Monte-Carlo for Kinetic Energy of Closed Vortices as Self-Avoiding Polygons

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Gustavus Adolphus College Mathematics Honors Presentation

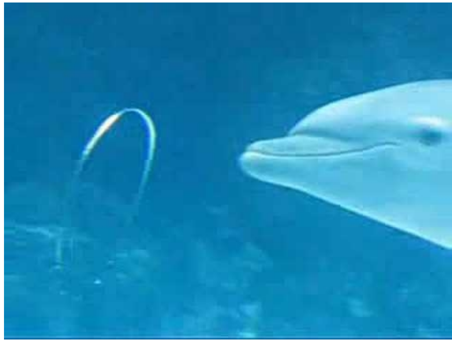
Overview

1) Model Introduction
2) Vortices in the Cubic Lattice
3) Statistical Background
4) Research Question and Former Work
5) Enumeration and Small N
6) New Maximum Configuration
7) Conclusion and Questions (Save for end)

Model Introduction

Vortices

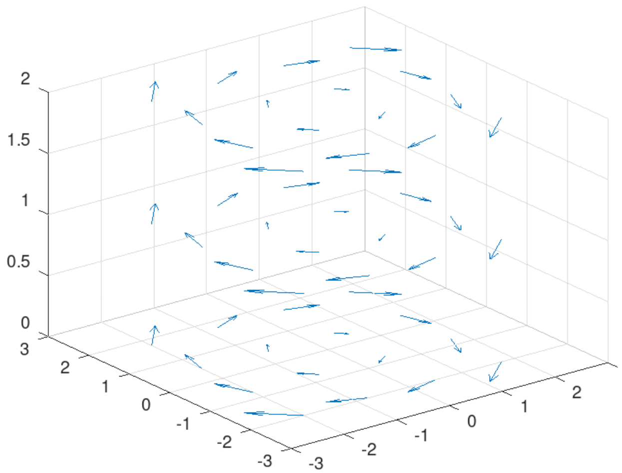
- Rotating mass of liquid or gas in a region
- Bounded at edges
- In tornadoes, found to begin as long, straight vortices that "fold up" on themselves as they dissipate energy to their surroundings



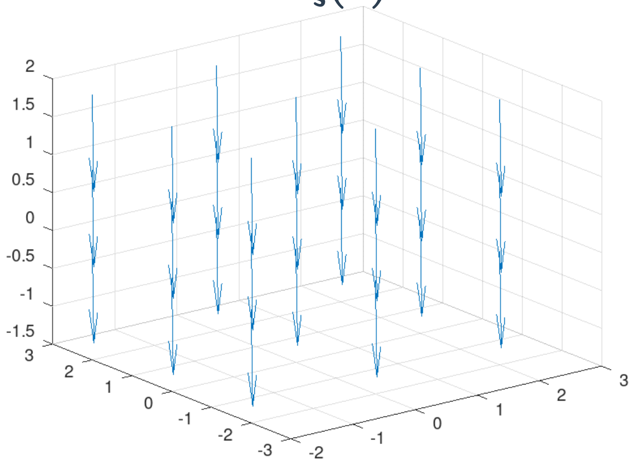
Vorticity Field

- Given vector field of velocity field $\mathbf{u}(\mathbf{x})$, construct the **vorticity field**, $\boldsymbol{\xi}(\mathbf{x}) := \text{curl } \mathbf{u}(\mathbf{x})$
- A **vortex** is a collection of integral curves of the vorticity field, $\boldsymbol{\xi}(\mathbf{x})$

$\mathbf{u}(\mathbf{x})$



$\boldsymbol{\xi}(\mathbf{x})$



Energy of a Vortex

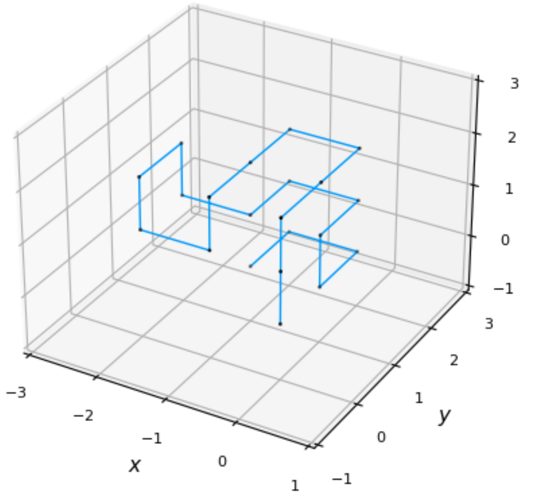
- Assume that vorticity is only non-zero in a collection of thin **vortex tubes**, $\boldsymbol{\tau}$, or if infinitely thin, **vortex filament**
- Energy of such vortex given below

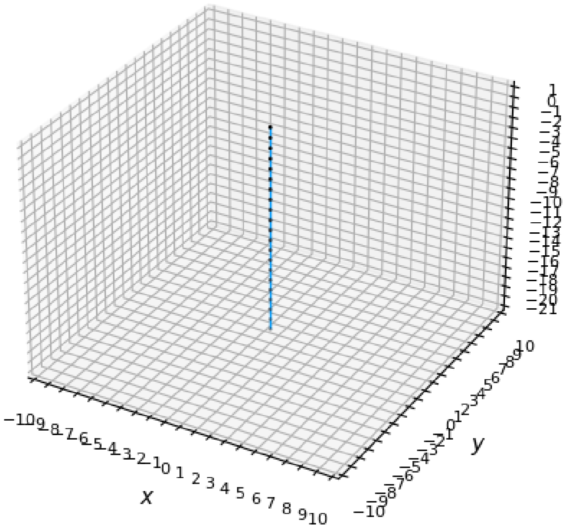
$$E = \frac{1}{8\pi} \int_{\mathcal{T}} \int_{\mathcal{T}} \frac{\boldsymbol{\xi}(\mathbf{x}) \cdot \boldsymbol{\xi}(\mathbf{x}')}{|\mathbf{x} - \mathbf{x}'|} \, d\mathbf{x}' d\mathbf{x}.$$

