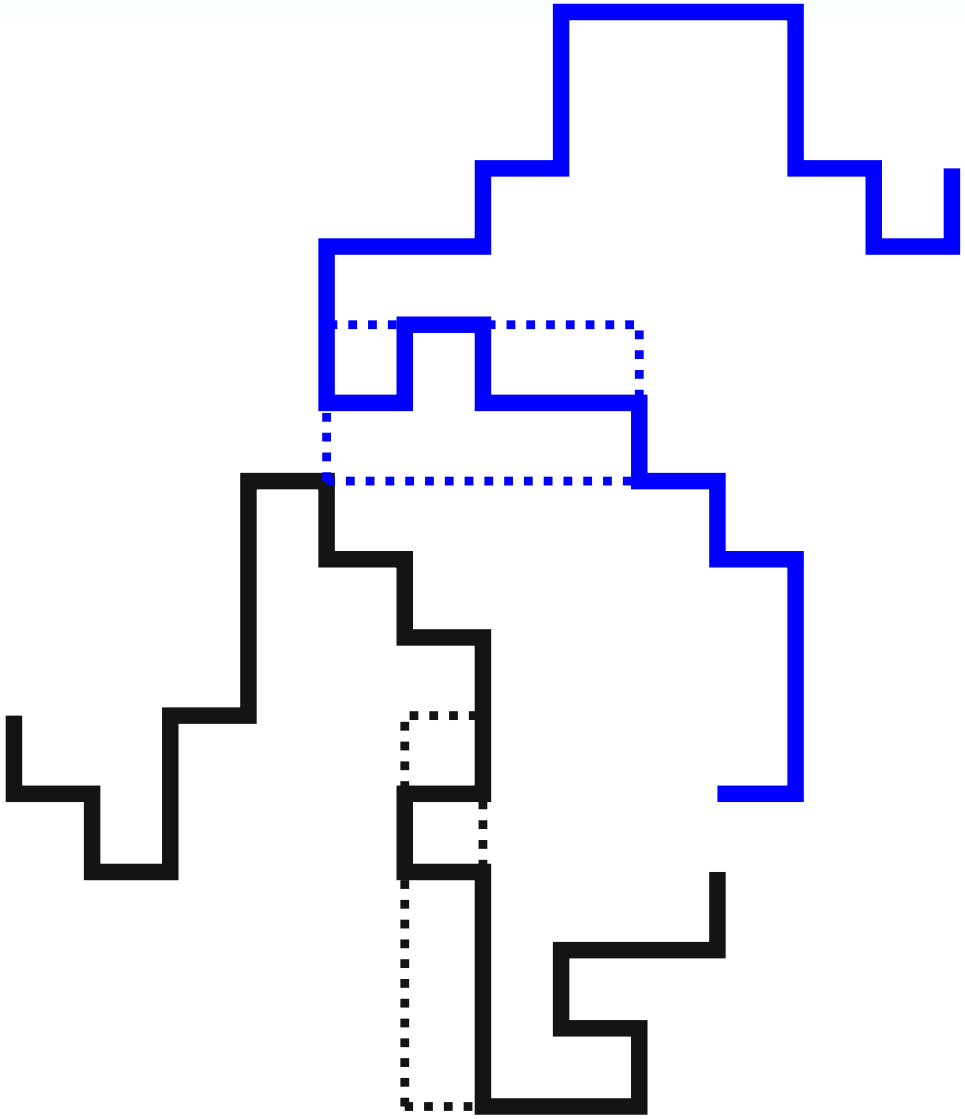


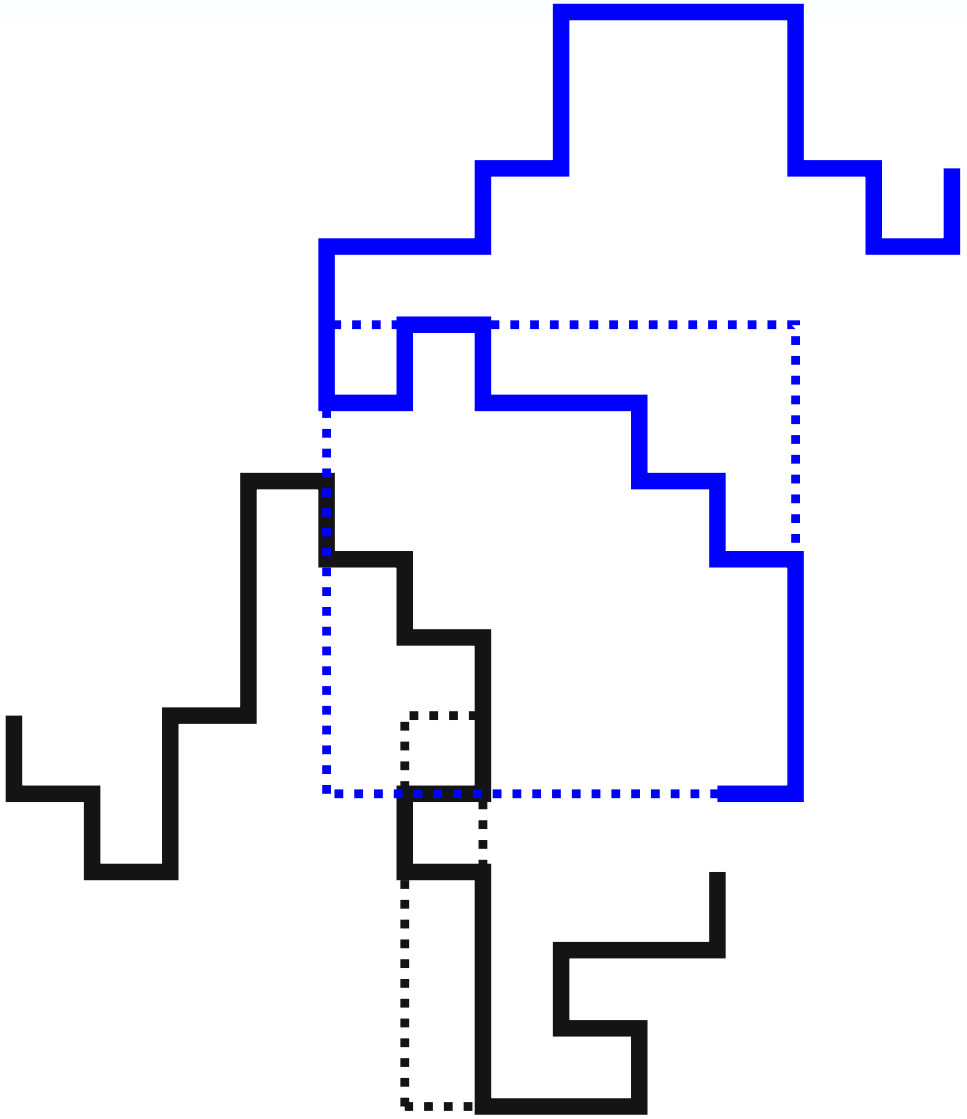


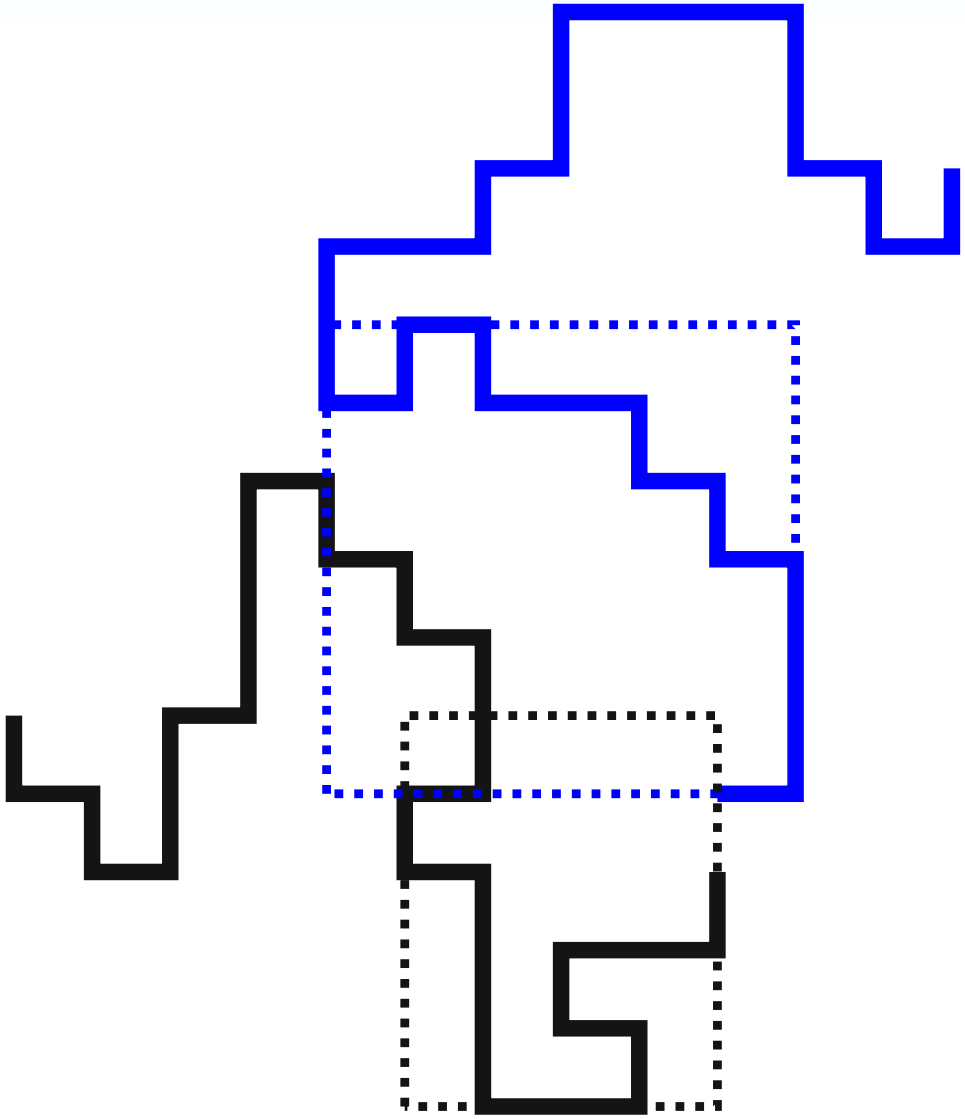


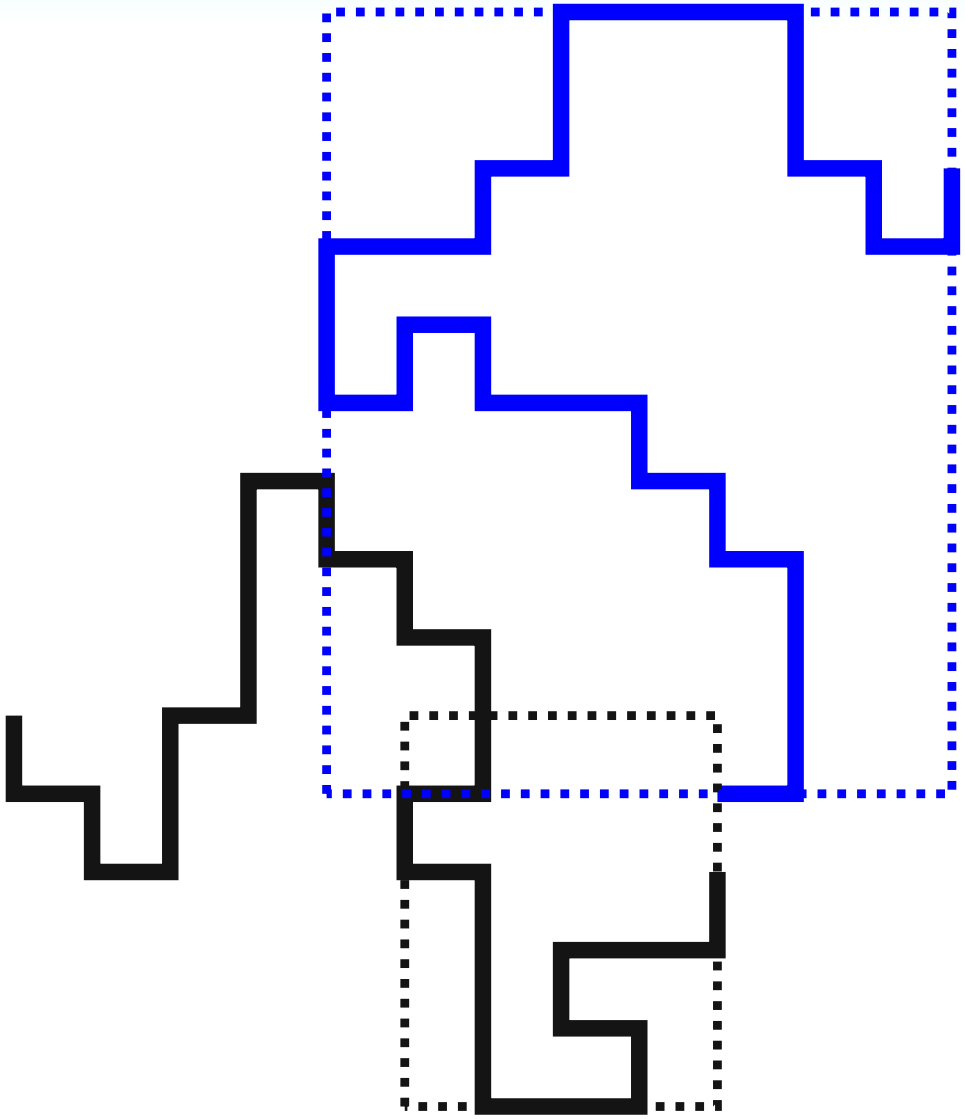


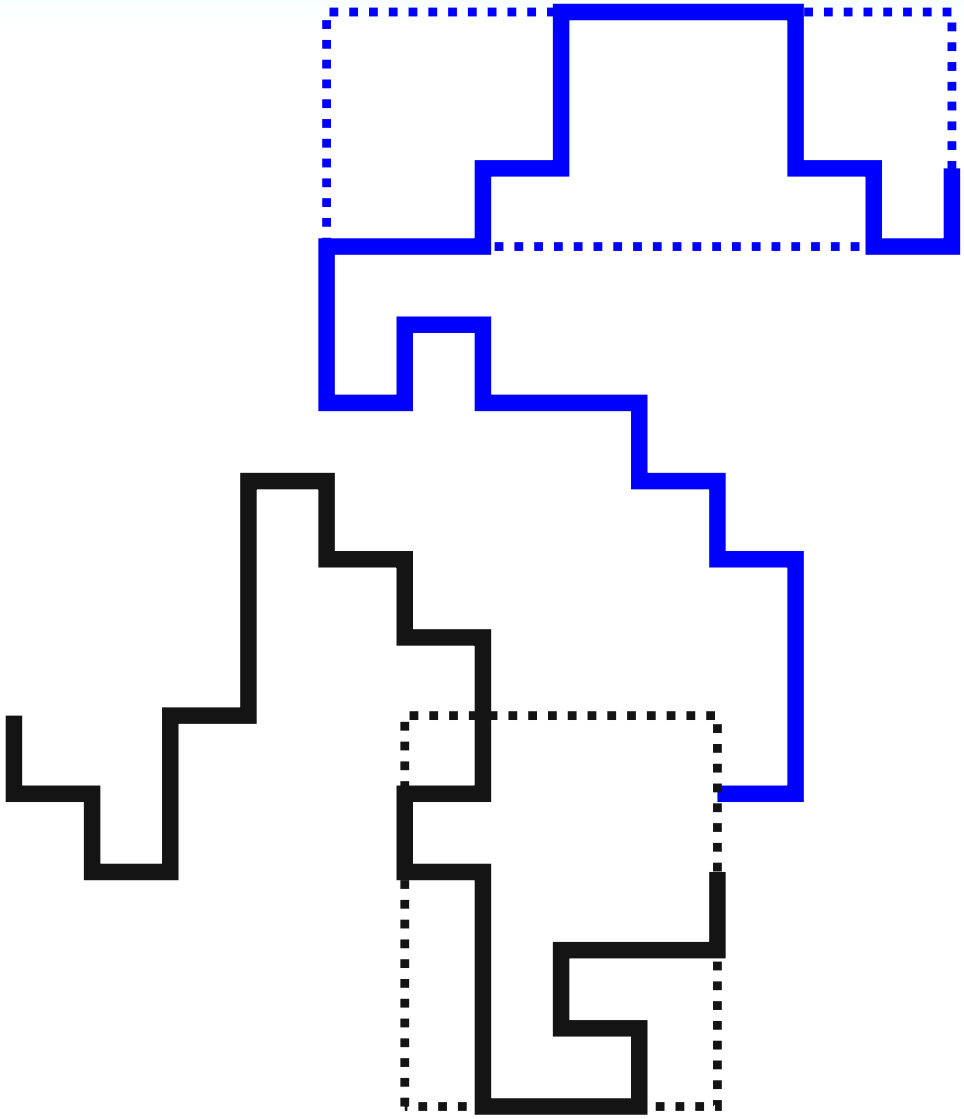


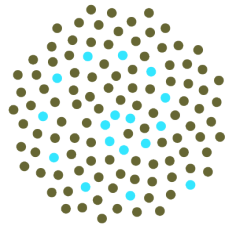


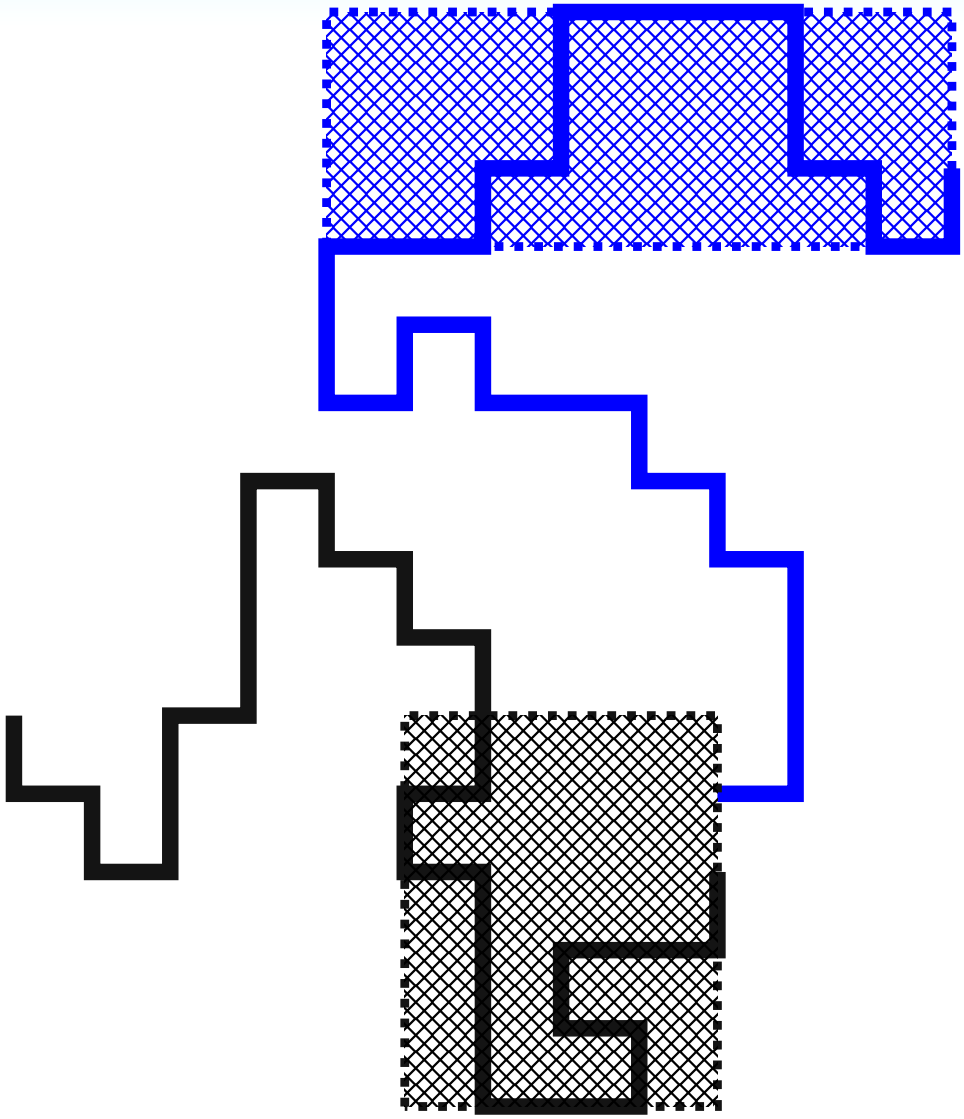


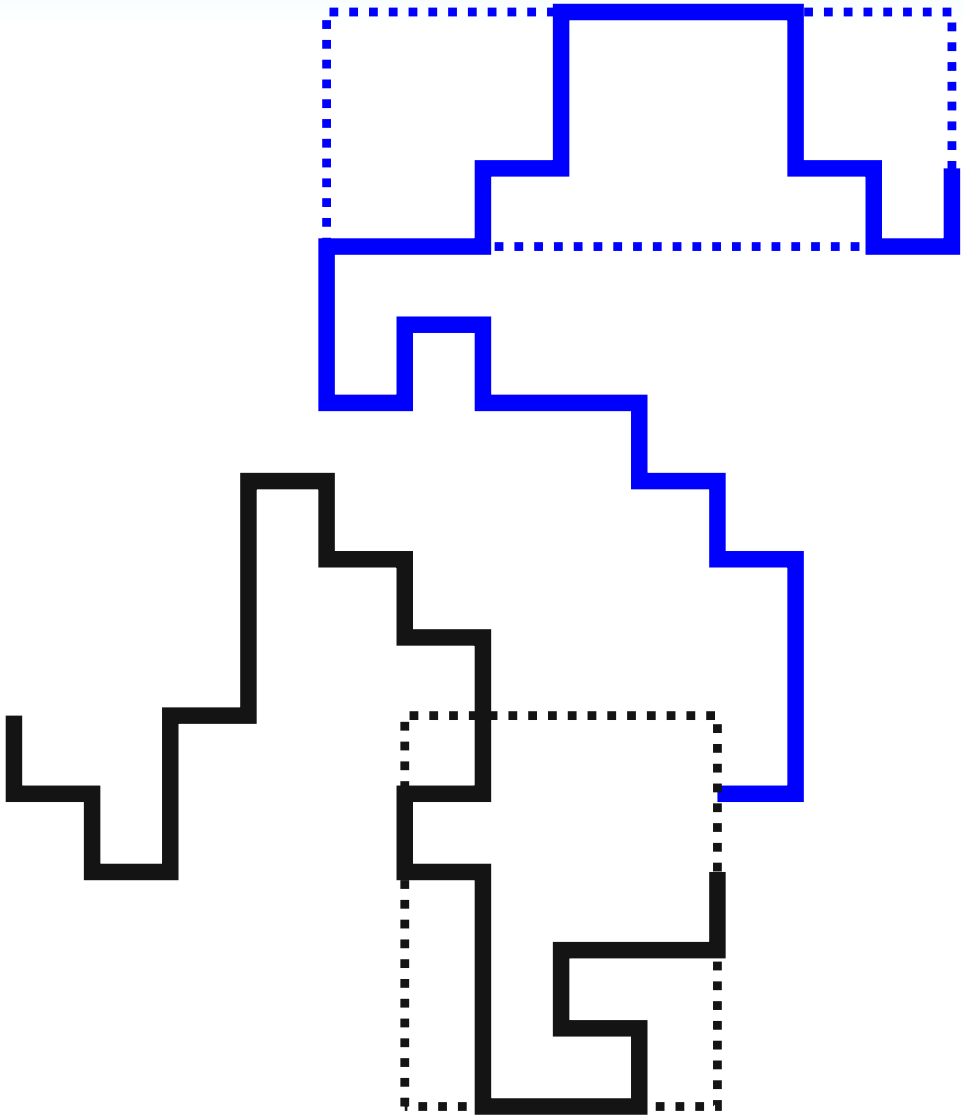


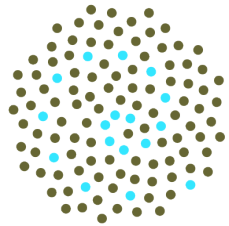


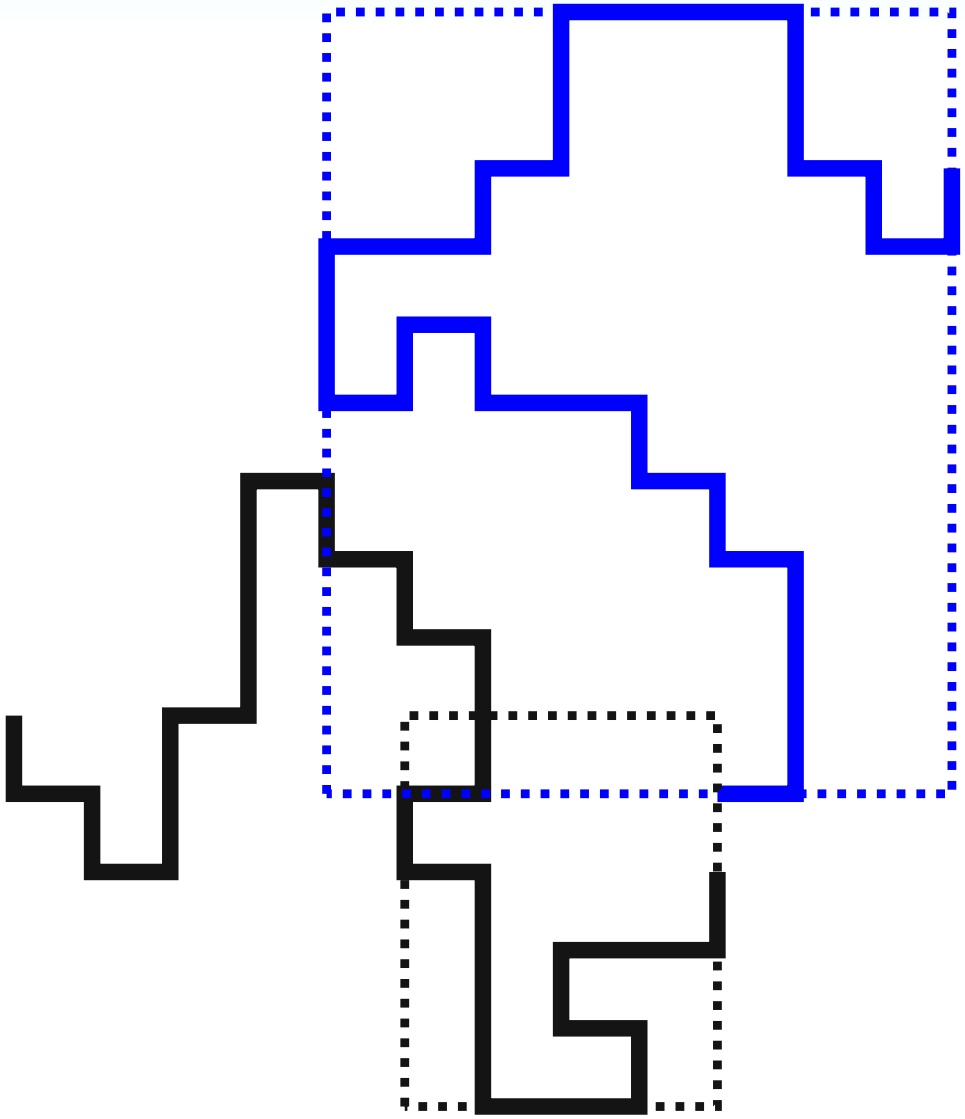


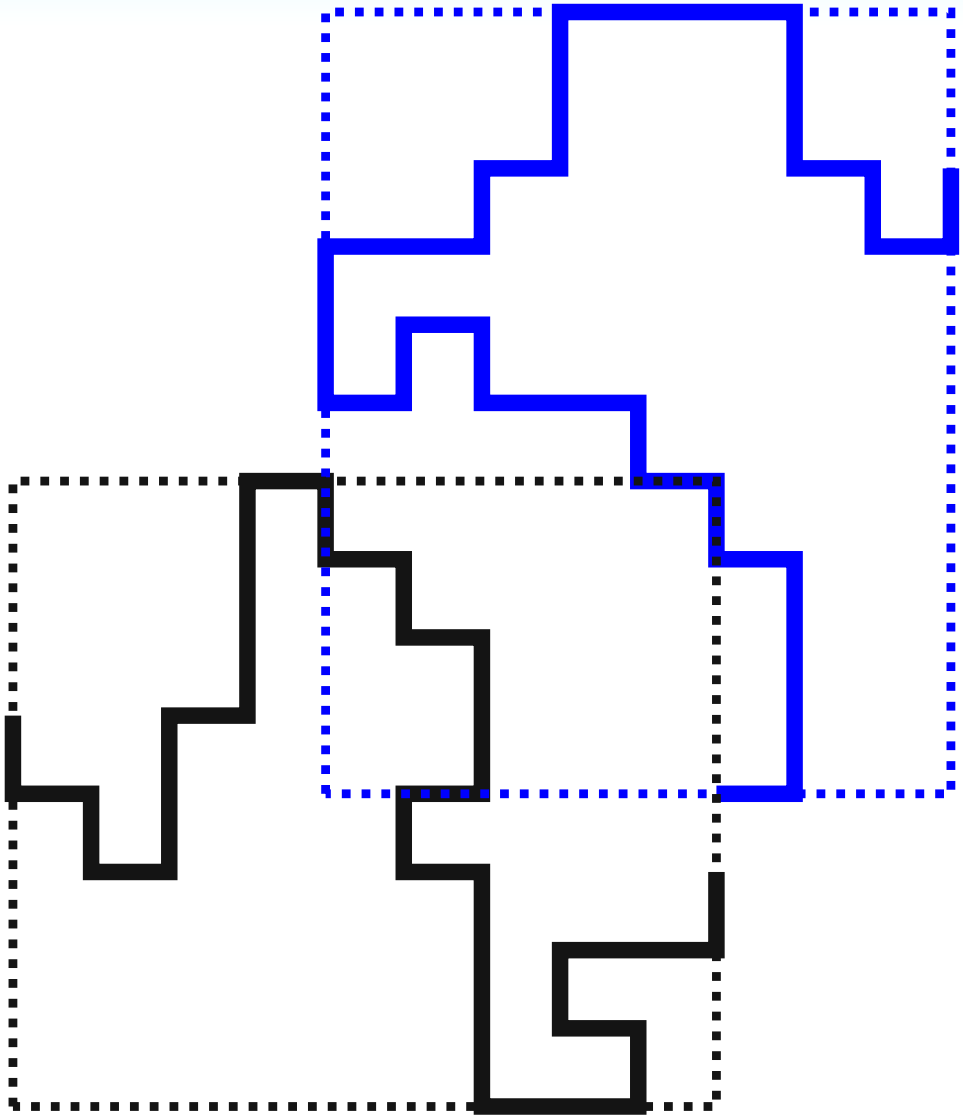


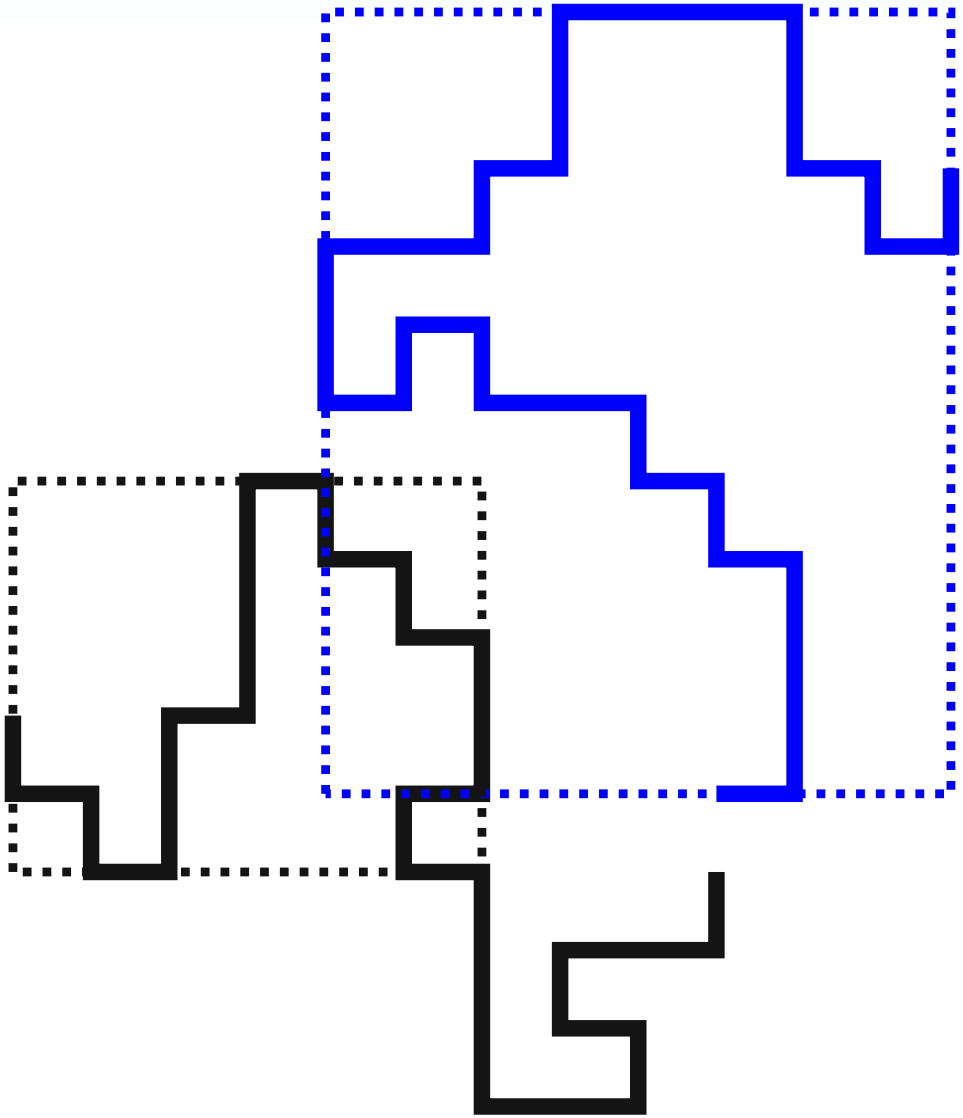


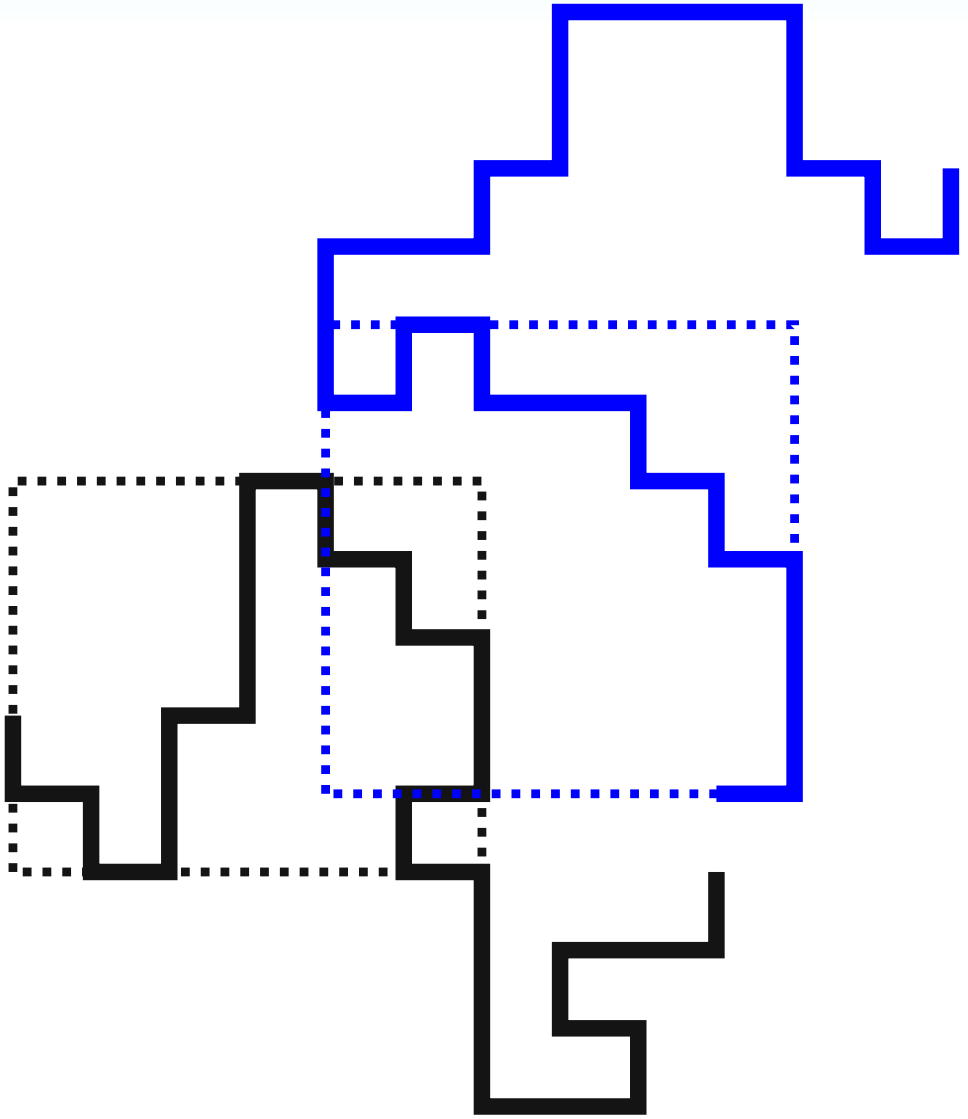


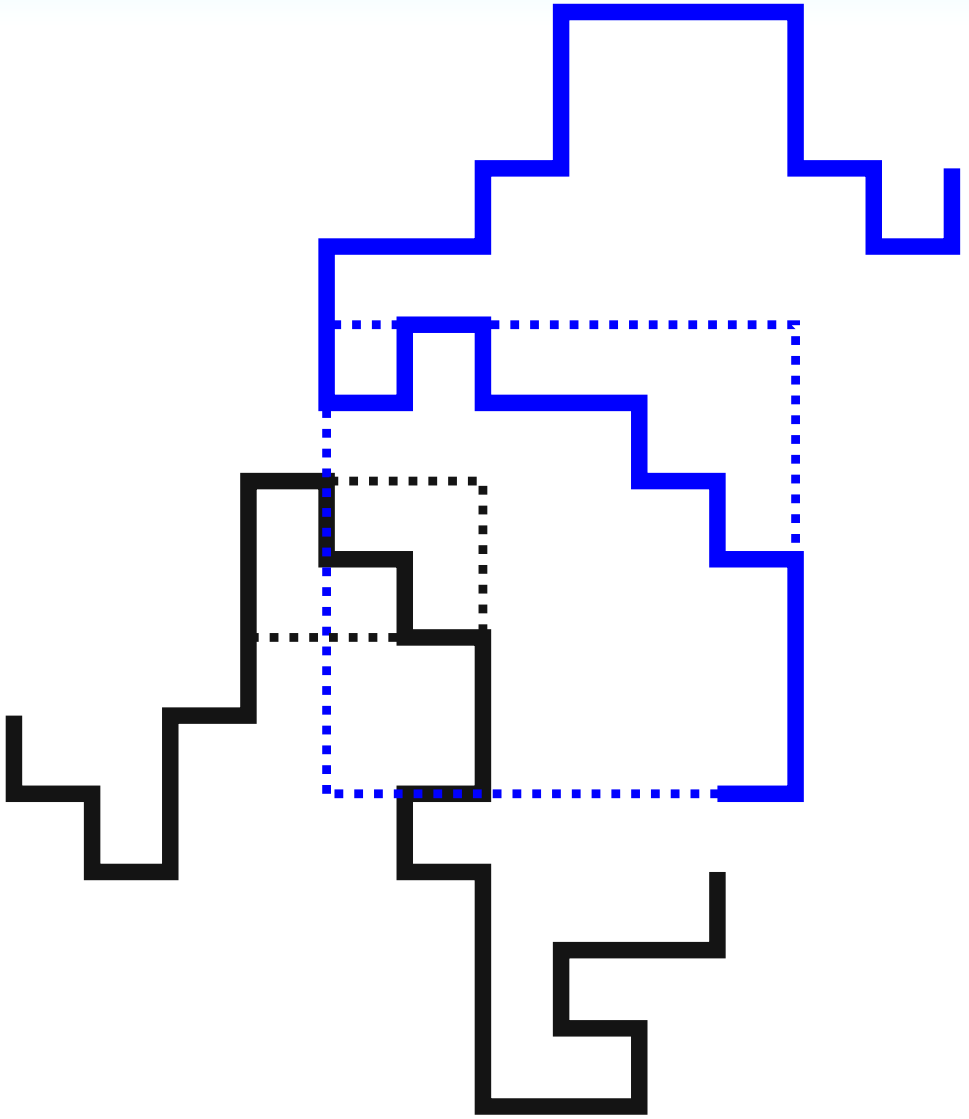


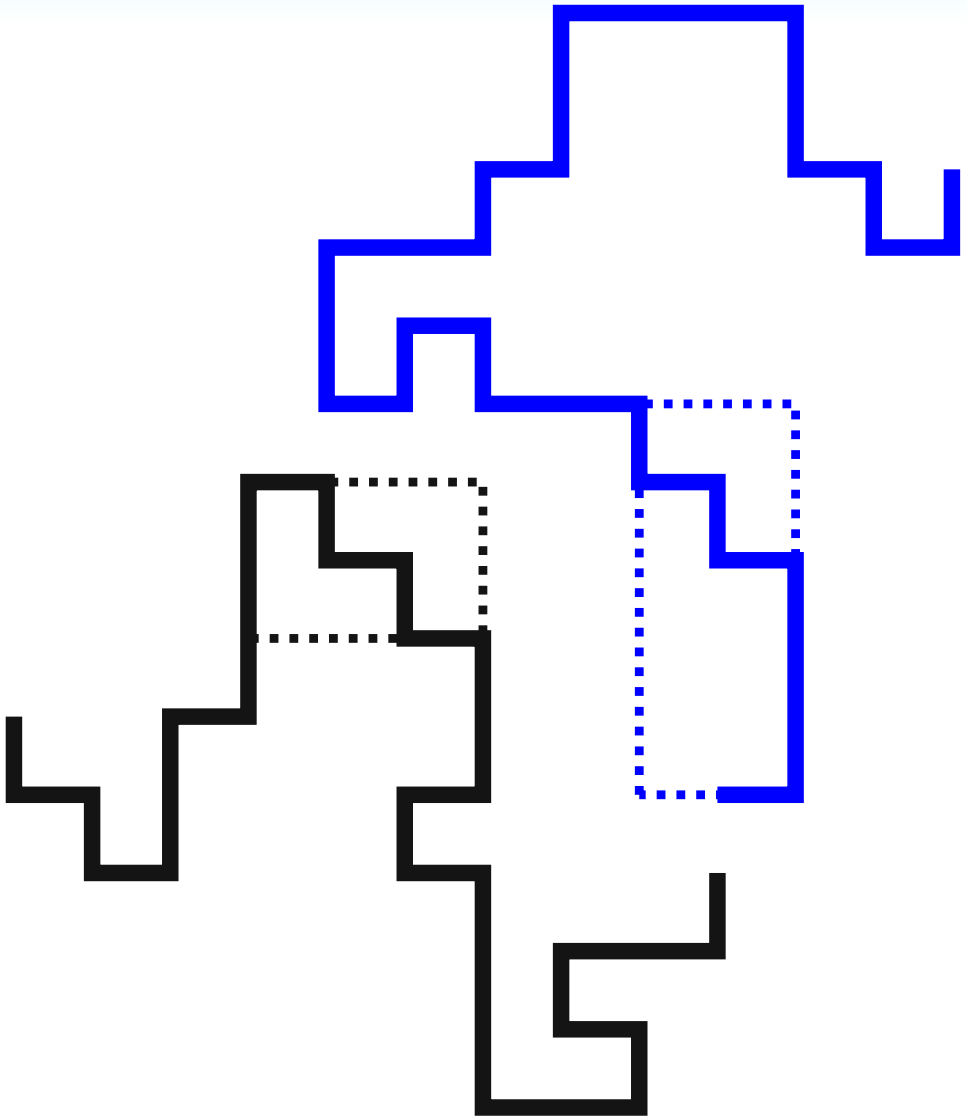


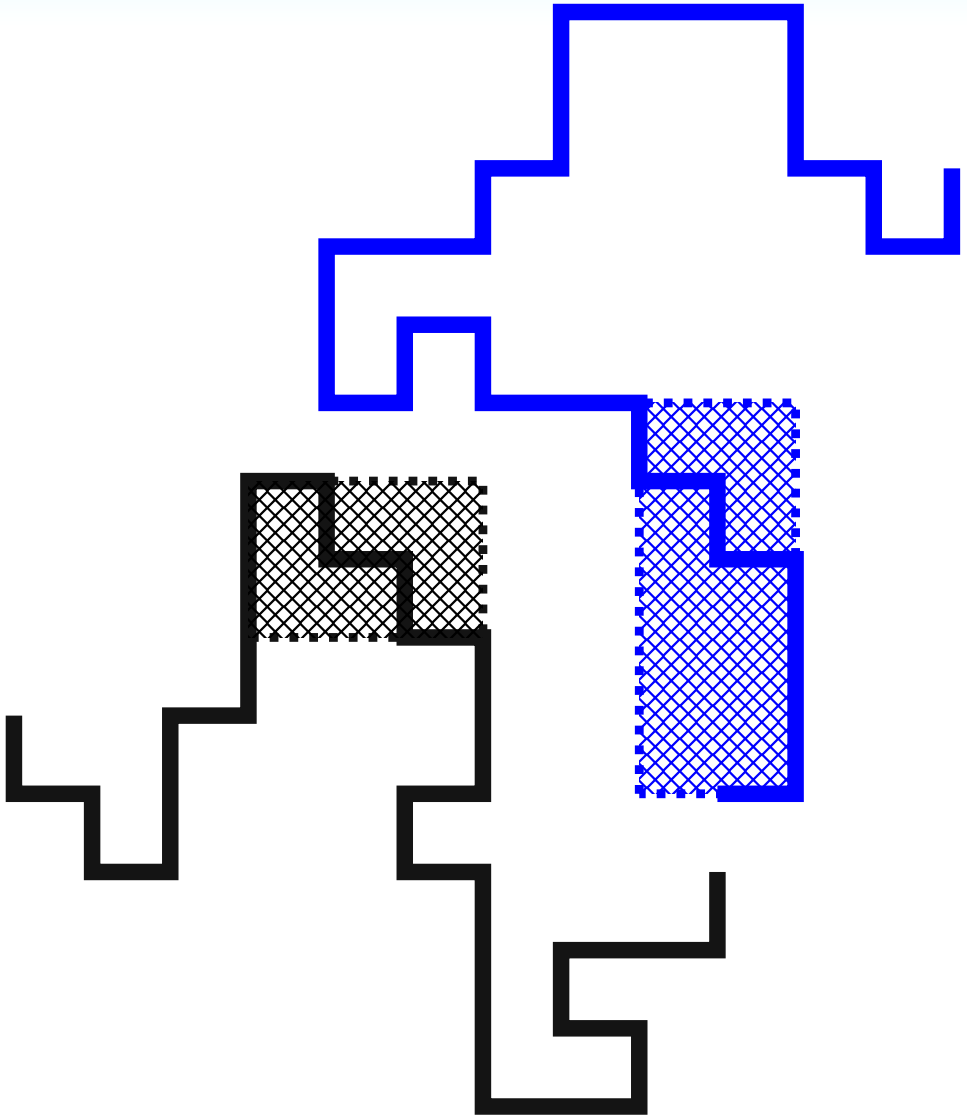


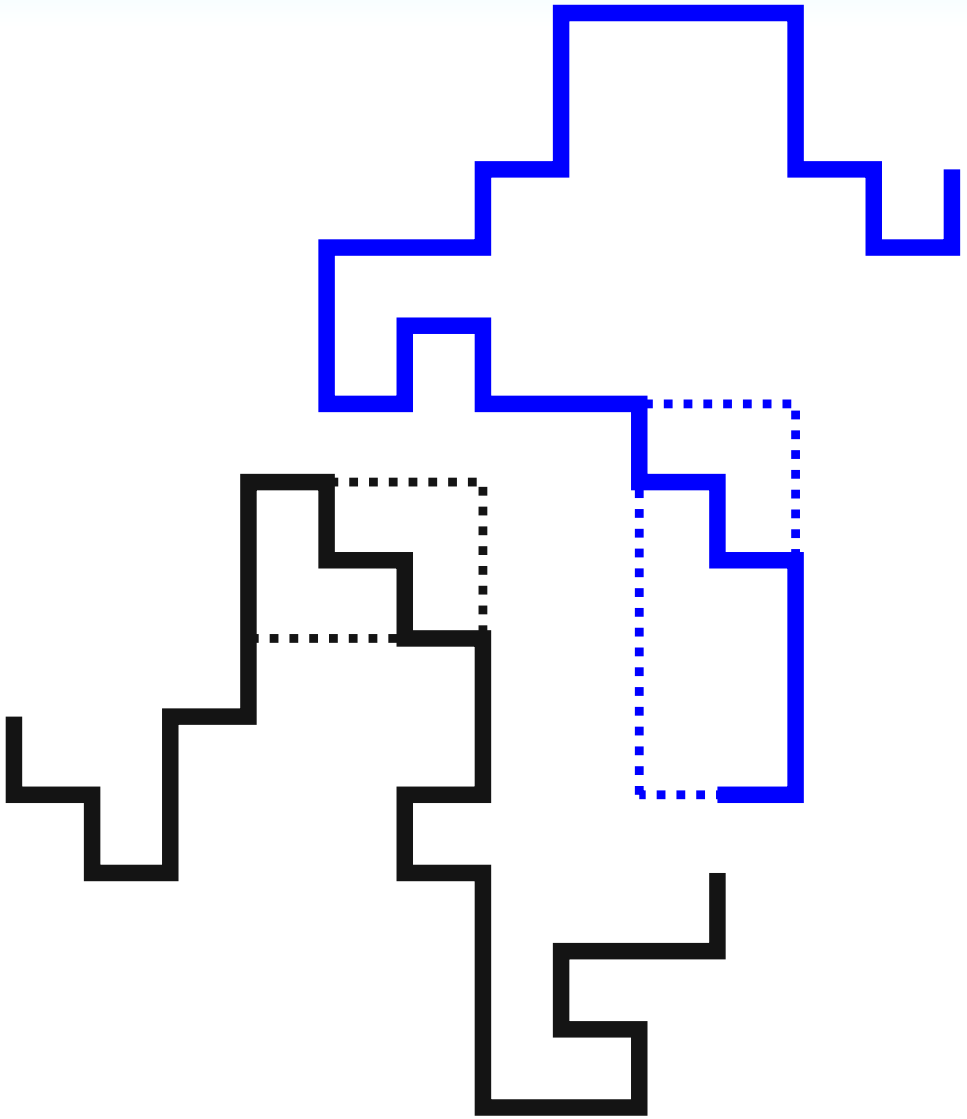


