# The importance of fast algorithms for simulating complex systems

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MASCOS, The University of Melbourne

Mathematics of Planet Earth Conference
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# Statistical mechanics

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- $\cdots$ but system may still have globally emergent changes called *phase transitions*.
- Collective, emergent behaviour is emblematic of *complex systems*.

# Two typical phase transitions are $\cdots$

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Liquid water boiling

(source: wikimedia commons)

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Ice melting

source: Ian Joughin, released under Creative Commons license www.imaggeo.net/view/984

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Study of long chain molecules, or polymers, is another important example.

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- In particular, can understand *how* phase transitions occur.
- These common features are *universal*.

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- Will show what a "good" computer algorithm looks like, and explain why good algorithms make a big difference.

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- A walk on a grid, with the rule that you can't revisit any grid points.
- Can study SAW in any dimension, most commonly 3 dimensions due to physical relevance, or in 2 dimensions because this is a rich and important topic in mathematical physics.

Simple random walk

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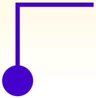

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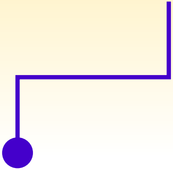

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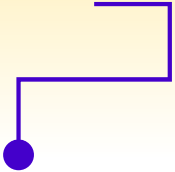

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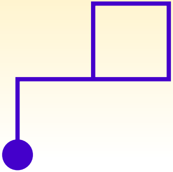

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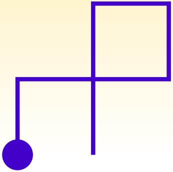

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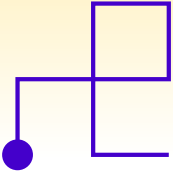

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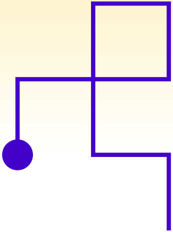

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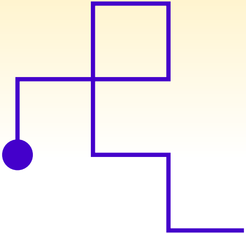

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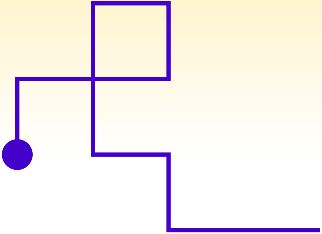

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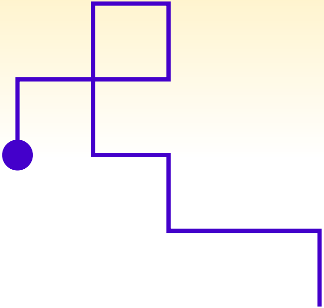

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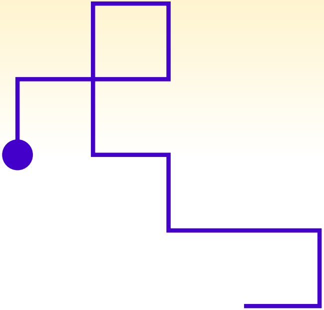

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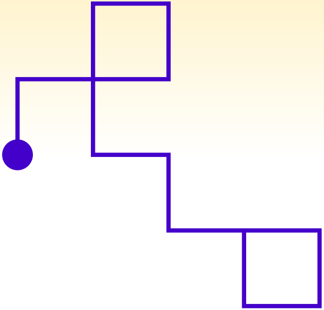

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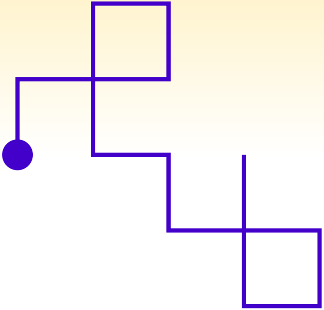

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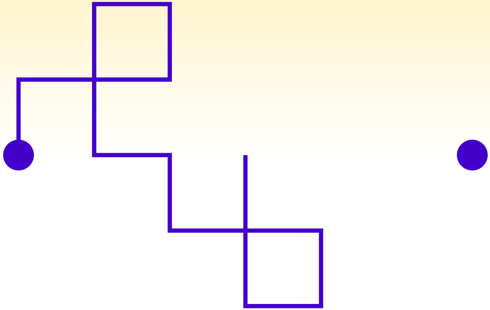