- Dot product of vorticities over distance of points
- Intuition: Nearby parallel components

Modeling Idea

- Construct a vortex filament path in the cubic lattice for modeling vortices: Analyze the patterns of configurations and their energies
- Former Work: Analyzed this model on open vortices
- Studied average energies, min and max configurations, patterns as N grows

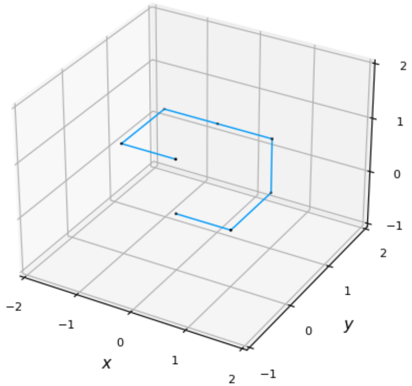


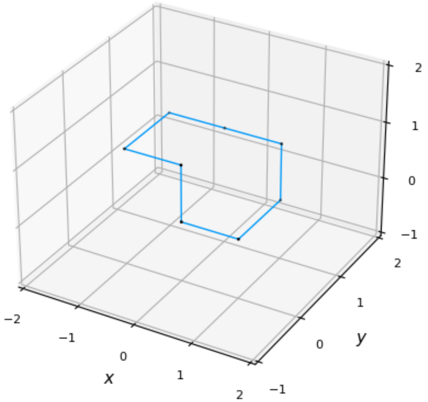


Vortices in the Cubic Lattice

Self-avoiding Walks and Polygons

- **Self-avoiding walk (SAW)** versus **self-avoiding polygon (SAP)** in $\mathbb{Z}^3$:





- SAWs can model open vortices, SAPs for closed-loop vortices

Discretization of Energy Formula

- Consider our original energy formula across vortex filament $\boldsymbol{\tau}$

$$E = \frac{1}{8\pi} \int_{\mathcal{T}} \int_{\mathcal{T}} \frac{\boldsymbol{\xi}(\mathbf{x}) \cdot \boldsymbol{\xi}(\mathbf{x}')}{|\mathbf{x} - \mathbf{x}'|} \, d\mathbf{x}' \, d\mathbf{x}.$$

- Reduce the formula to a double sum across the SAW or SAP

$$E = \frac{1}{8\pi} \sum_{i} \sum_{j \neq i} \frac{\boldsymbol{\xi}_i \cdot \boldsymbol{\xi}_j}{|\mathbf{m}_i - \mathbf{m}_j|}$$

Note: Negative energy configurations

Statistical Background

Boltzmann Probability Distribution – Statistical Mechanics

- Provided a set of states with corresponding energies $E_1,\ldots,E_n$
- Probability of achieving a single state given by

$$p_i = \frac{e^{-\beta E_i}}{Z}, \quad Z = \sum_{i=1}^{n} E_i$$

- β is inverse of k_B times statistical temperature T
- When $\beta=0$, each state equally likely, when $\beta>0$, lower energy configurations more likely, when $\beta<0$, high energy
- Can calculate average energy: $\hat{E} = \sum_{i=1}^{n} p_i E_i$

Metropolis Markov-Chain Monte Carlo

- The **Metropolis MCMC Algorithm** allows us to generate a sequence of samples and accept/reject to approximate distribution
- Given a SAP s_{t-1}, and a new proposal for sequence n_t, acceptance probability given by

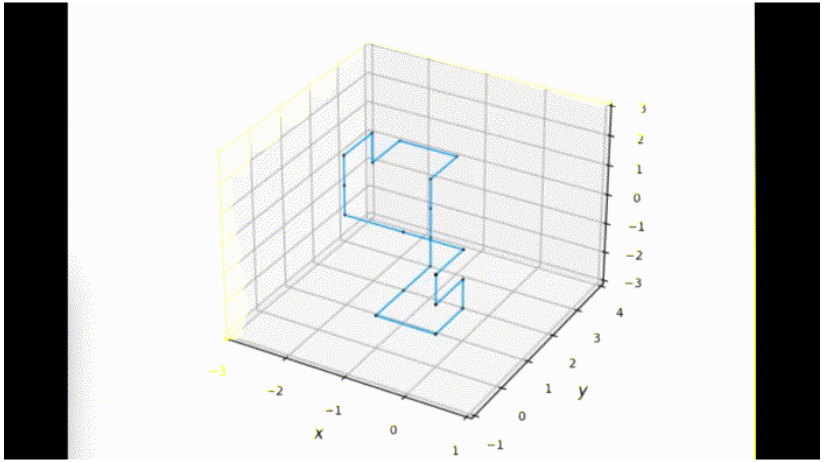
$$p_t = \min(\frac{f(n_t)}{f(s_{t-1})}, 1)$$

$$= \min(e^{-\beta(E_{n_t} - E_{s_{t-1}})}, 1)$$

$$f(s) = \frac{e^{-\beta E_s}}{Z}, \quad Z = \sum_{s \in SAP_N} e^{-\beta E_s}$$

Transformations

- What is finally required is a set of transformations that given a current SAP s_{t-1}, can propose a new SAP n_t which is accepted with probability described before
- Use transformations described by Madras, Orlitsky, Shepp symmetries
- Ergodicity, symmetric, local



