HONORS PROPOSAL: MONTE-CARLO FOR KINETIC ENERGY OF VORTICES AS SELF-AVOIDING POLYGONS (UNDER THE SUPERVISION OF DR. PAVEL BĚLÍK)

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1. Introduction

A vortex may be described as a mass of liquid or gas that rotates about a given region. More specifically, it can be described as a collection of integral curves of vorticity, often in a tube-like region, in which vorticity is significantly stronger than in its surroundings. Examples of vortices in nature include a tornado hitting earth and water swirling into a drain. Former work has been done in modeling the equilibrium kinetic energy of such vortices [1] where it was shown that narrow vortices within a tornadic flow, so-called supercritical vortices, begin as long, straight vortices that fold up on themselves and dissipate as they transfer energy to their surroundings. As is commonly stated in fluid dynamics, such vortices must be bounded at their edges or wander off to infinity [2]. So while the vortices we have described so far are typically thought of as being bound at two distinct locations, it is possible for a vortex to be bounded by looping back upon itself. One common example of this is when someone puffs a ring of smoke. Dolphins and whales have even been found to be able to blow bubble rings underwater and play with them by moving them around.

We are interested in understanding and modeling the kinetic energy of vortices that loop back on themselves. Motivated by the results in [1], we will model looping vortices in the three-dimensional cubic lattice as self-avoiding polygons and calculate their energies directly through a simplified integral formula for continuous vortices. In [1], non-looping vortices are modeled, such as the supercritical vortices in tornadoes, as self-avoiding walks and Monte-Carlo methods are used to study the energies and entropies of such configurations [1]. It was found that minimum energy walks tended to end with the last point of the walk

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Figure 1. Dolphin and vortex ring - https://www.youtube.com/watch?v=2m6ie3MVIAw

near the first point, as if they were vortices which wanted to loop back on themselves. Under that context, studying the case in which vortices do create a loop may provide further insight into the minima problem for non-looping vortices. In addition, self-avoiding polygons have been studied as both a combinatorics problem of enumeration and for modeling polymers in a dilute solution [5].

We will use Monte-Carlo methods to approximate the maximum, minimum, and average energies of different length self-avoiding polygons at differing statistical temperatures, with the goal of finding optimal transformations for the Monte-Carlo process and approximating the long-term behavior of maximum and minimum energy polygons over different lengths.

2. Mathematical Background

More formally, given a three-dimensional velocity vector field $\mathbf{u}(\mathbf{x})$ of a gas or liquid matter, its vorticity field is the vector field of the curl at each point $\mathbf{x}$, i.e., $\boldsymbol{\xi}(\mathbf{x}) = \nabla \times \mathbf{u}(\mathbf{x})$. As is described by the right-hand rule, a path followed by a particle through the vorticity field gives the direction in which the surrounding matter has the most counterclockwise rotary motion. These paths are called vortex lines, and regions containing vortex lines are called vortex tubes [2]. Assuming a simplified scenario where in a homogeneous liquid of uniform density vorticity is non-zero only in a collection of thin vortex tubes, denoted by $\mathcal{T}$, the formula for kinetic energy is given as follows [6].

$$E = \frac{1}{8\pi} \int_{\mathcal{T}} \int_{\mathcal{T}} \frac{\boldsymbol{\xi}(\mathbf{x}) \cdot \boldsymbol{\xi}(\mathbf{x}')}{|\mathbf{x} - \mathbf{x}'|} \, d\mathbf{x}' d\mathbf{x} \tag{2.1}$$

In (2.1), $\boldsymbol{\xi}(\mathbf{x}) \cdot \boldsymbol{\xi}(\mathbf{x}')$ refers to the dot product of the two vorticity vectors, and $|\mathbf{x} - \mathbf{x}'|$ represents the distance between the two location vectors. Intuitively, this means that nearby components with large parallel vorticity will contribute the most to the energy, nearby components with large opposite vorticity will contribute the most negatively to the energy, any components with perpendicular vorticity do not contribute to the energy, and far apart components contribute little to the total energy.

When reduced to the discrete three-dimensional lattice under the assumption of infinitely thin vortex tubes, referred to as vortex filaments, (2.1) is simplified to a double summation across all steps $\boldsymbol{\xi}_i$, each of which has a magnitude of one and runs parallel to one of the Cartesian axes. Hence all dot products will come out to be zero, negative one, or positive one. Also note that since we are summing across entire segments, the denominator uses $\mathbf{m}_i$ which refers to to the midpoint of section i [1].

$$E = \frac{1}{8\pi} \sum_i \sum_{j \neq i} \frac{\boldsymbol{\xi}_i \cdot \boldsymbol{\xi}_j}{|\mathbf{m}_i - \mathbf{m}_j|} \tag{2.2}$$

One side-effect of this discrete simplification is that we neglect the theoretically infinite terms where $\mathbf{x}$ approaches $\mathbf{x}'$, or in formula (2.2), where $j = i$. This has the result that we may underestimate the total energy of such a vortex, and as a result, energies of vortices modeled in the integer lattice are not bounded below by zero.