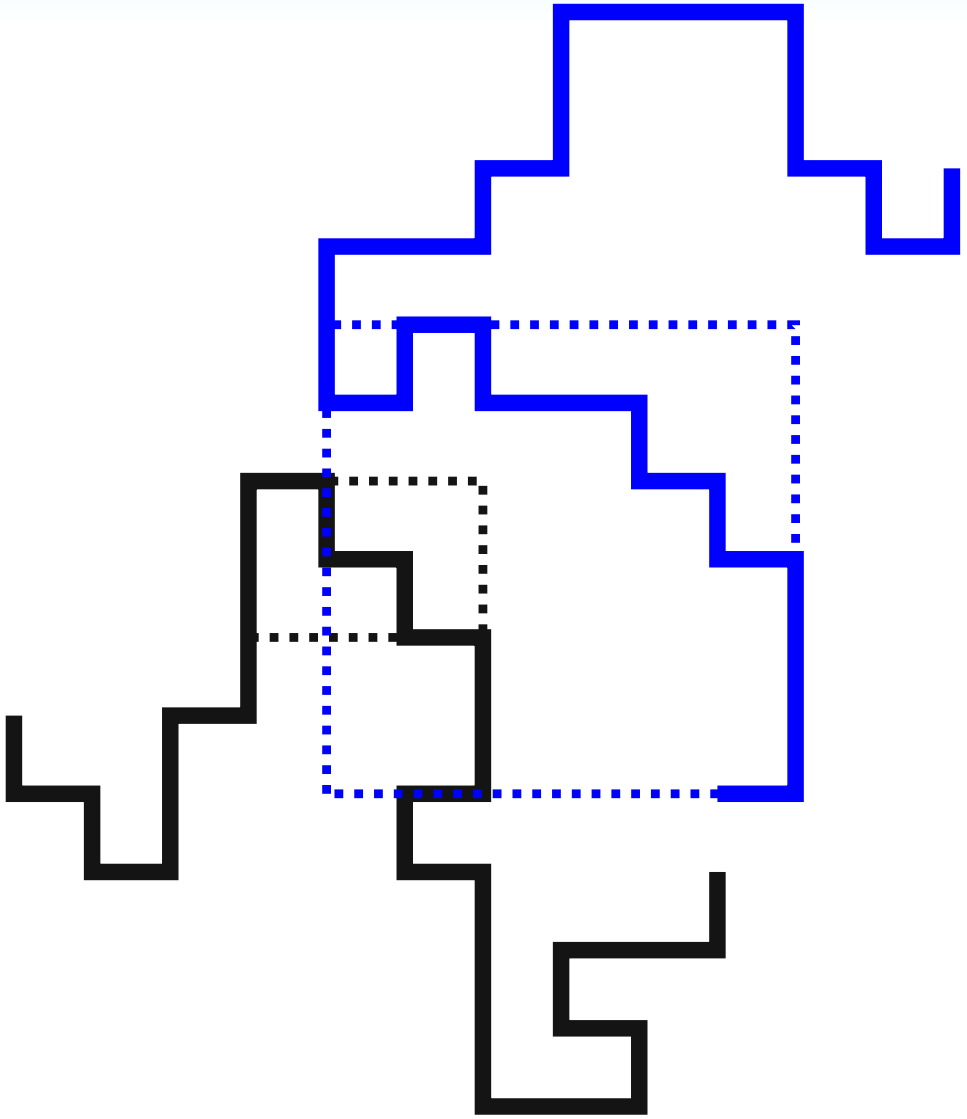


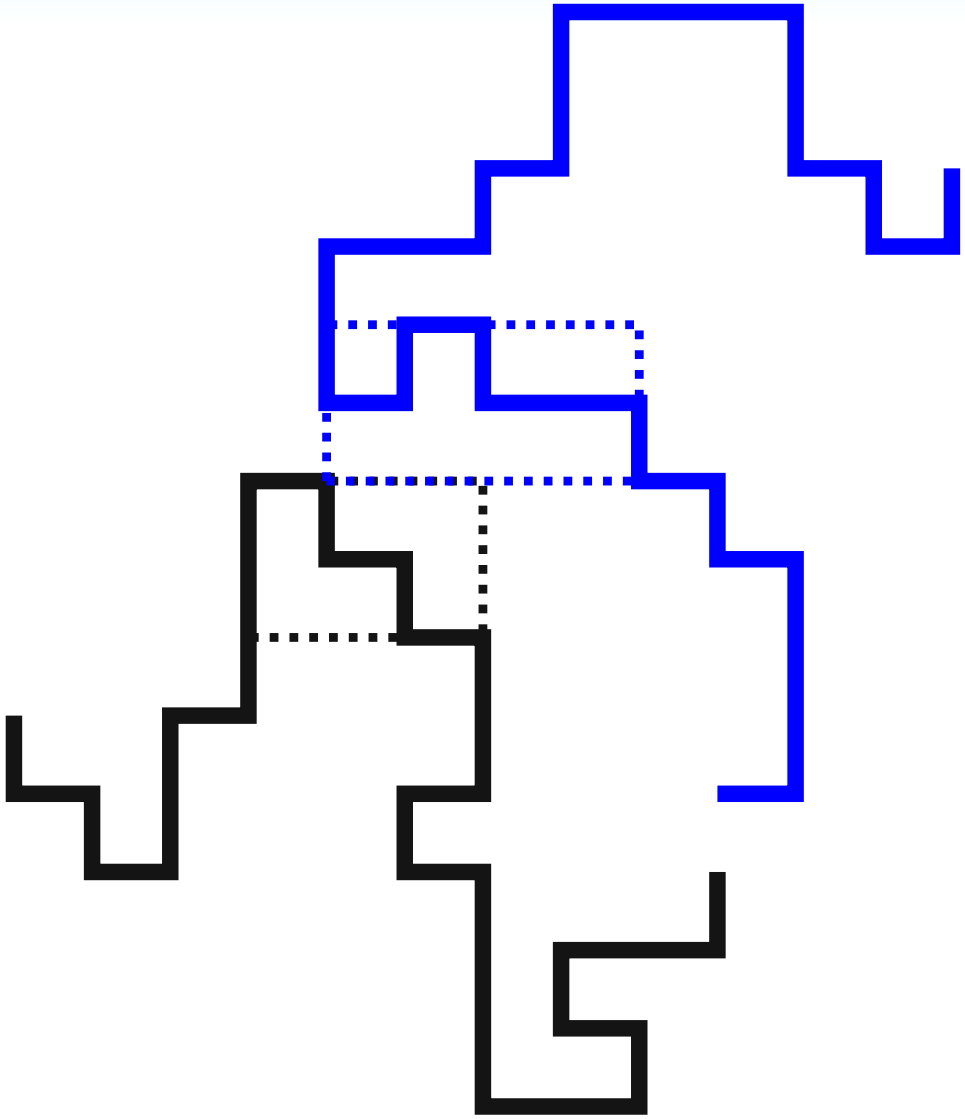


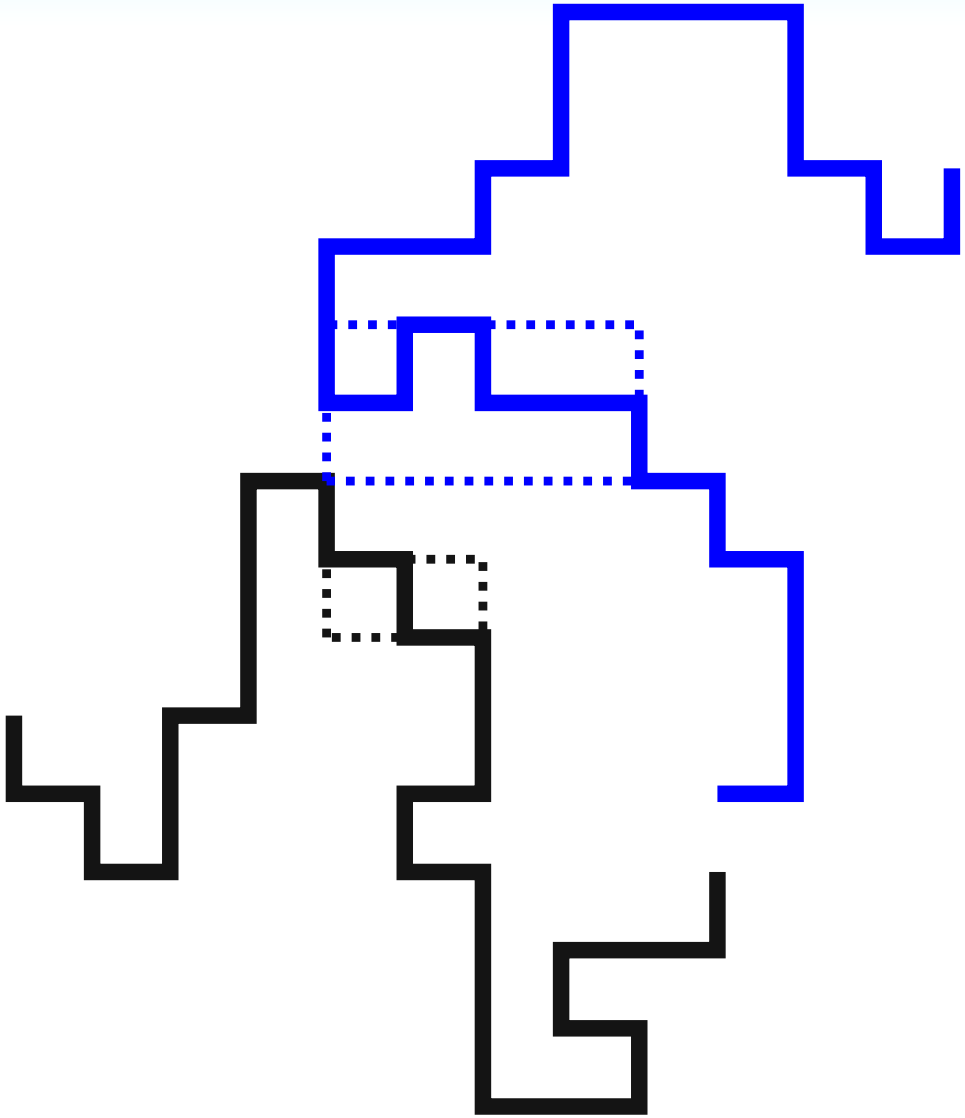


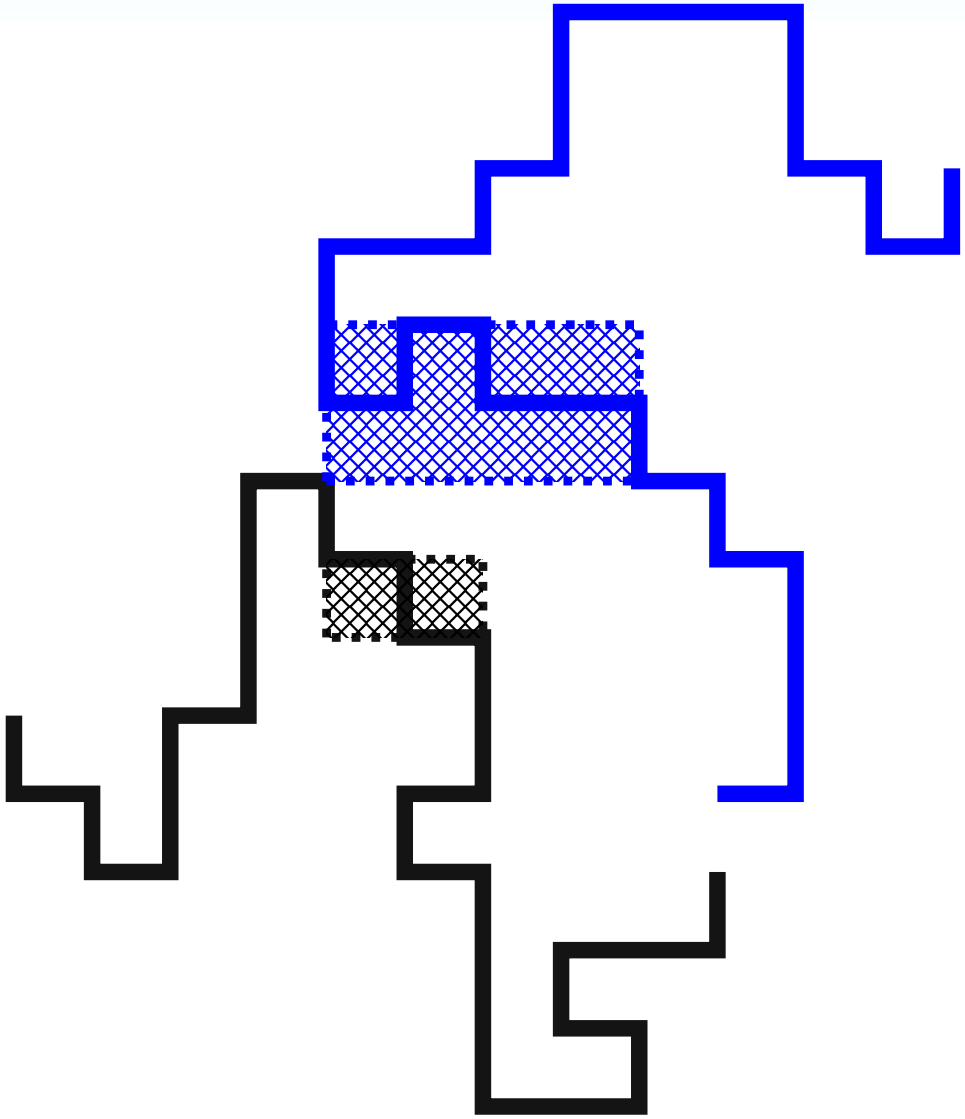


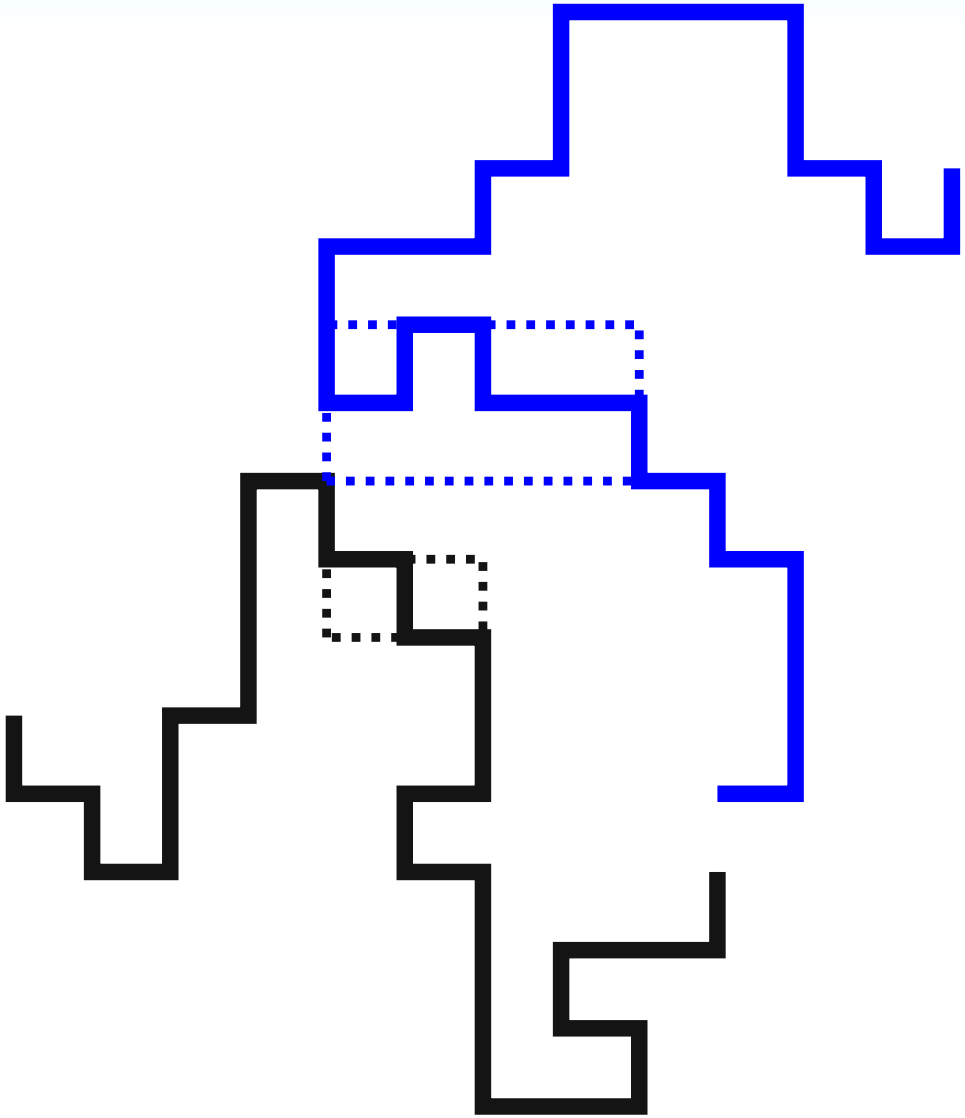


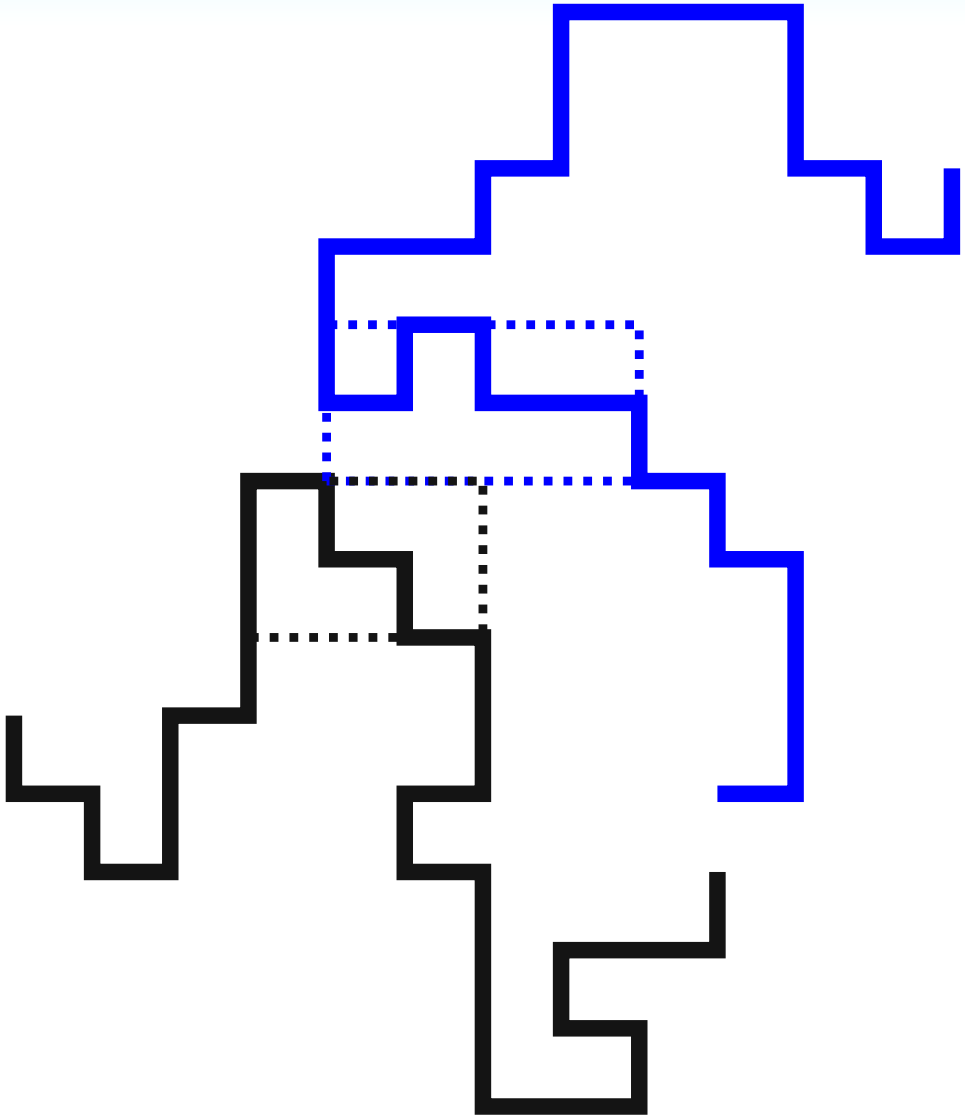


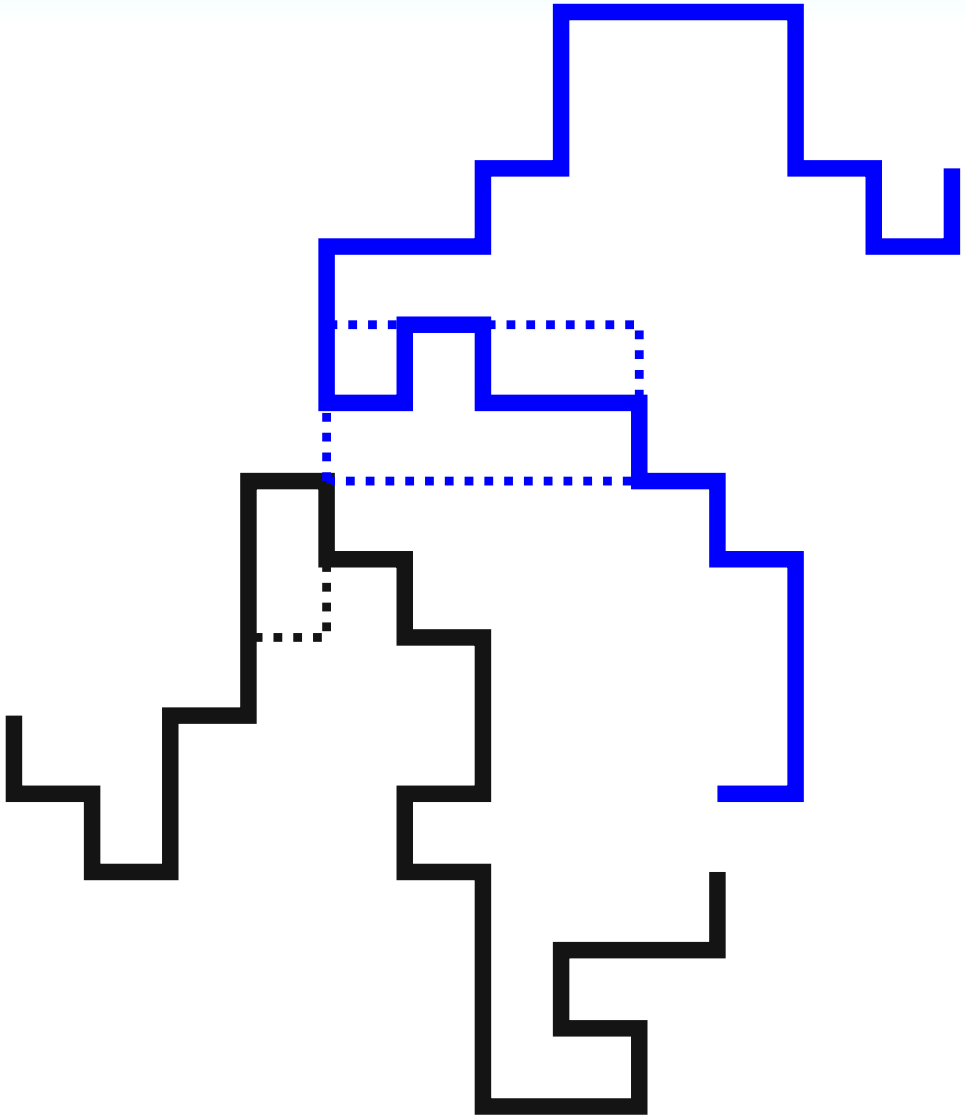


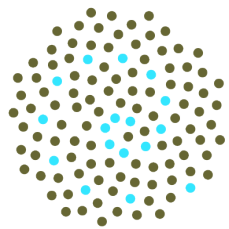


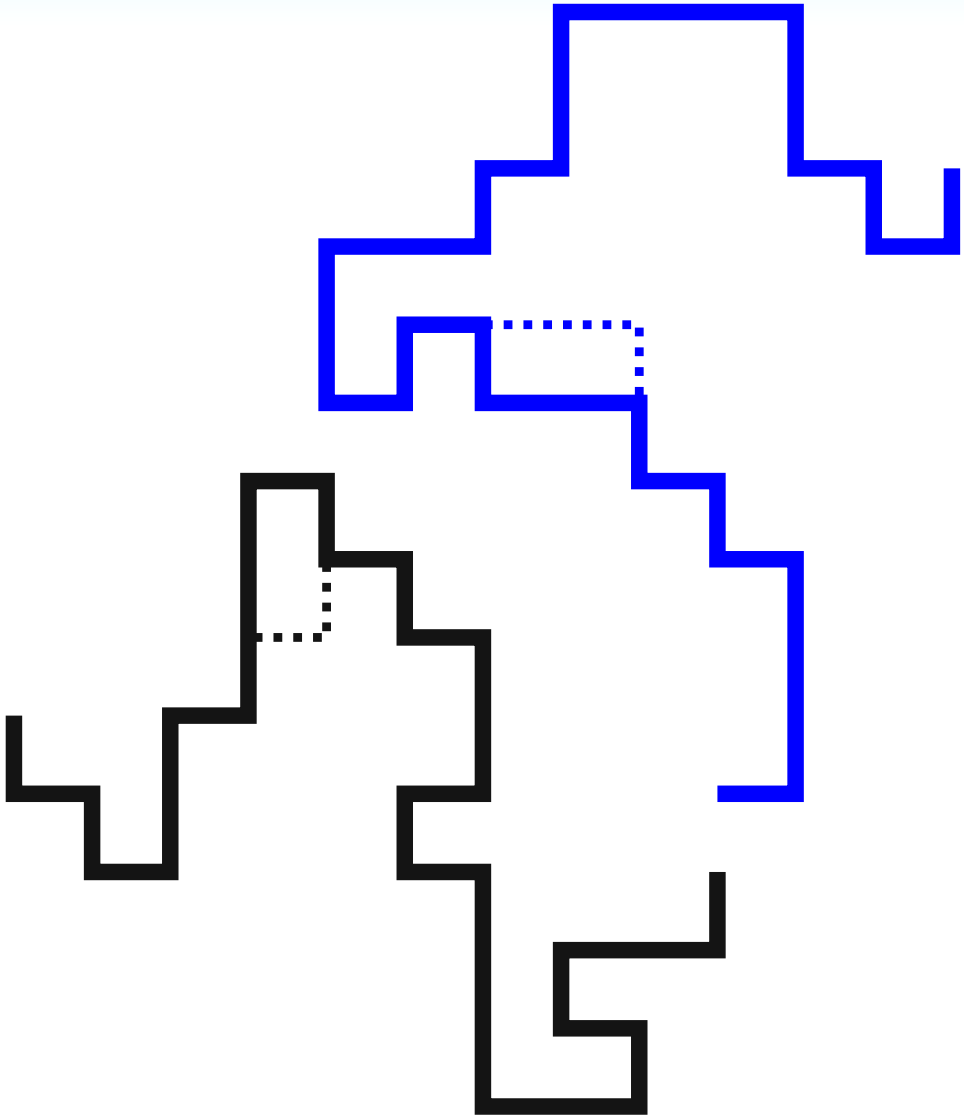


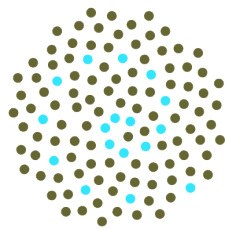


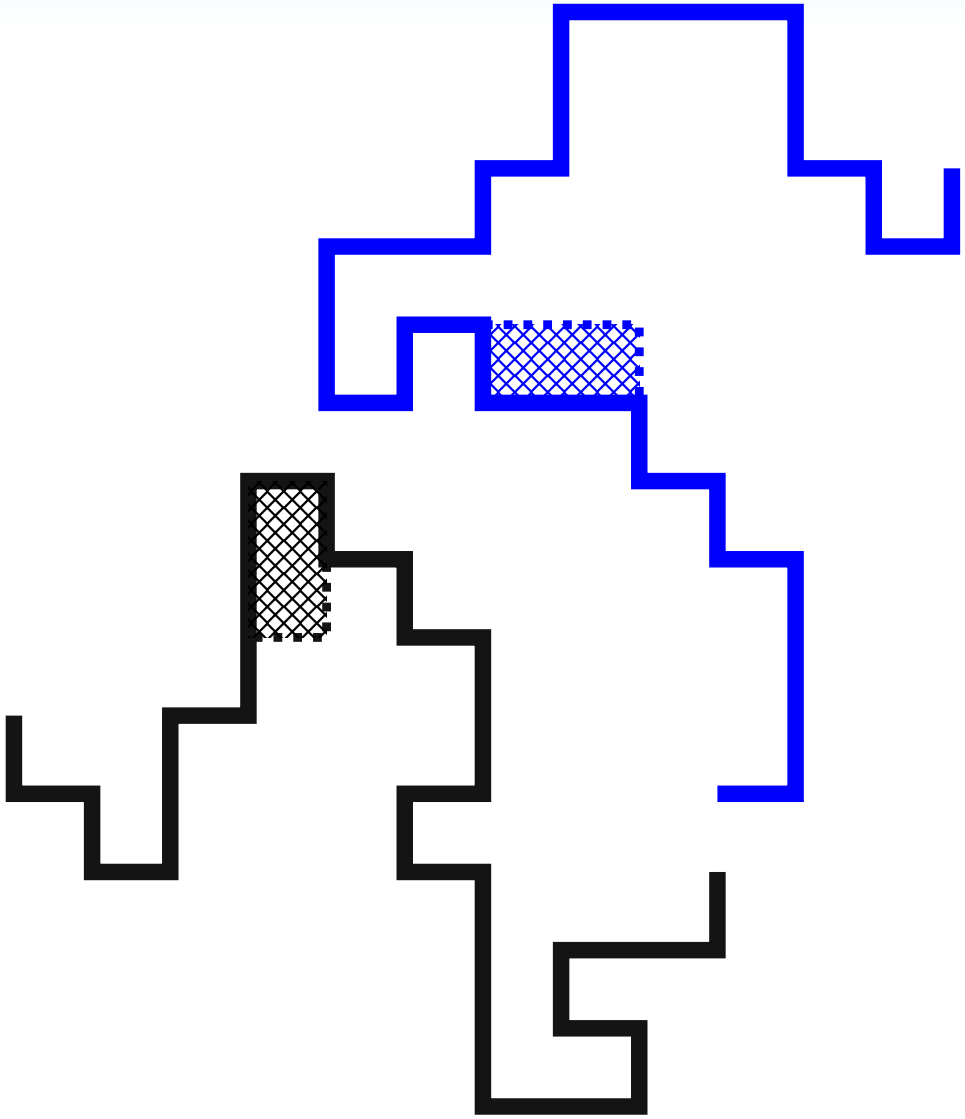


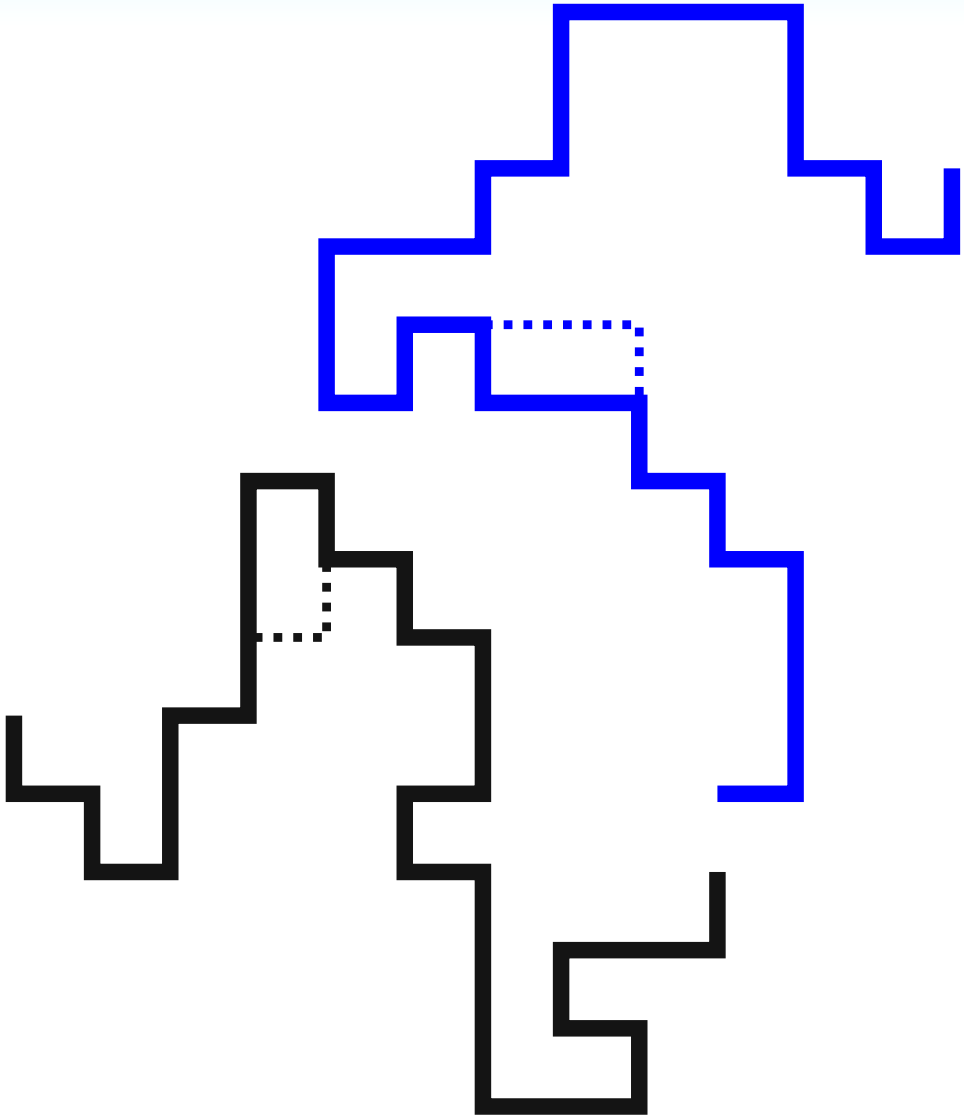


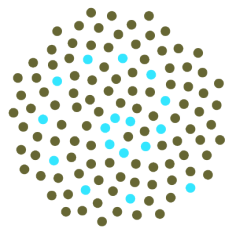


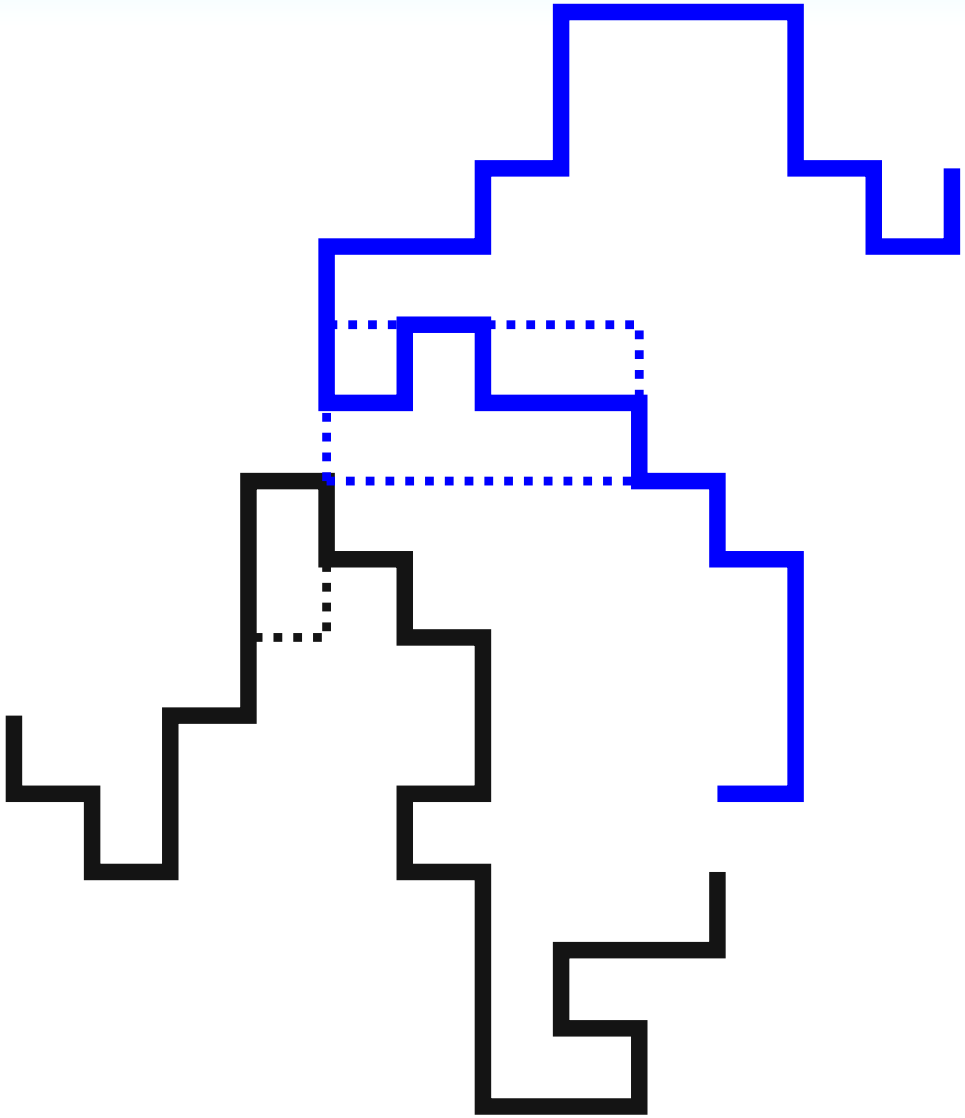


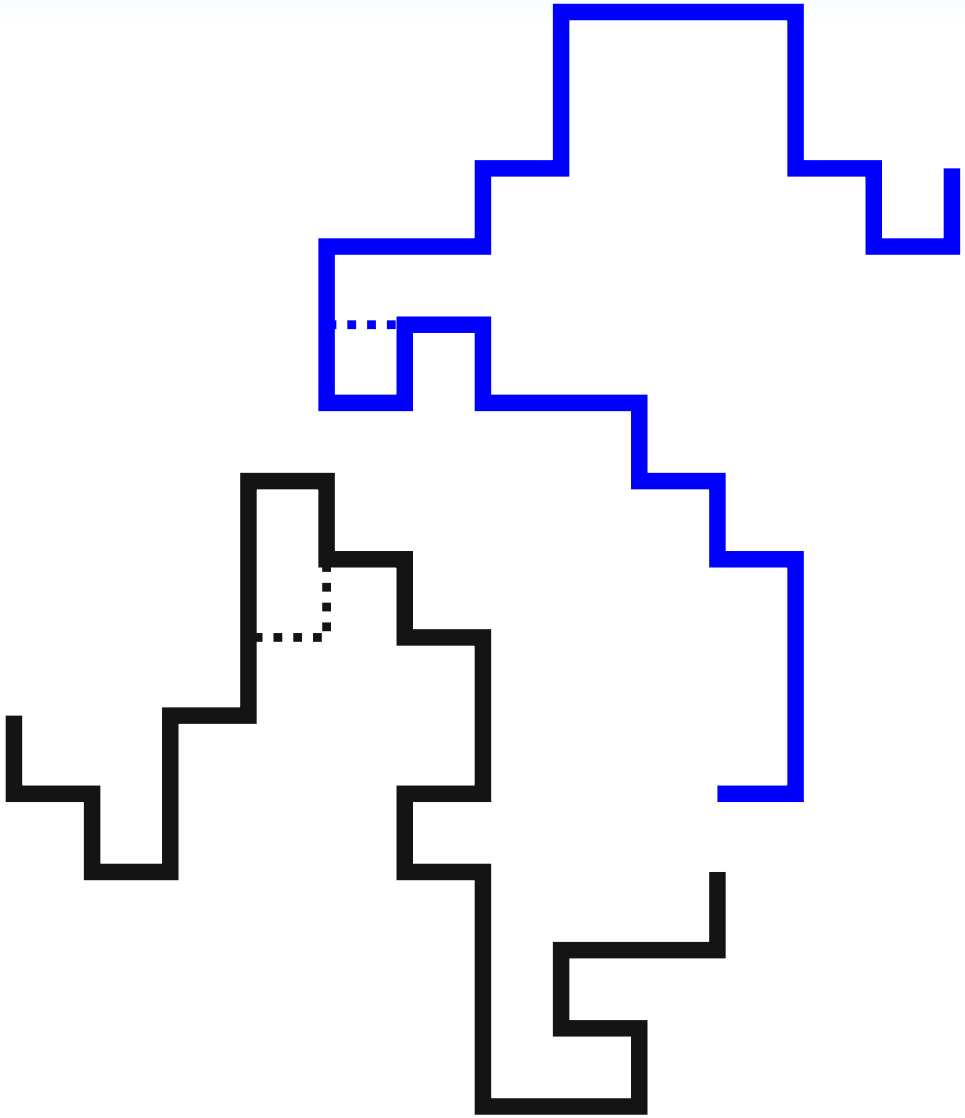


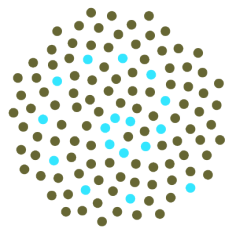


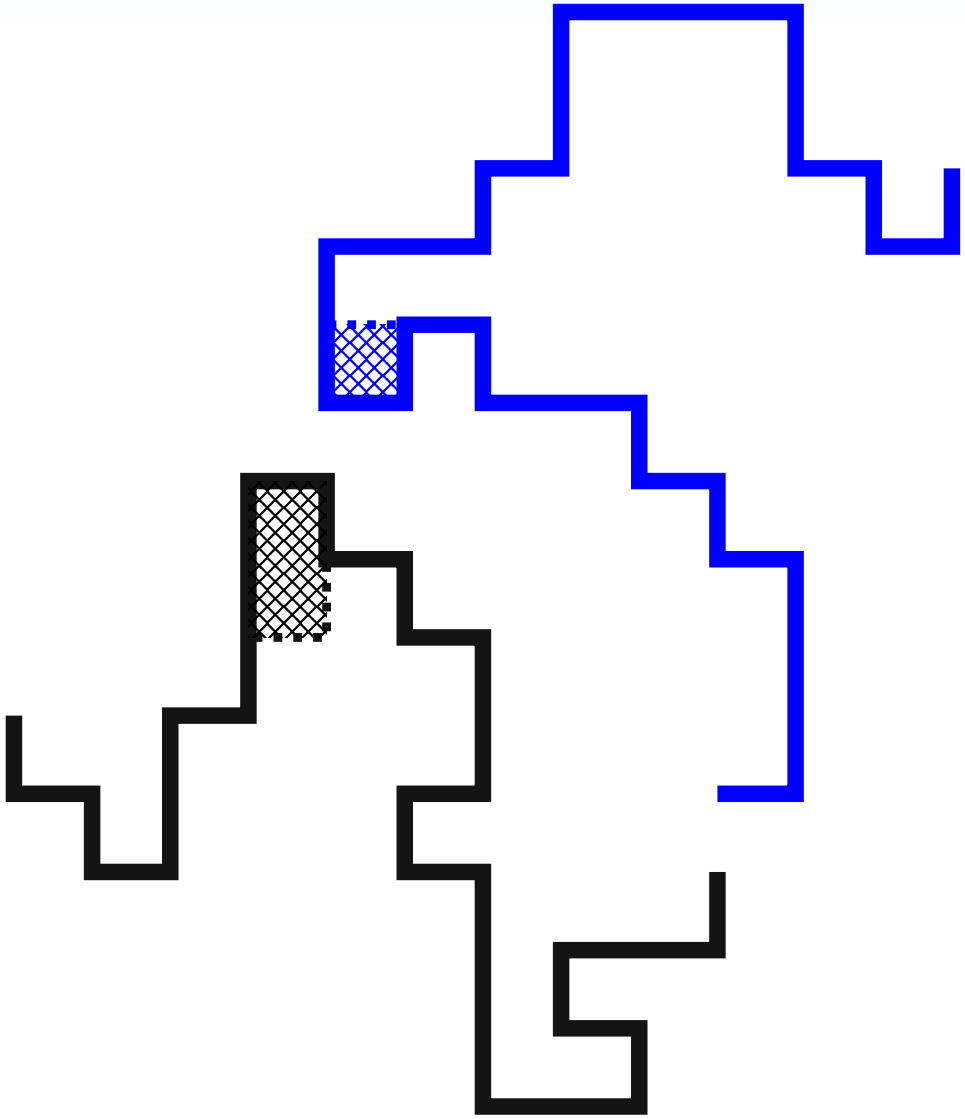


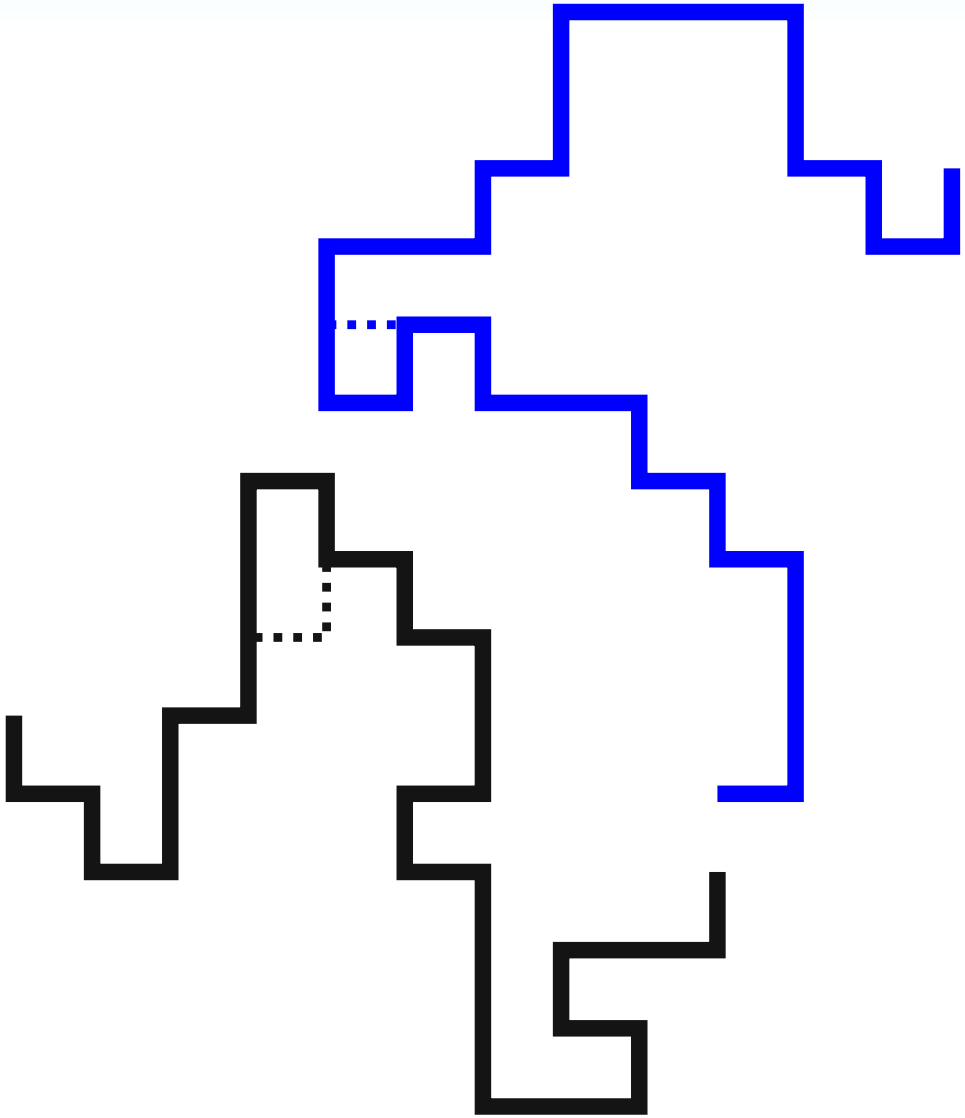