Research Question and Former Work

- Former work done in modeling open tornadic vortices as SAWs
- Maximum energy configuration proven to be straight
  - Maximum energy follows N log(N) pattern where N is SAW length
- Minimum energy configurations can be tricky to find
  - Minimum energy follows linear decreasing pattern
  - Small, balled-up or folded-up configurations
  - Start point near endpoint, suggesting "wanting to close"
- **Q: How does this model hold over closed-loop vortices as SAPs?**
- **Q: Do minimum energy SAPs correspond with minimum energy SAWs**

Enumeration and Small N

Number of SAPs

- As length of configuration, N, grows, number of configurations grows exponentially
- Enumerated SAPs up to length 16 by backtracking, calculated energies directly

N	$\|SAP_N\|$	Min Eng	Max Eng
4	3	-0.15915	-0.15915
6	22	-0.21542	-0.15233
8	207	-0.36493	0.01680
10	2 412	-0.39523	0.13567
12	31 754	-0.51877	0.34702
14	452 640	-0.59807	0.53220
16	6 840 774	-0.68339	0.78257

TABLE 1. Number of SAPs of length N from length 4 to 16 with minimum and maximum energies to five decimal points.

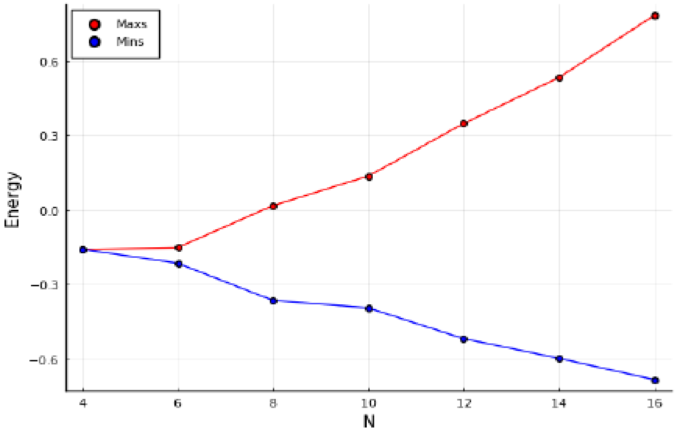


FIGURE 13. Plot of minimum and maximum energies for lengths 4 through 16.

Maximum and Minimum Configurations

- Maximum energy configurations simple, nearest-square configuration
  - For N divisible by 4, N/4 by N/4 square
  - Otherwise, (N-2)/4 by (N+2)/4 rectangle
- Similar to SAWs, minimum energy configurations more interesting
  - Folded-up configurations
  - Seemingly linear decreasing pattern
  - Trickier to “guess”