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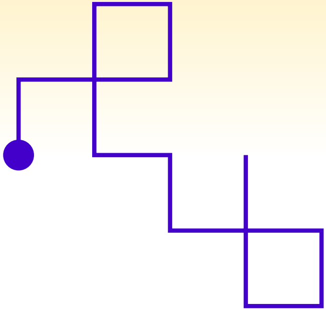

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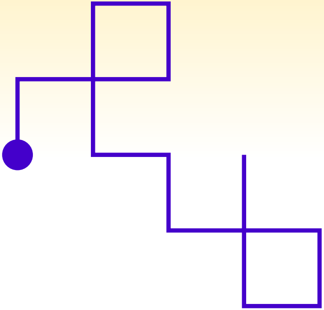

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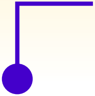

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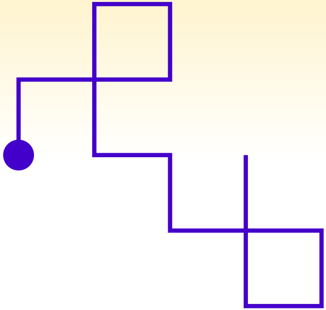

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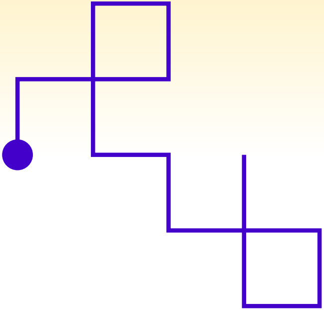

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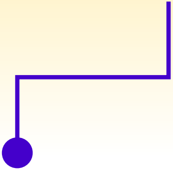

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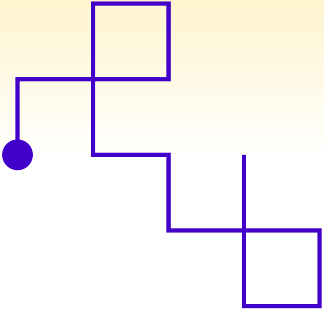

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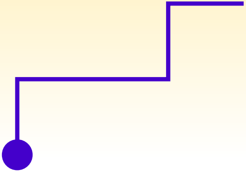

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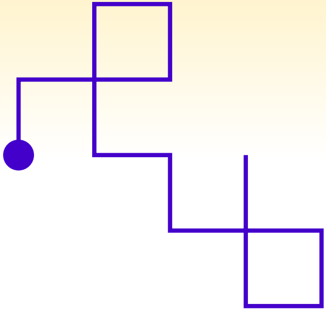

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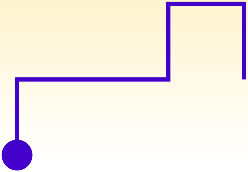

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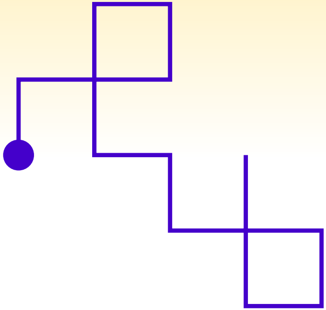

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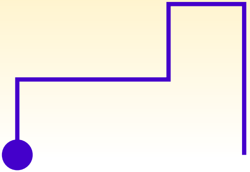

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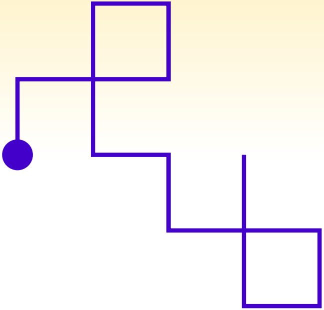

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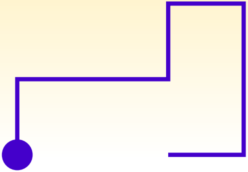

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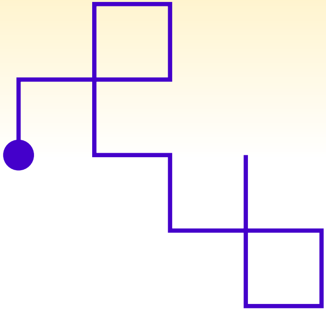