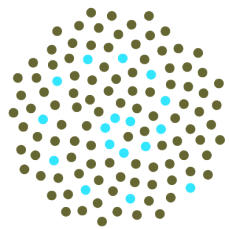


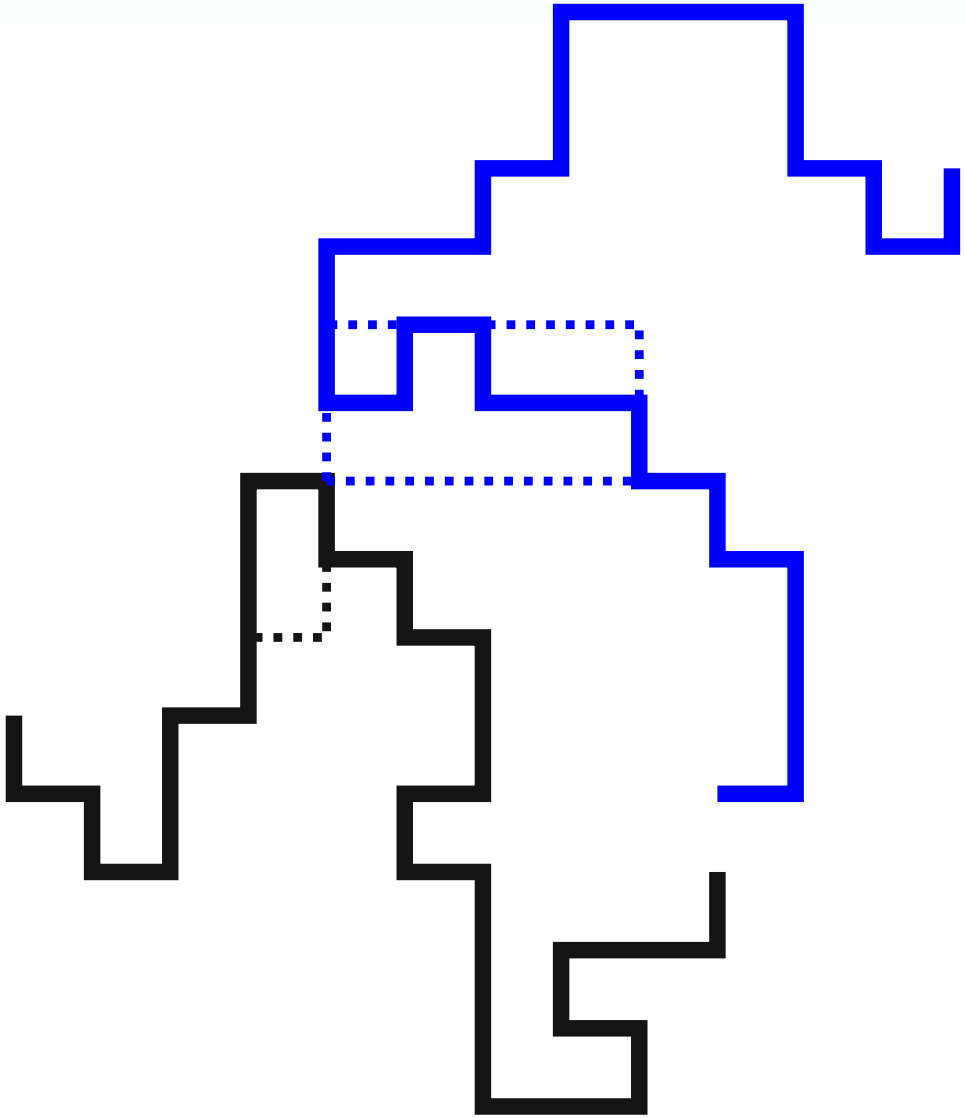


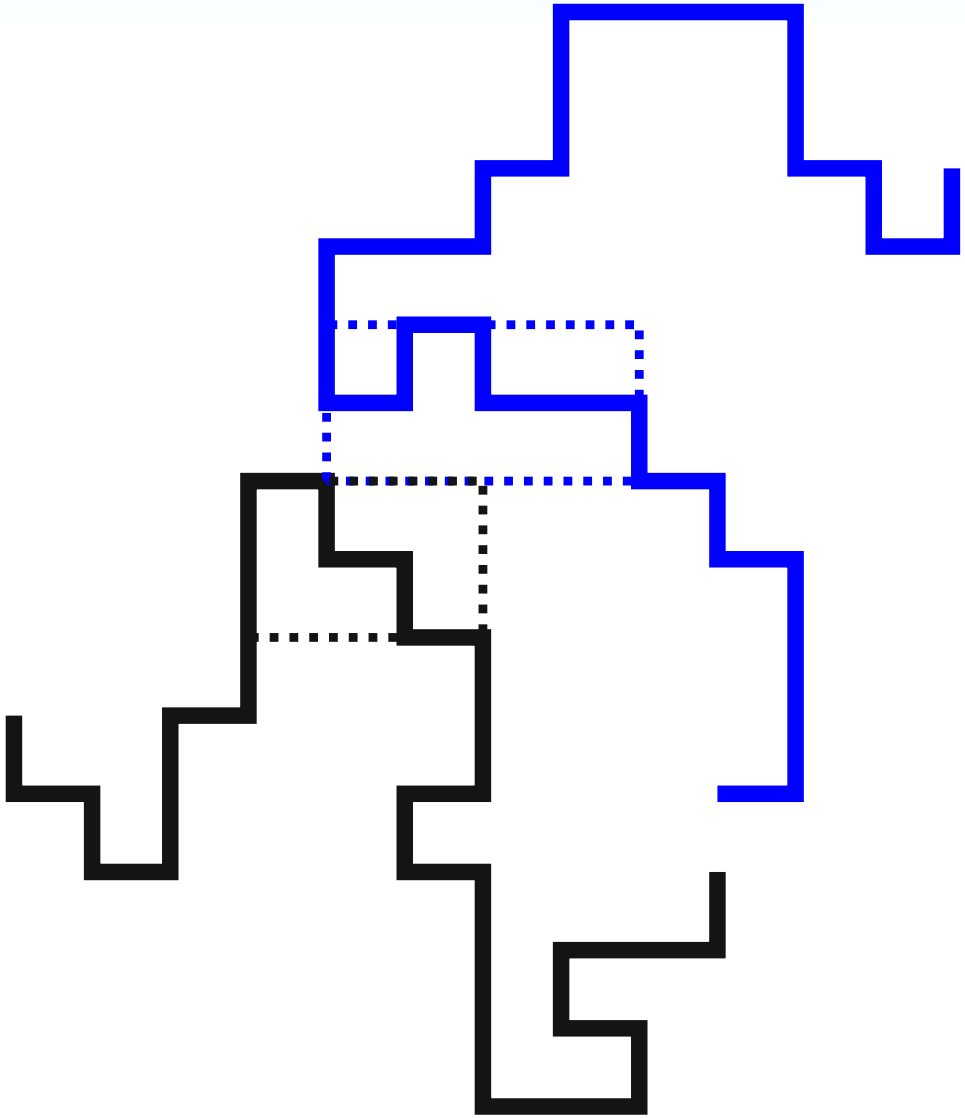


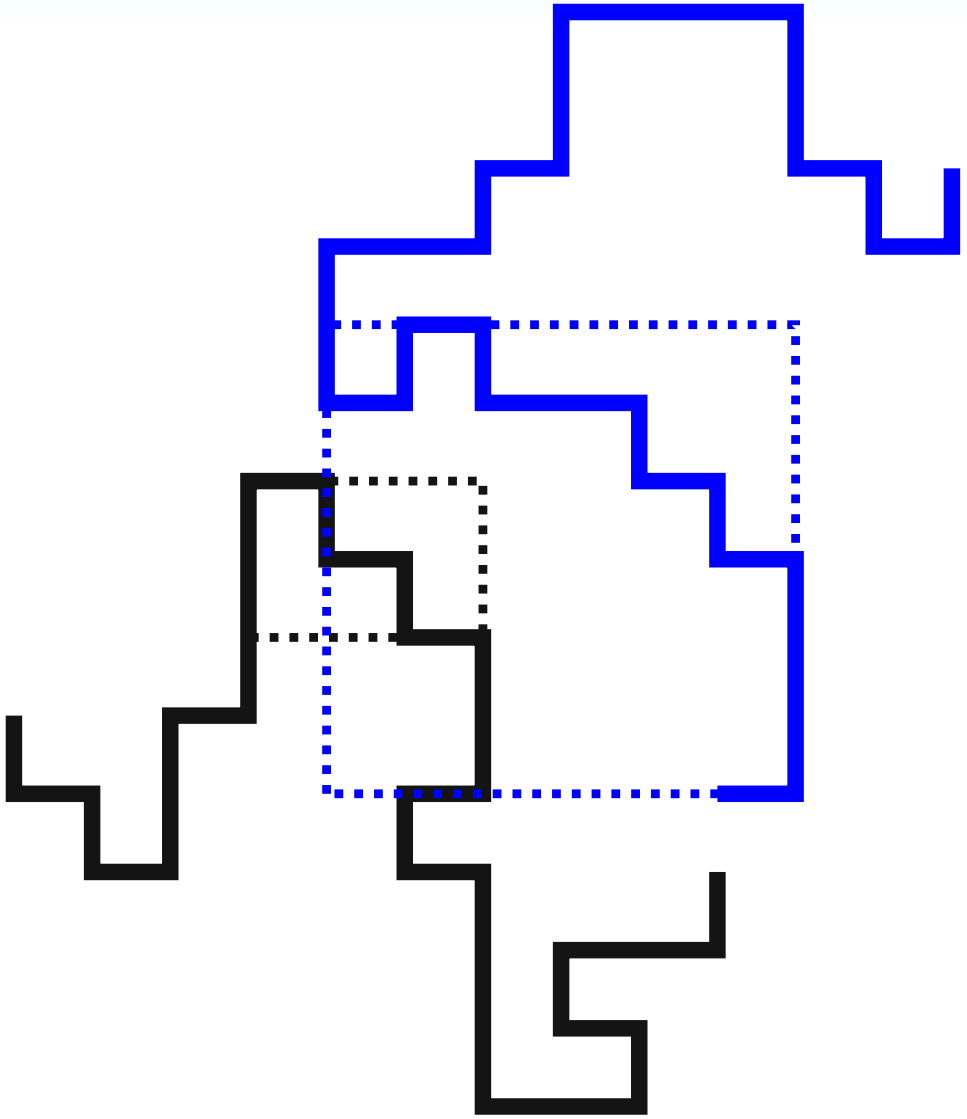


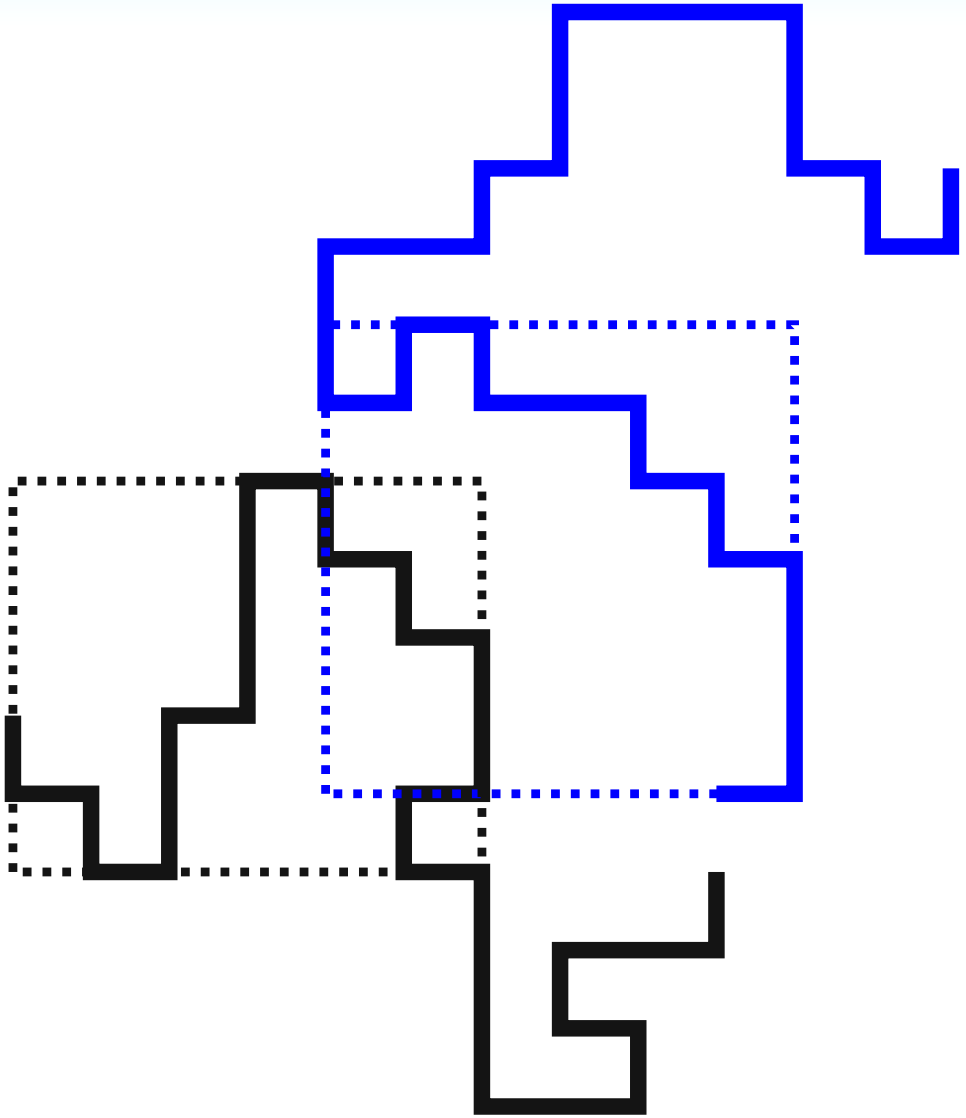


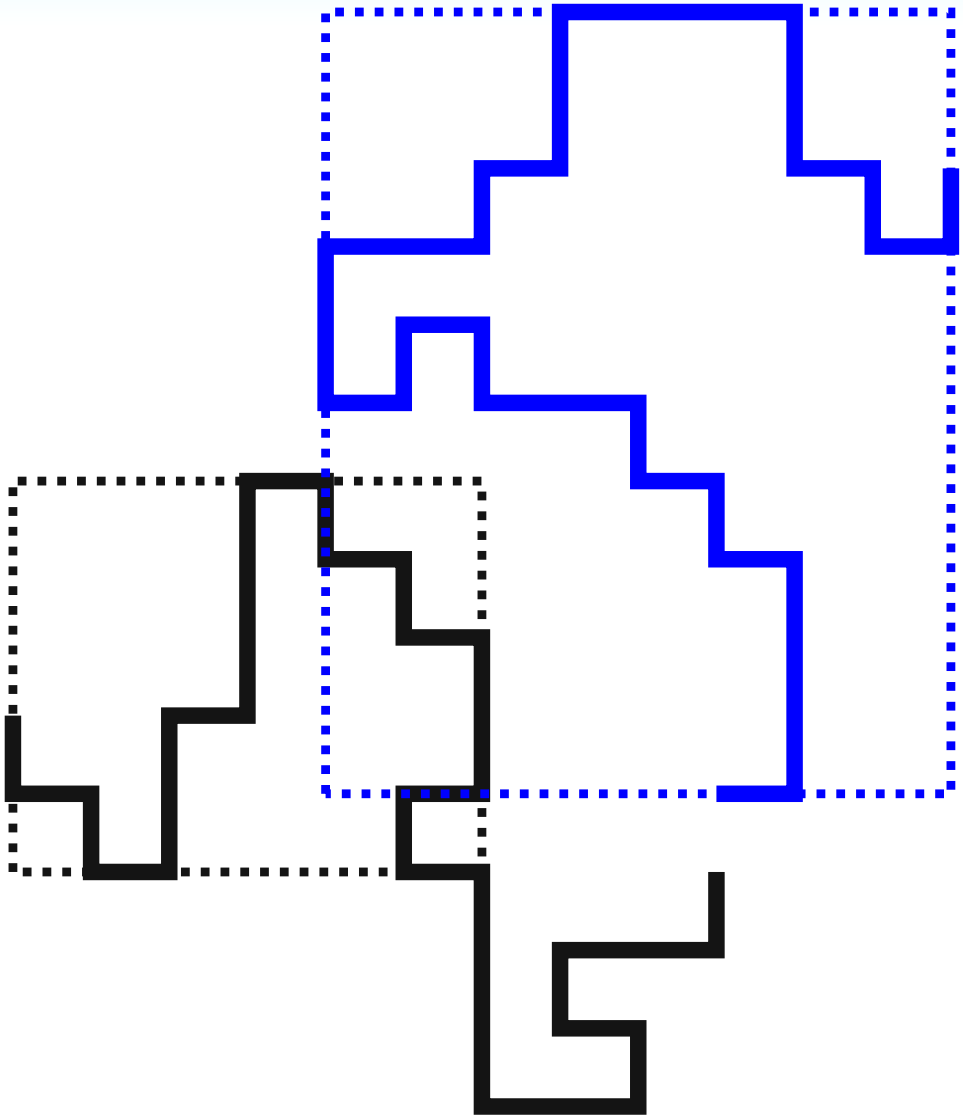


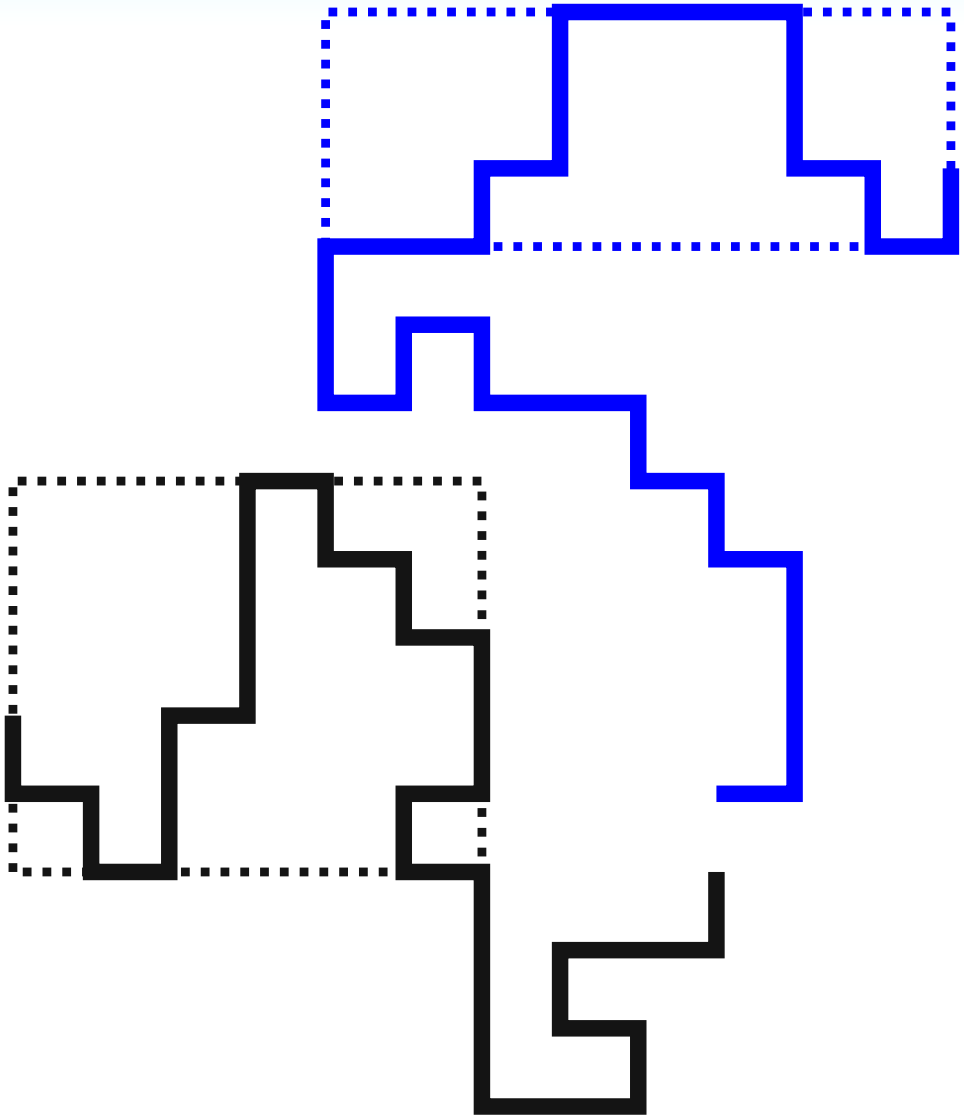


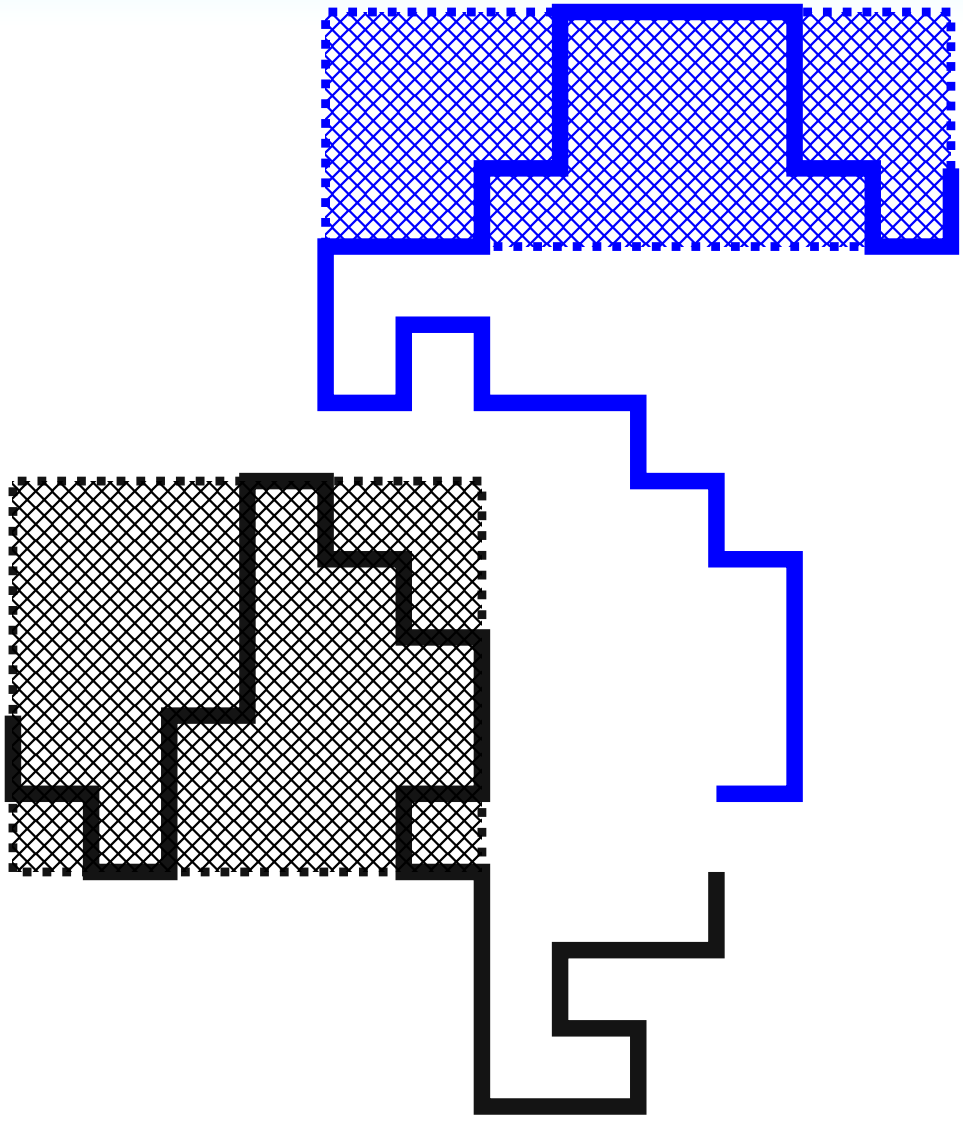


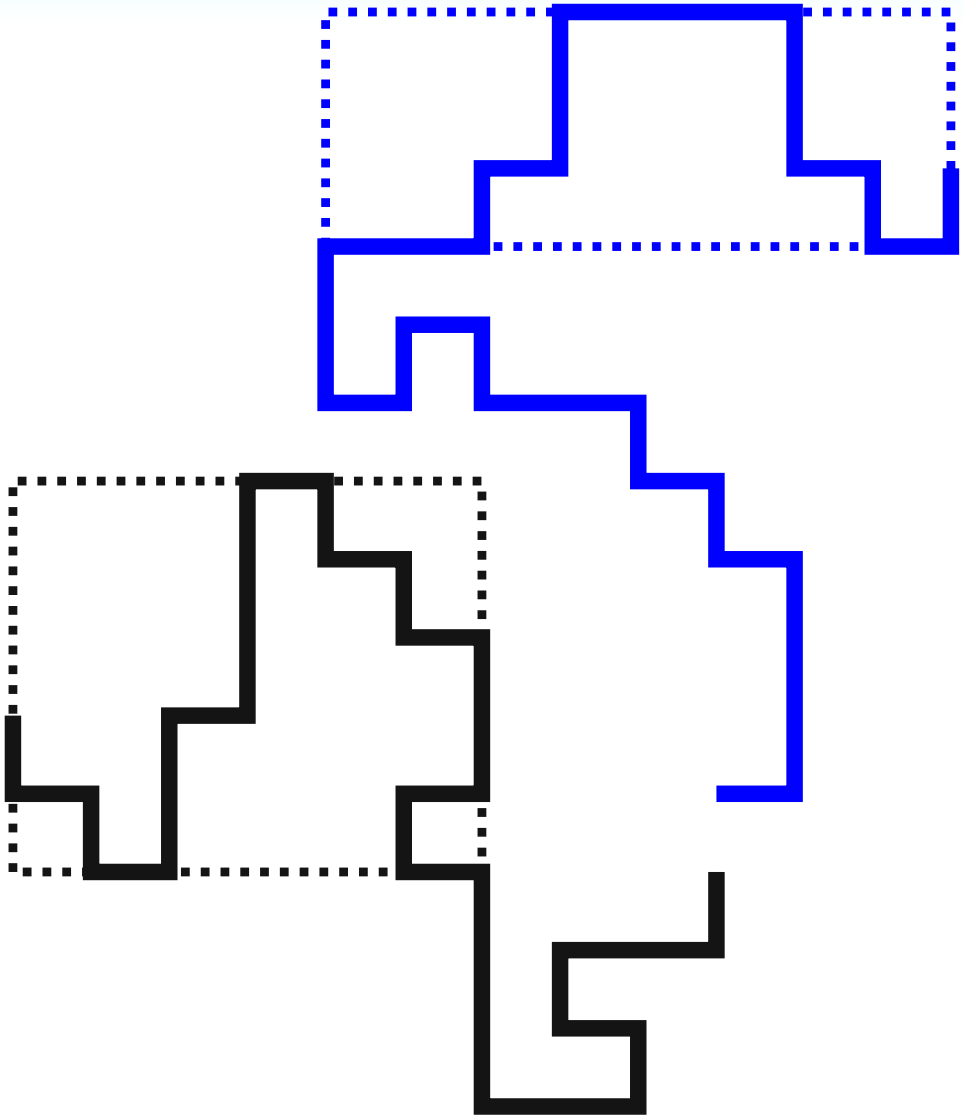


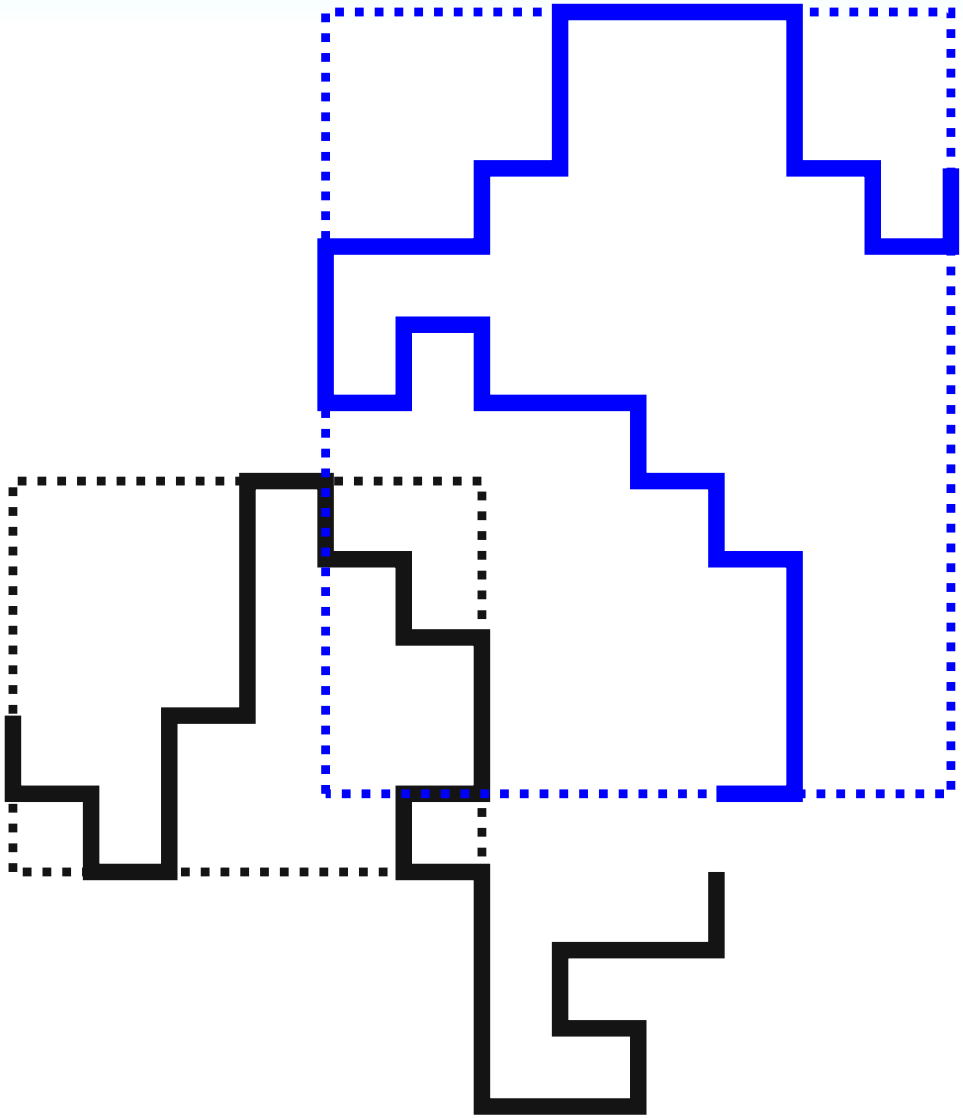


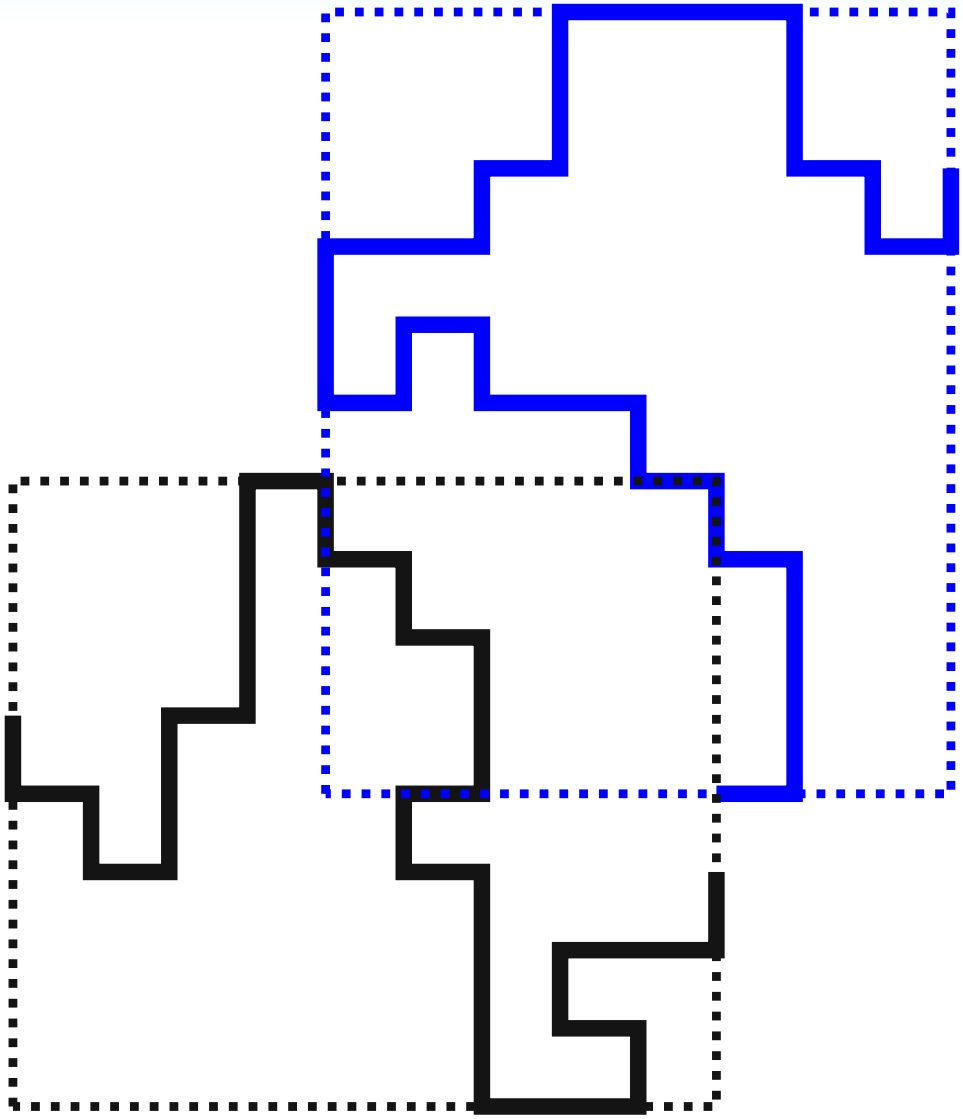


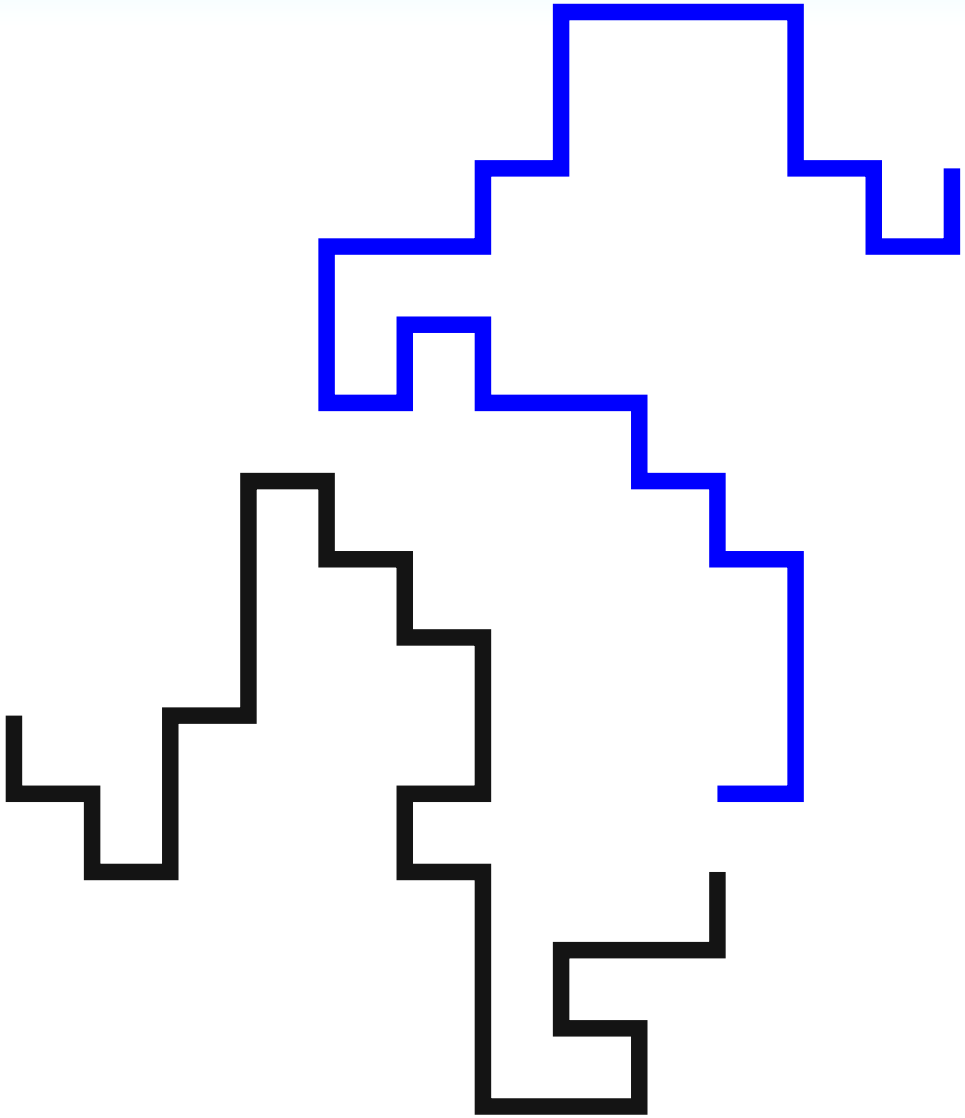




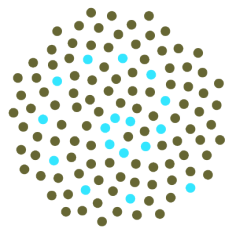






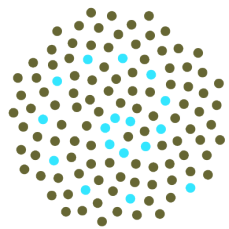


- For SAWs, there are $O(1)$ nearest neighbour contacts between two halves.
- Polymer with N monomers $\Rightarrow$ height of tree $O(\log N)$.