- See configurations on next slide

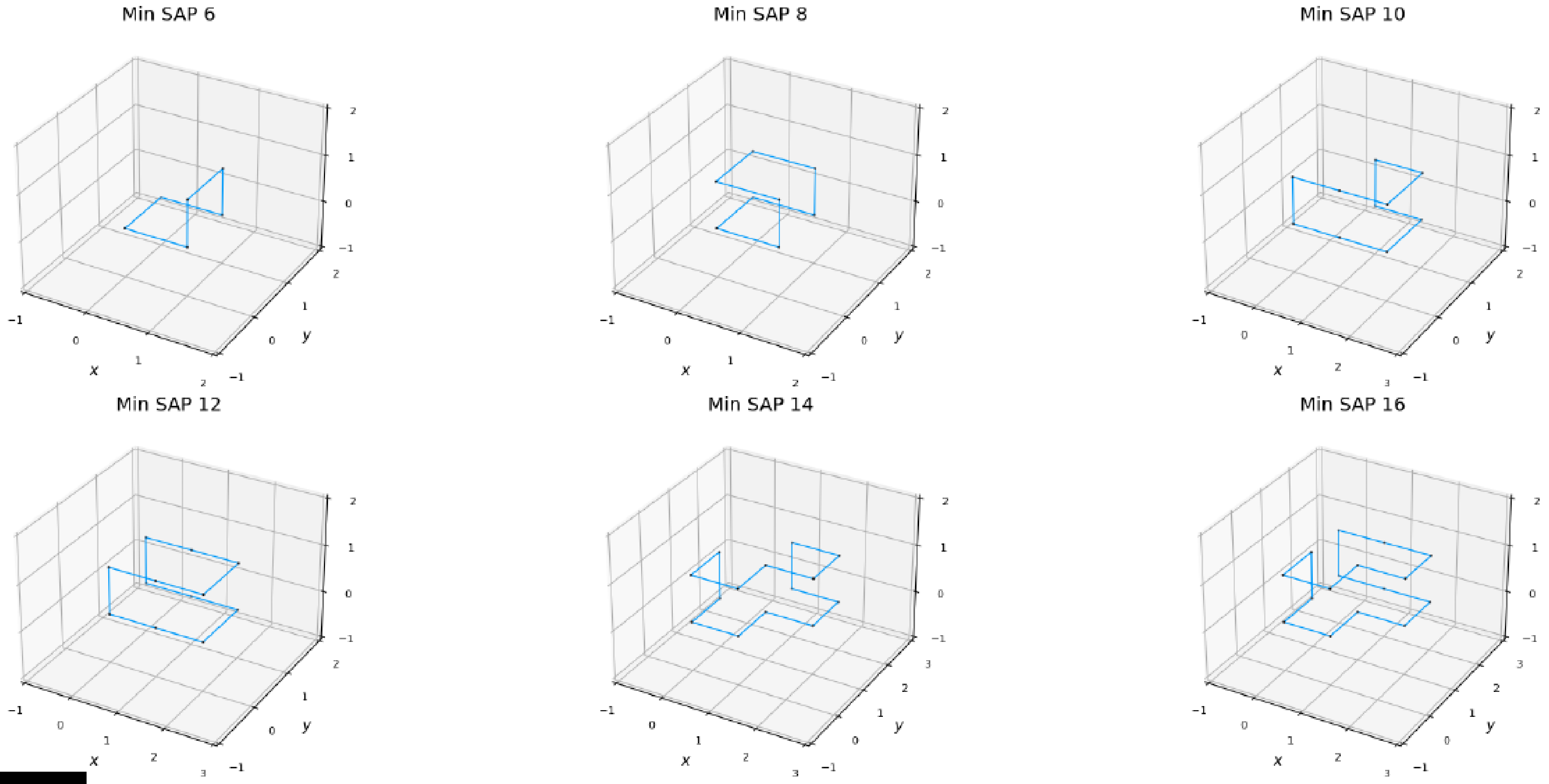
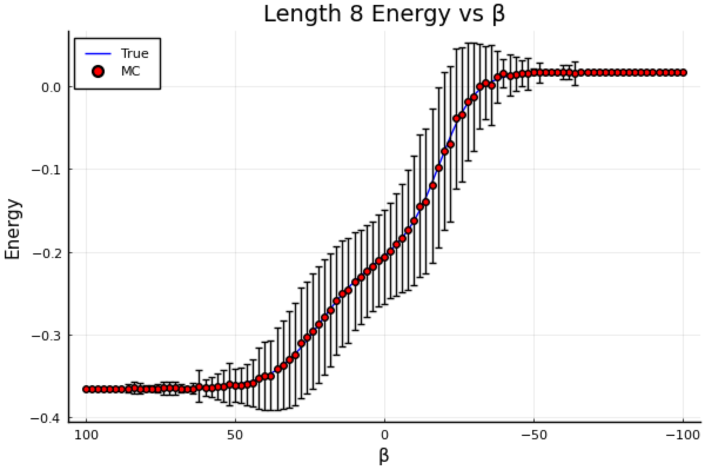
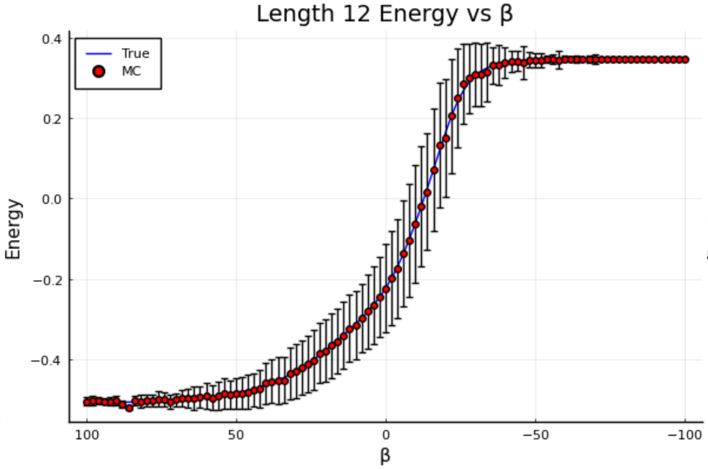
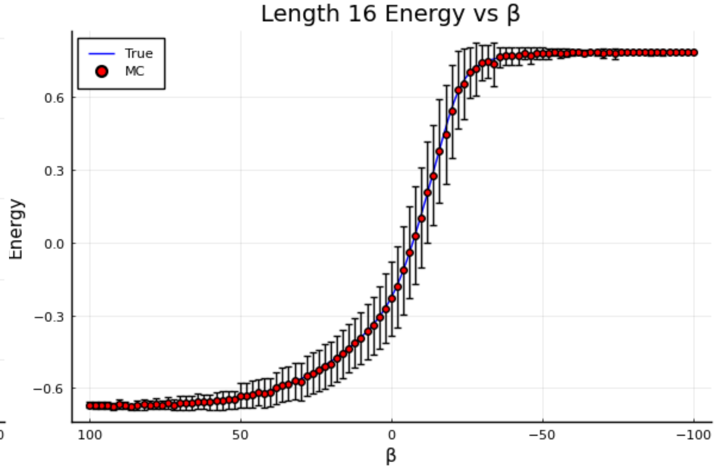


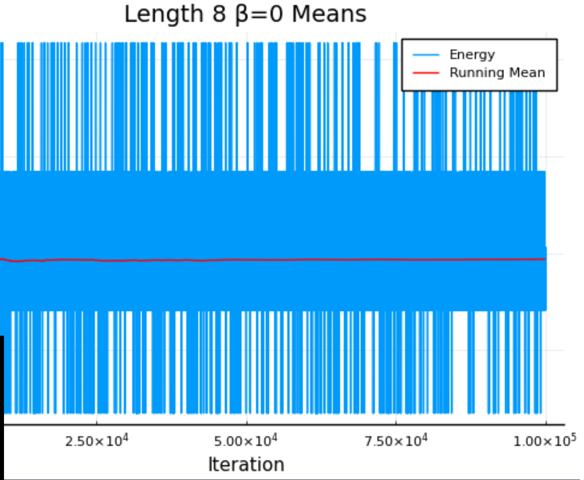
FIGURE 14. Minimum energy SAPs for lengths 6 though 16.