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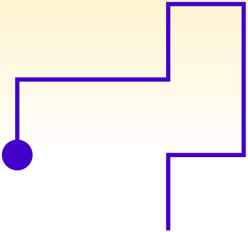

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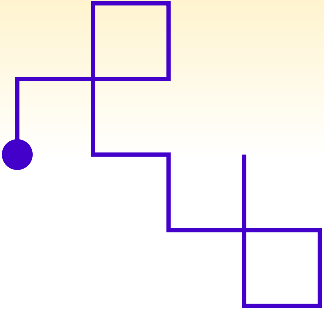

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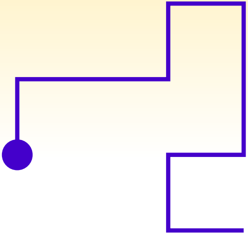

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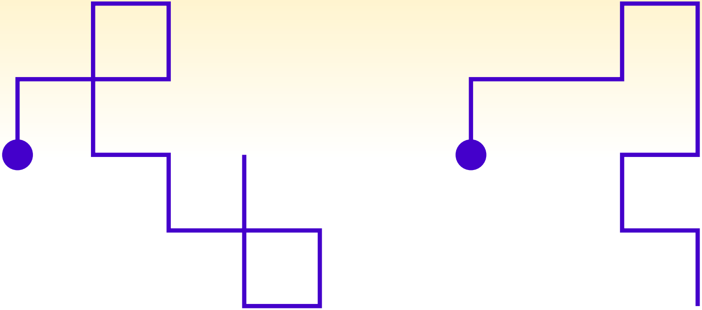

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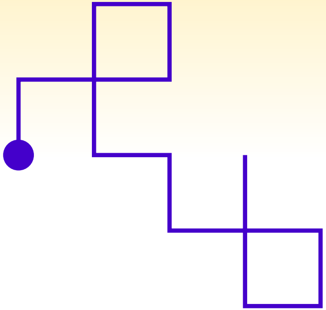

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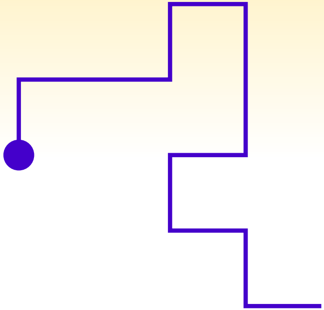

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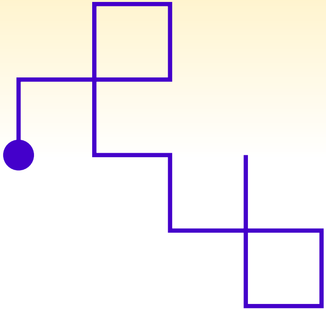

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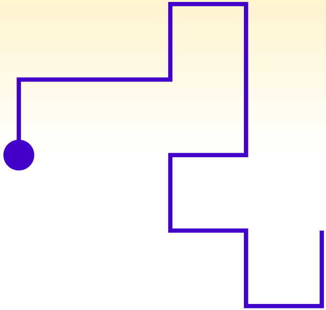

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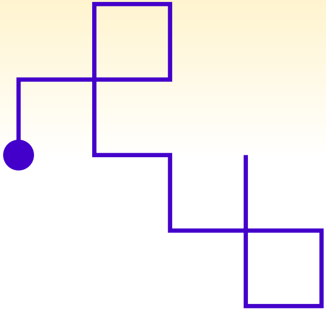

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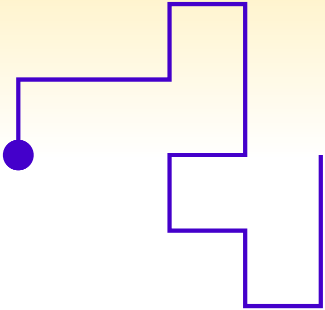

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- Clearly, can't have two atoms in the same place, and it turns out that this is the key property of polymers in a good solvent.
- In fact SAW *exactly* captures universal properties of polymers, such as the way in which the typical size of a polymer grows with the number of atoms in the chain.

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- SAW are *fractal* objects, and $1/\nu$ is their fractal dimension.