- When a successful pivot is made $\Rightarrow$ CPU time = $O(\log N)$.
- By universality, will be same for SAW-like polymers.



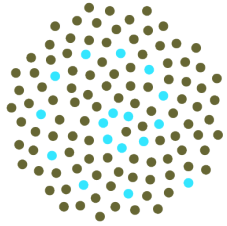
Markov chain:

- Select a sub-chain; split polymer into either 2 or 3. chains, i.e. split SAW-tree in 2 or 3 pieces, $O(\log N)$.
- Apply *move* to sub-chain, $O(1)$.
- Calculate change in interaction energy by finding all interacting monomer pairs between sub-chain and rest of polymer, $O(\log N)$.
- Accept / reject move.
- Merge chains.



Performance

- Madras and Sokal (1988): hash table implementation.
- Kennedy (2002): complicated data structure.



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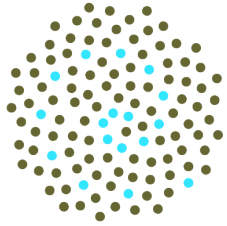
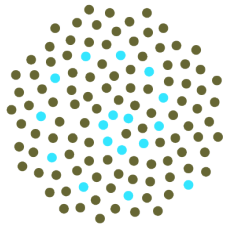


Performance

- Madras and Sokal (1988): hash table implementation.
- Kennedy (2002): complicated data structure.

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

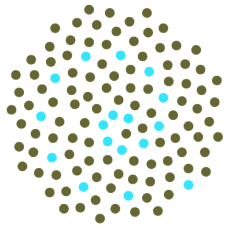
Lattice	Madras and Sokal	Kennedy	SAW-tree
Square	$O(N^{0.81})$	$O(N^{0.38})$	$o(\log N)$
Cubic	$O(N^{0.89})$	$O(N^{0.74})$	$O(\log N)$



Performance

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



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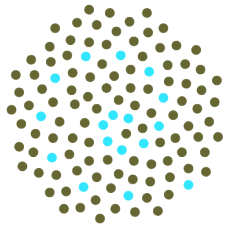
Principal limitation for studying long walks is memory; so far have simulated equilibrium SAWs on $\mathbb{Z}^3$ up to $N = 2^{28} \approx 270$ million.



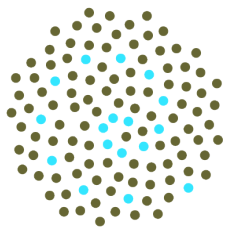
