Applying Various Movesets to the Lattice-SAW Model of High Intensity Vortices

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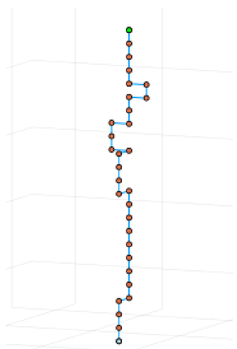
Introduction

A Self-Avoiding Walk (SAW) is a structure that can be used to mathematically model some kind of linear path through space. Two such models, which we were concerned with here, are for a vortex filament in a tornado and for a long protein chain. Using the similarities of these two contexts, we examined multiple approaches to the problem of energy sampling in order to determine which is most efficient and reliable.

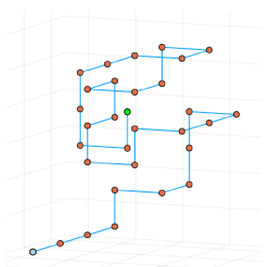
SAWs and Energy

For the sake of simplicity, we worked exclusively with SAWs that are constrained to the lattice grid in three dimensions, resulting in the more "blocky" visualisations here. A caveat to this: as we increase the size of the SAW, it does not necessarily correspond to a "larger" structure but rather one which is more precise.

The chief metric with which we were concerned here is the energy of a configuration, a measure of its compactedness.



(a) A high-energy SAW, largely extending in one direction



(b) A low-energy SAW, occupying a more compact volume of space

For an environmental parameter β, we used a Markov Chain Monte Carlo technique to determine the average energy of the vortex model at progressively longer SAWs. Our primary goal was to compare a few combinations of movesets that specify how the next state can be constructed from the previous.

Movesets Explored

LT Moves

Proposed in [1] as an alternative to the Pivot algorithm, Localised Transformations (LT) work by randomly reconstructing (or permuting) the steps of some subsection of the SAW.

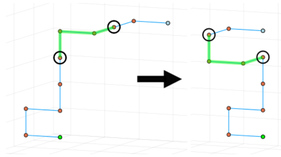


Figure: A single LT move, reconstructing the highlighted segments.

Pull Moves

As detailed in [3], pull moves displace a single point and then "pull" the subsequent steps along until a new valid configuration is reached.

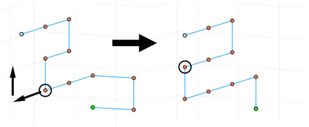


Figure: A single pull move, starting with the circled point

Bond-Rebridging Moves

Rebridging moves, devised in [2], replace one set of parallel adjacent segments with another, re-routing the SAW through the same volume.

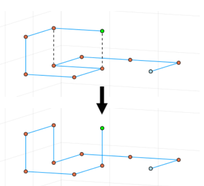


Figure: A single rebridge move, placing new segments at the dotted lines

Madras Moves

The moveset described by [4] works by rotating or reflecting some subsection of the SAW, leaving the ends of the subsection unmoved.

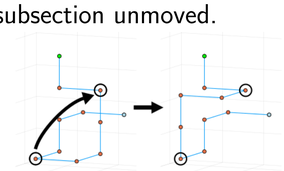


Figure: A single Madras move, rotating the section between the circled points

Moveset Comparison

After implementing the model and movesets in the Julia programming language, we ran many averaging trials, using different parameters for the length N, the environmental parameter β, and the combination of movesets employed.

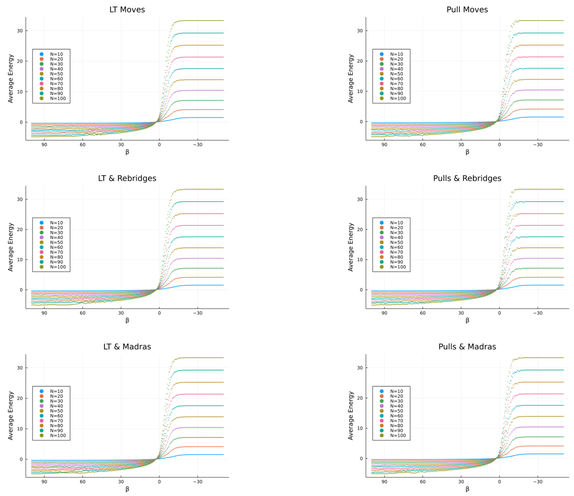


Figure: Simulation-generated average energies for $10 \leq N \leq 100$, $\Delta N = 10$, $-50 \leq \beta \leq 100$

While all movesets were functional, as evidenced by the macroscopically smooth curves in the above images, we were able to draw some conclusions about the relative performance of each moveset:

- The LT moves are more reliable for negative β/high energy states.
- The pull moves are more reliable for large, positive β/low energy states.
- Both rebridging and Madras moves act as a stablising force for positive β when used in conjunction with LT or pulls.

References

[1] P. Bělík et al. "Equilibrium Energy and Enrtopy of Vortex Filaments on a Cubic Lattice: A Localized Transformations Algorithm". (2021)

[2] J. M. Deutsch. "Long range moves for high density polymer simulations". The Journal of Chemical Physics 106.21 (1997), pp. 8849–8854.

[3] N. Lesh et al. "A Complete and Effective Move Set for Simplified Protein Folding". (2003)

[4] N. Madras et al. "The pivot algorithm: A highly efficient Monte Carlo method for the self-avoiding walk". In: Journal of Statistical Physics 50 (1988), pp. 109–186.

Minima

A secondary objective of ours was to investigate the minimum energy values for different lengths of SAWs. Using the model with these different movesets, we employed a Simulated Annealing schedule for β and recorded the lowest-energy configuration found in each trial. This method yielded potential minima for $3 \leq N \leq 90$, most of which were supported by multiple trials. Previous work had determined the minima for $3 \leq N \leq 21$, and [1] had suggested a linear trend given those values. These new values, which must be greater than the true minima if not equal, allow us to refine the linear trend as well as suggest a better-fitting $N \log(N)$ curve.

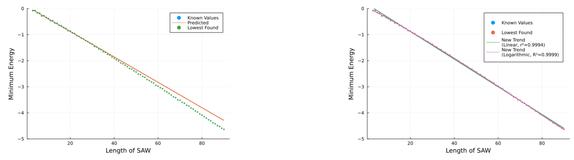


Figure: Minimum energy values for $3 \leq N \leq 90$, with trend lines. The left image shows the predictions of Bělík et al. based off of minima for $3 \leq N \leq 18$. The right shows new best fit linear and $N \log(N)$ curves.

There seem to be some patterns in the contruction of the configurations themselves, most notably in a tend towards bilateral symmetry, which had been previously noted in [1].

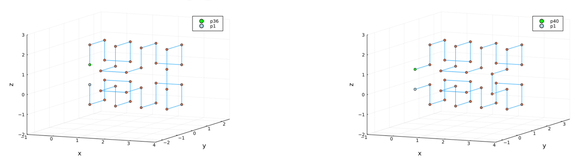


Figure: Minima found for $N = 35$ and $N = 39$, exhibiting bilateral symmetry and showing similar and repeating structures

While these patterns could potentially be utilised to easily find the minimum-energy configuration of any-length SAW, more research is needed to determine those mechanisms.

Acknowledgements

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