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Typical simple random walks and self-avoiding walks

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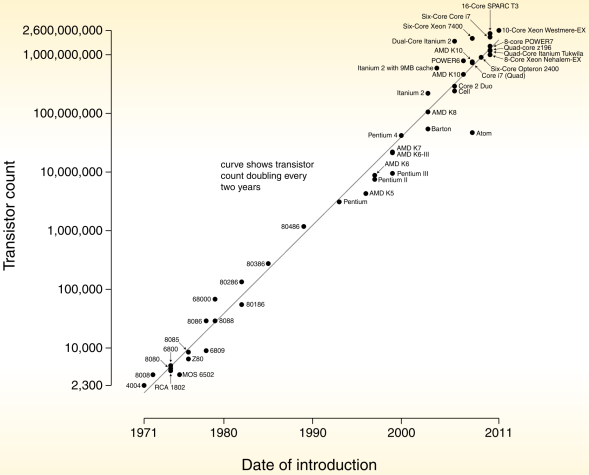
- This rule of thumb has held to a good approximation ever since, i.e. available computing power per $ has increased exponentially.

Microprocessor Transistor Counts 1971-2011 & Moore's Law




Line shows doubling every 2 years. Source: Wikipedia.

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- This makes a *big* difference to the quality of computer simulations, and the size / resolution of the systems that can be simulated.

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- Molecular dynamics (very important for understanding polymer dynamics)
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- Markov chain Monte Carlo (MCMC) sampling, and other Monte Carlo methods.

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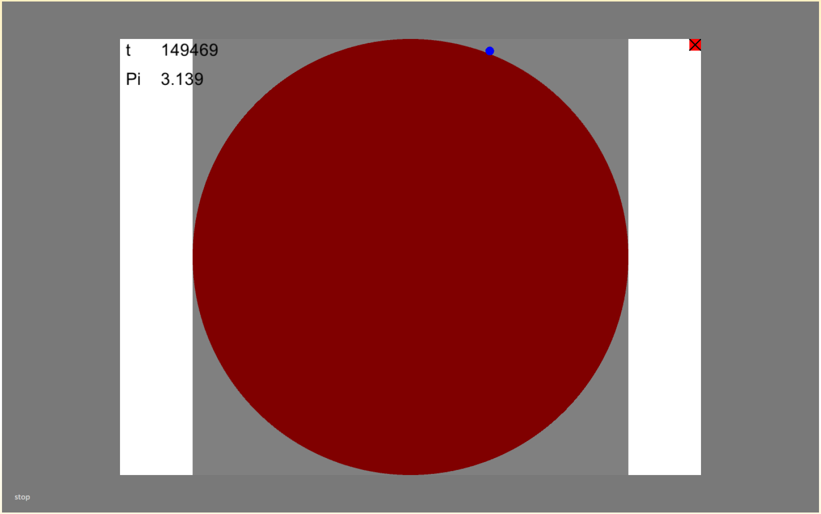
MCMC estimation of $\pi$


t 149469
Pi 3.139
stop

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- CPU time $O(N)$ for an essentially new configuration.
- Made it possible to study dramatically longer SAW (from hundreds of steps, to tens of thousands).

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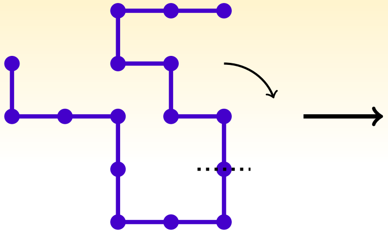
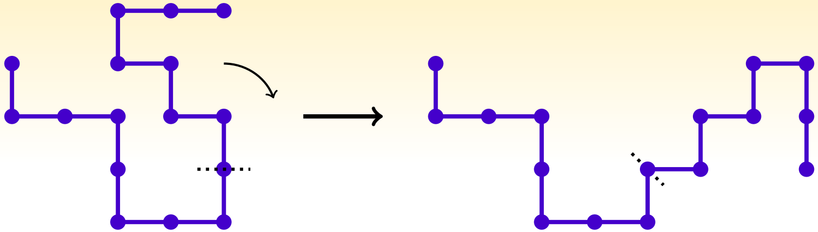
- "Global" because on average half of the monomers are moved.