Critical phenomena

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

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

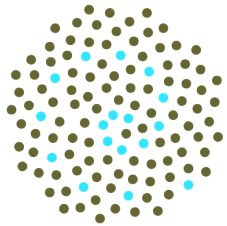
- Mean square end to end distance tells us about the size of a typical SAW:

$$\langle R_e^2 \rangle_N \sim D_e N^{2\nu}\, [1 + \text{corrections}]$$

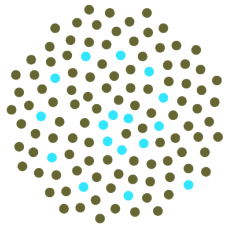


Results

- Experiment 1: $\mathbb{Z}^3$, estimated $\nu = 0.587597(7)$ cf. 0.5874(2) (MC, Prellberg, 2001) and 0.58756(5) (MCRG, Belohorec, 1997).
- Experiment 2: $\mathbb{Z}^3$, estimated $\gamma = 1.156957(9)$, cf. 1.1573(2) (MC, Hsu & Grassberger, 2004), 1.1575(6) (MC, Caracciolo et al. 1998), and 1.1569(6) (enumeration, Clisby et al. 2007).
- Experiment 3: $\mathbb{Z}^3$, estimated $\mu = 4.6840398(9)$ (data run not yet complete), cf. 4.684038(6) (MC, Hsu & Grassberger, 2004), 4.684043(12) (enumeration, Clisby et al., 2007).

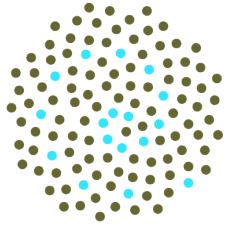


- So far, implemented pivot algorithm for SAWs on $\mathbb{Z}^d$.
- In the process of generalising to:
  - other non-local moves: cut-and-paste, pivot with fixed endpoints;
  - other lattices / off-lattice;
  - arbitrary short-range interactions (e.g. Domb-Joyce, ISAWs, truncated power law);
  - copolymers;
  - Later: branched polymers, confined polymers.
- Will release as an open source software library.



Summary

- Tree data structure has resulted in much faster implementation of pivot algorithm for SAWs.
- Will soon be generalised to other models with short-range interactions, other global moves.
- Can study extremely long polymers.
- Open source software library to be released soon.



References

- Nathan Clisby, *Accurate estimate of the critical exponent ν for self-avoiding walks via a fast implementation of the pivot algorithm*, Phys. Rev. Lett. **104** (2010), 055702.
- N. Clisby, *Efficient implementation of the pivot algorithm for self-avoiding walks*, J. Stat. Phys. **140** (2010), 349–392.
- N. Clisby, *Accurate estimate of the critical exponent γ for three-dimensional self-avoiding walks*, in preparation.
- N. Clisby, *Determination of the connective constant for self-avoiding walks via the pivot algorithm and the method of atmospheres*, in preparation.