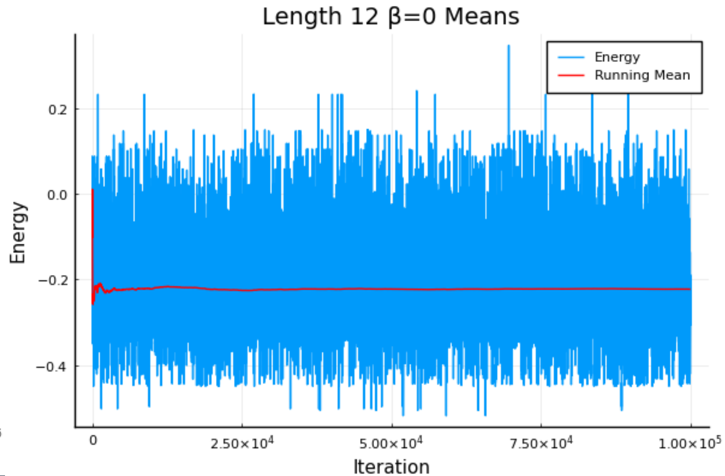
Average Energy vs β Curves

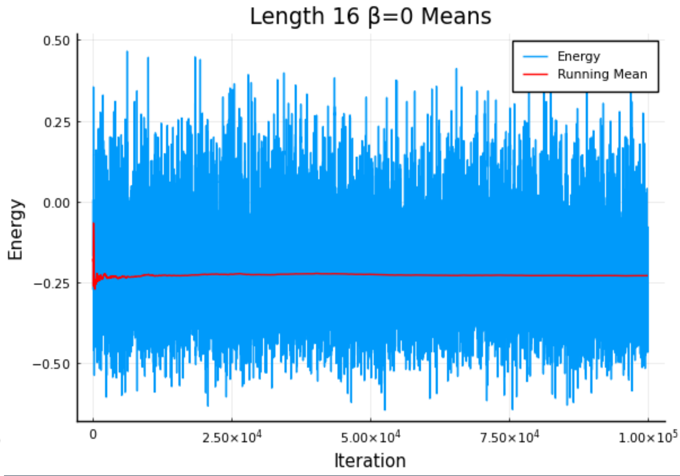






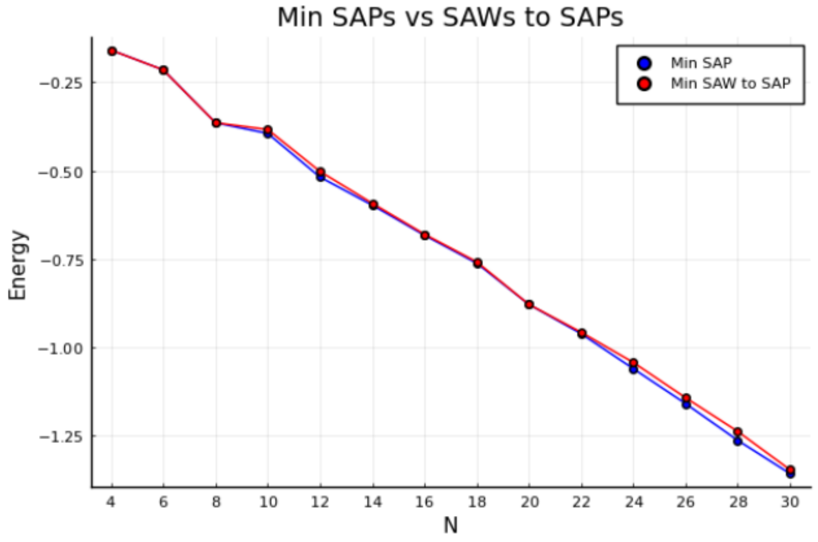


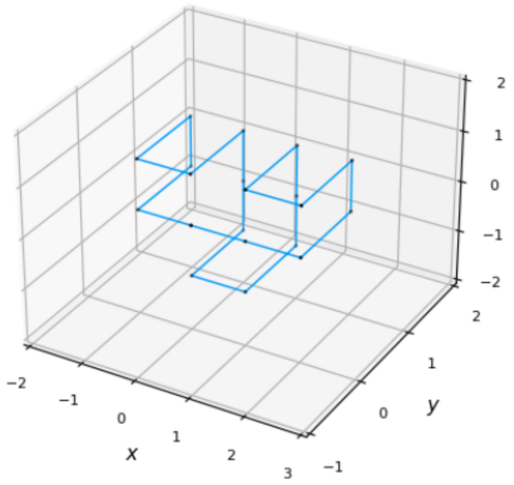


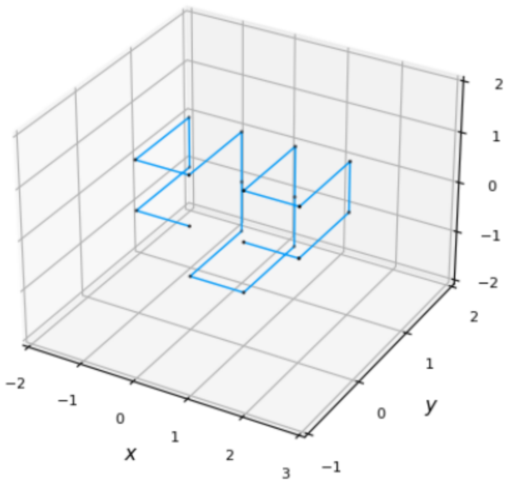


Comparison of Minima SAPs and SAWs

- For small N, directly compared minimum energy SAWs to SAPs due to SAWs wanting to close on themselves