Example pivot move



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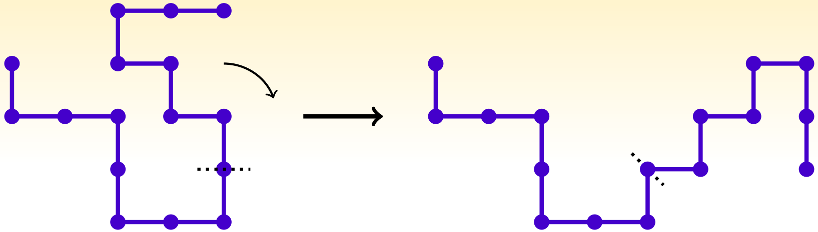

Example pivot move

Run simulation

# Why is it so effective?

- Every time a pivot attempt *is* successful there is a large change in global observables.

# Why is it so effective?

- Every time a pivot attempt *is* successful there is a large change in global observables.
- Only need $O(1)$ successful pivots before we have an *essentially new* configuration.

More to the story: pivot moves are in fact *local* moves if you think of them the right way.

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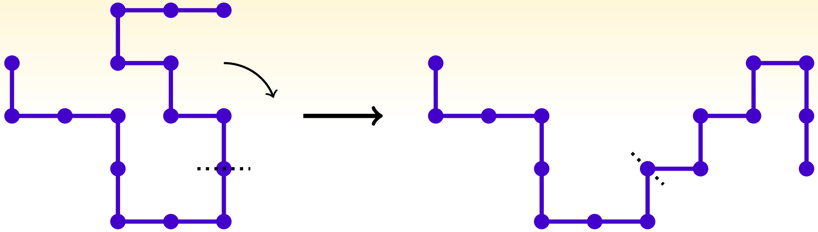

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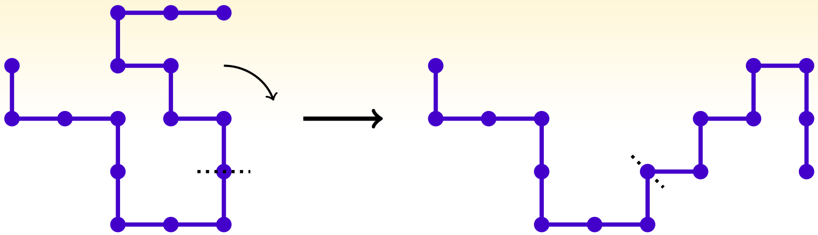

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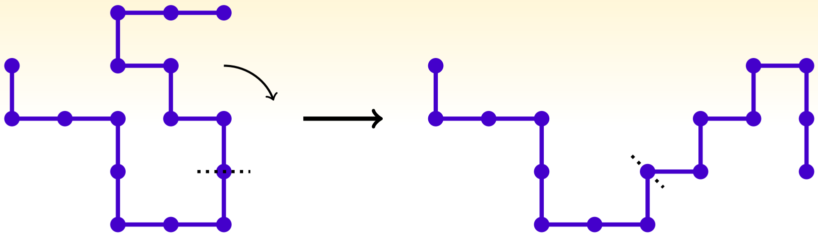

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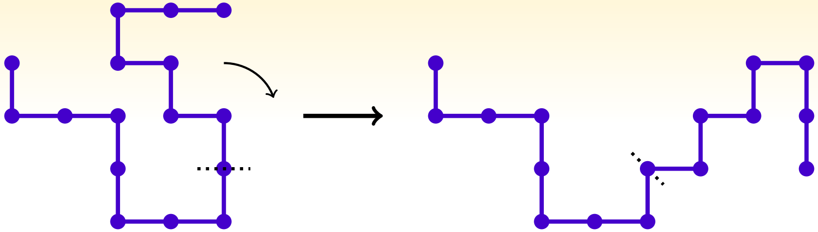

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With the right implementation, pivot move has *global effect* for *local cost*. Tricky part is checking that after subwalk is rotated the walk remains self-avoiding.

Following simulation based on timings from 3 years ago. $1s$ in animation corresponds to $10\mu s$ of computer time.

Comparison of hash table and SAW-tree implementations

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## Comparison of hash table and SAW-tree implementations

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

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

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

| | $\mathbb{Z}^2$ | | | $\mathbb{Z}^3$ | | |
|---|---|---|---|---|---|---|
| $N$ | S-t ($\mu s$) | M&S/S-t | K/S-t | S-t ($\mu s$) | 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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- This is not the end of the story for polymer knotting - other hard problems must also be solved.

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- Challenge: find efficient algorithms and computer implementations for other systems. (Very active research area, e.g. cluster algorithms, Wang-Landau method, PERM, worm algorithms.)