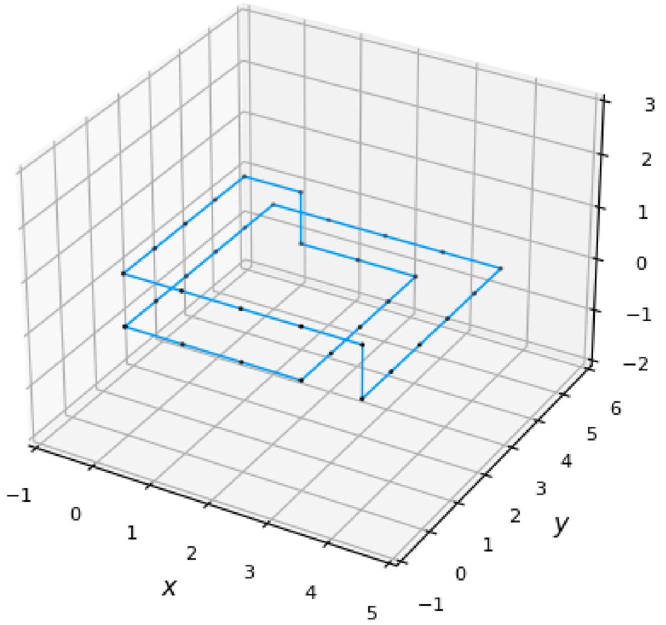




New Maximum Configuration

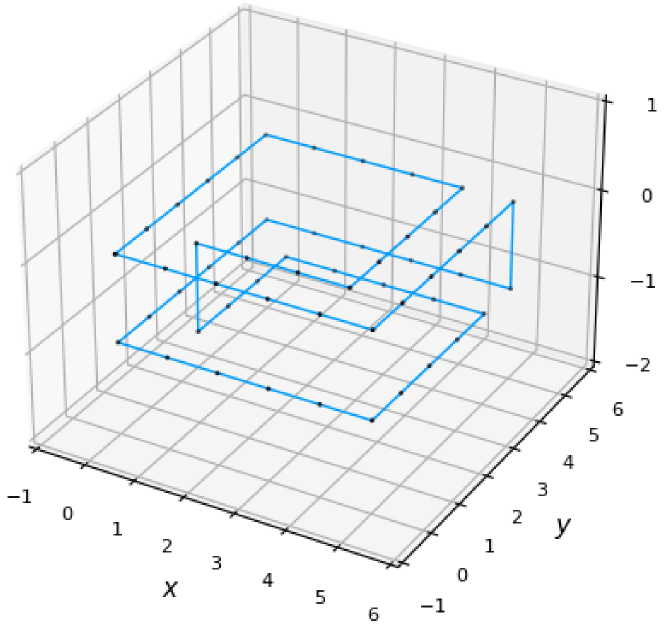
Double-Loop Configuration

- Interesting new pattern discovered for $N \geq 34$



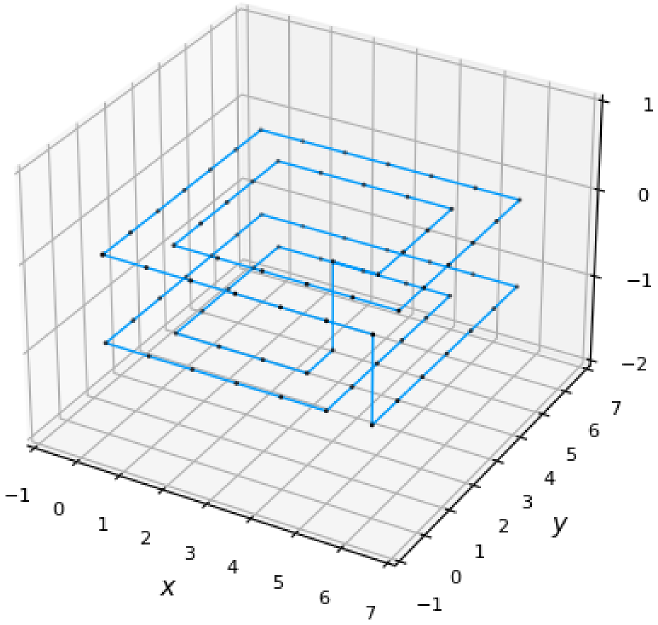
Triple-Loop Configuration

- Pattern for $N \geq 54$

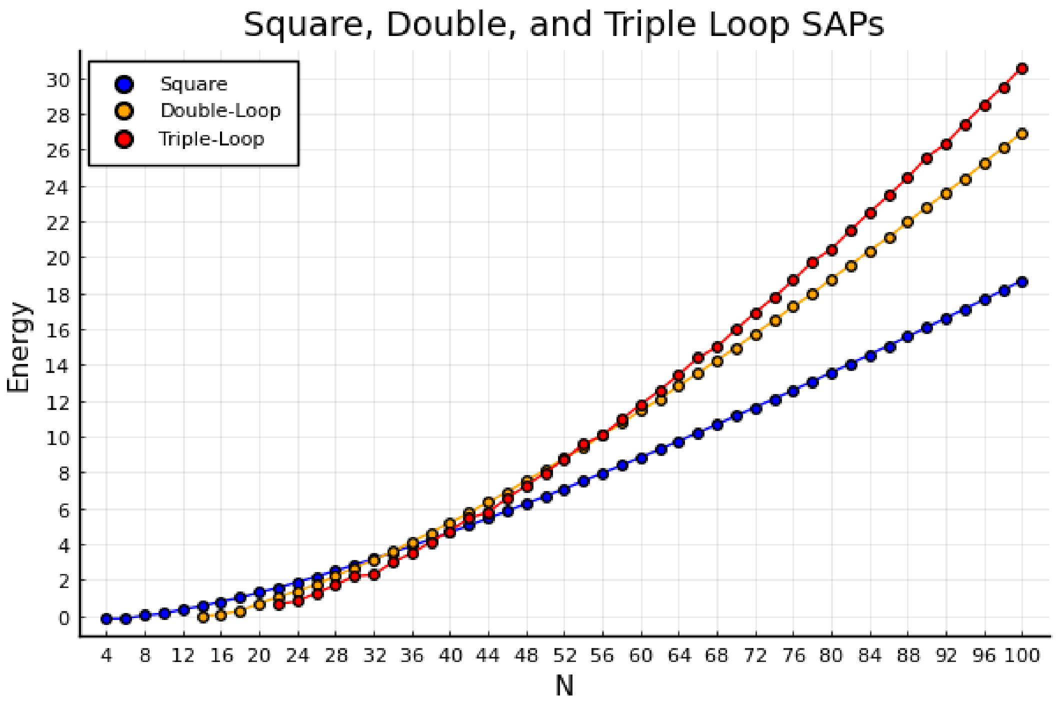


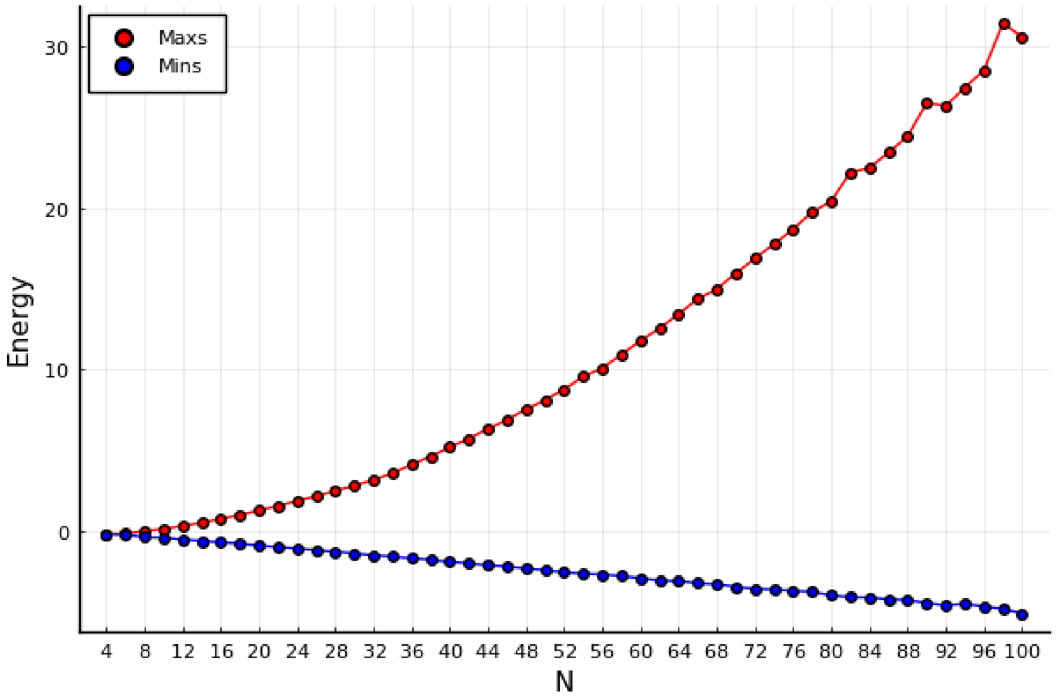
Quadruple-Loop Configuration

- $N = 82$

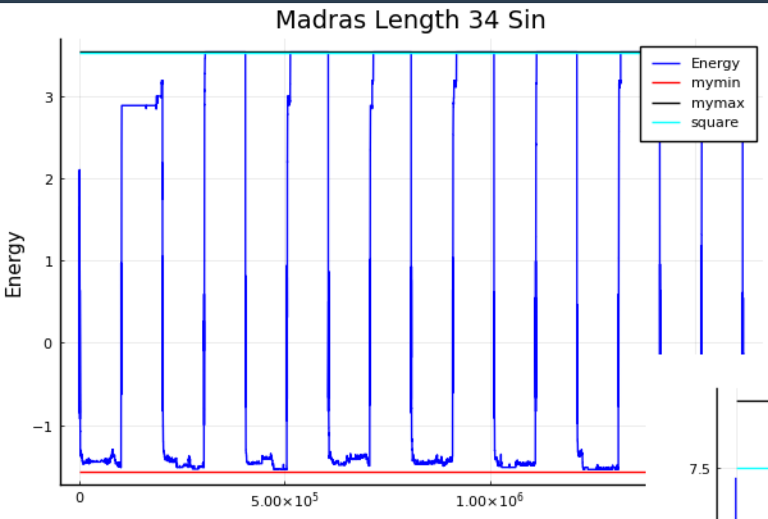


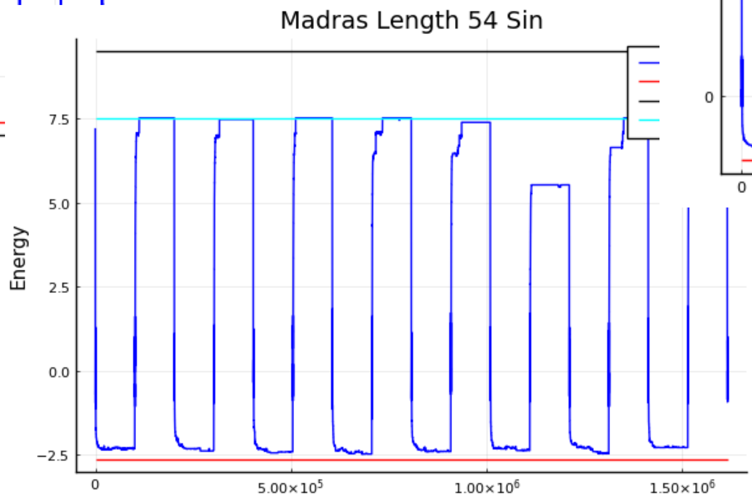
Double and Triple-Loop Energies

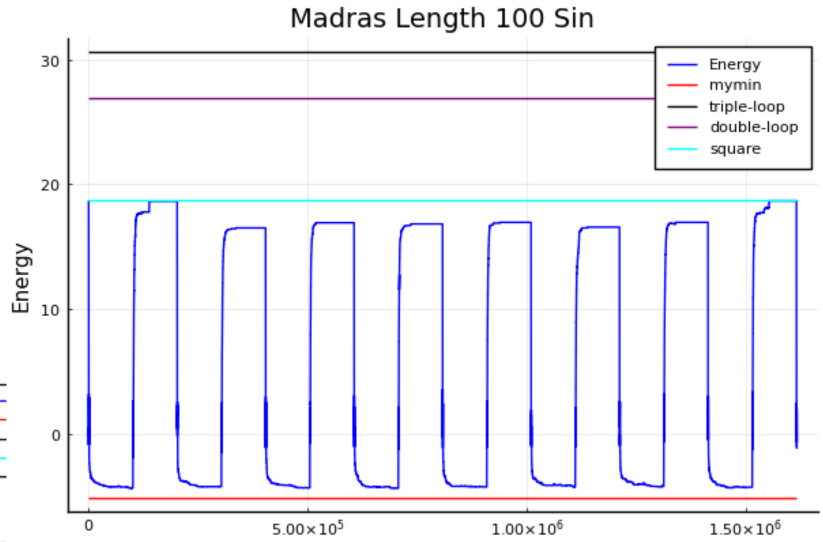




Issue with MCMC







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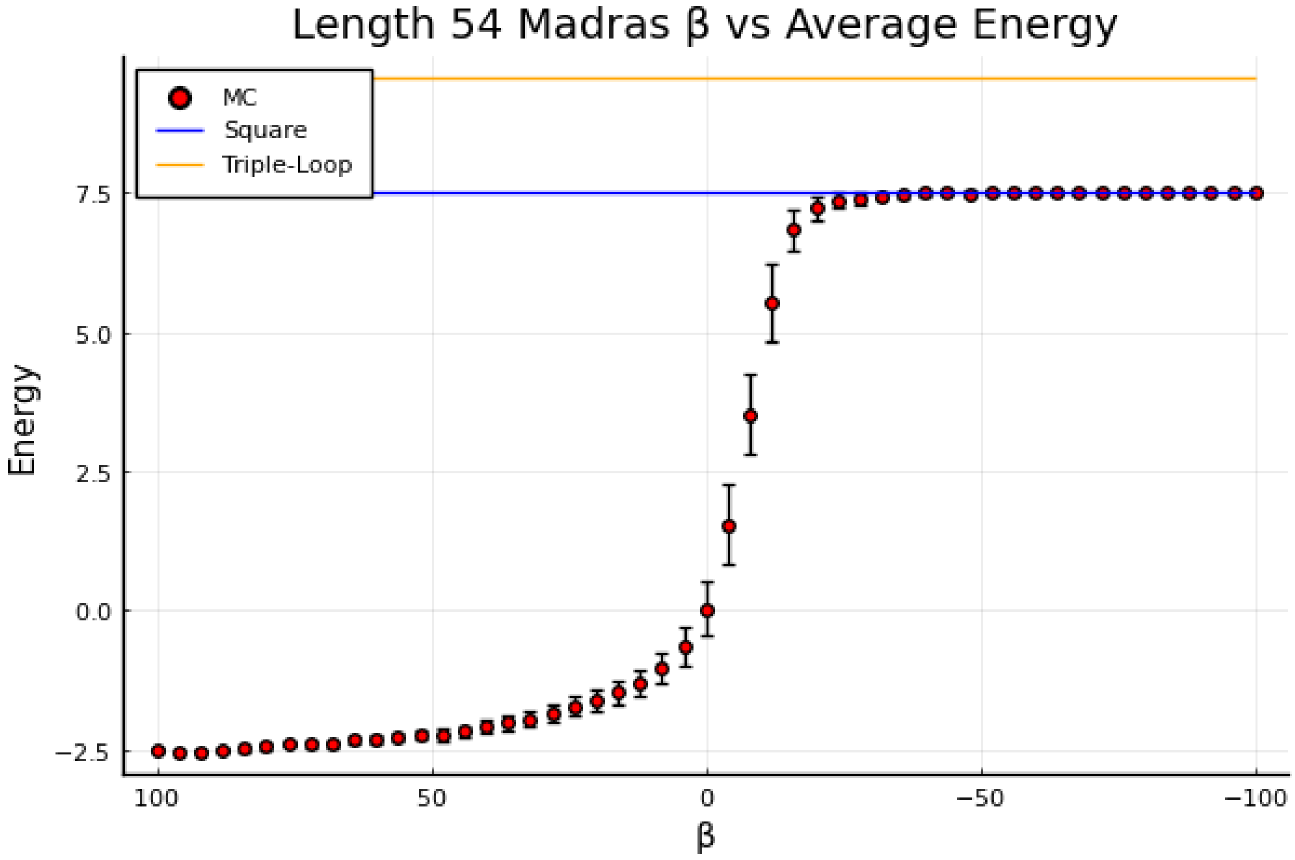

Conclusion

Takeaways and Future Work

- Enumeration through length 16, exact minima
- Implementation of transformations for MCMC with SAPs
- Minimum energy SAPs and SAWs were not exact in general (19)
- Discovery of new maximum energy configuration
- **Future Work**: Test/create new moves to discover multi-loops

Thank you!!
Questions?

Citations

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