3. Modeling on the Cubic Lattice

As was suggested earlier, a vortex can be modeled on the three-dimensional cubic lattice as a sequence of adjacent points. A *length N self-avoiding polygon* (SAP) in $\mathbb{Z}^3$ is a sequence of points $w_1, w_2, \ldots, w_N, w_{N+1}$ contained in $\mathbb{Z}^3$ such that $w_1, w_2, \ldots, w_N$ are all distinct, $w_{N+1} = w_1$, and the Euclidean distance $|w_{i+1} - w_i| = 1$ for $1 \leq i \leq N$. Define the *steps* of a length N SAP as the sequence $s_1, s_2, \ldots, s_N$ where $s_i = w_{i+1} - w_i$ for $1 \leq i \leq N$. Similarly, the *length N self-avoiding walk* (SAW) in $\mathbb{Z}^3$ as a sequence of distinct points $w_1, w_2, \ldots, w_N$ contained in $\mathbb{Z}^3$ such that $|w_{i+1} - w_i| = 1$ for $1 \leq i \leq N$, with the $N - 1$ steps defined the same way as with SAPs. Note that a length N SAP can be regarded as a length N SAW where the Nth point is a distance of one away from the first point. Finally, define *self-avoidance* in a length N walk or polygon to mean that points $w_1, w_2, \ldots, w_N$ are all distinct. A length N SAP is considered self-avoiding even though $w_1 = w_{N+1}$.

4. Probability Distribution

Before continuing, we will define the *Boltzmann probability distribution* of a set of states with associated energies. Let M denote the number of length N SAPs, and consider the set of M length N SAPs $\{x_1, x_2, \ldots, x_M\}$. Let $E(x_i)$ denote the energy of SAP x_i defined in (2.2). Then the probability of such a state occurring is given by

$$p(x_i) = \frac{e^{-\beta E(x_i)}}{Z}, \quad Z = \sum_{k=1}^{M} e^{-\beta E(x_k)}. \tag{4.1}$$

Here $\beta = \frac{1}{k_B T}$, where k_B is the Boltzmann constant and T is the statistical temperature; β is sometimes called the "coldness" as it is the reciprocal of the statistical temperature. Note that when $\beta = 0$, all states are equally likely, when β is a large positive number, then low energy states are more likely to occur, and when β is a negative number then higher energy states are more likely to occur. Using this metric, we can calculate or approximate the average energy of all SAPs of length N at a given coldness β or a given temperature T [1].

5. Monte-Carlo Transformations on SAPs and SAWs

We wish to be able to analyze energies of all length N SAPs. For relatively small values of N, we can enumerate and directly calculate their average energy per value of β. However, due to their exponential growth in count relative to N, this approach becomes quickly infeasible [4]. Therefore, the task becomes one of sampling as to properly approximate average energies by temperature.

One method of doing this is through a Monte-Carlo approach with a series of transformations that hopefully allow us to properly sample from the distribution of SAPs of length N. Given a starting SAP and a value for β, we attempt to perform a transformation, and then accept or reject the new SAP by the Metropolis-Hastings algorithm [7]. Although we don't know the exact probability of the current and next states, we know the ratio of the probabilities as the cumulative Z terms in (4.1) cancel out, as can be seen in (5.1) below. The algorithm states that if the ratio is greater than one, we immediately accept the new configuration, if the ratio is less than one, we accept it with probability of the ratio:

$$\frac{p(x_i)}{p(x_j)} = \frac{e^{-\beta E(x_i)}}{Z} \cdot \frac{Z}{e^{-\beta E(x_j)}} = e^{-\beta[E(x_i) - E(x_j)]}. \tag{5.1}$$

One set of transformations we wish to investigate are described in [**?**]. They define for SAWs in three-dimensions the inversion transformation, the reflection transformation, and the interchange transformation. They also prove that their set of transformations are *symmetric*, *aperiodic*, and *ergodic*. Given a starting SAW x_0, and then performing transformations such that for all $i \in \mathbb{N}$, x_i is created by a transformation from x_{i-1}, we have a chain of SAWs. The transformations are symmetric as the probability of some SAW x' occurring immediately before another x'' somewhere in the chain is equal to the probability of x'' occurring immediately before x'. They are aperiodic as there is a non-zero probability of any SAW occurring twice in a row in the chain. And the transformations are ergodic as given any starting SAW, there is a non-zero probability of eventually reaching any other SAW. Additionally, they perform modifications of continguous subsets of a given SAW, leaving the parts before and after the modified subset intact, making this algorithm suitable for modeling SAPs. These four features are important as they allow for a Monte-Carlo procedure to properly explore the entire space of length N SAWs or SAPs [**?**].

Another set of transformations is described by Wüst and Landau [8] and involves two types of moves: pull moves and bond-rebridging moves. Those are of interest as in addition to following ergodicity, they either displace a small segment or rearrange the steps while maintaining the same set of points. This can be helpful in the case when we are targeting minimal energy configurations when the SAPs are more likely to be small and balled up. With an already low-energy configuration, performing moves that incur larger changes are either likely to increase the energy resulting in a less desirable configuration or are more likely to displace in such a way that the resulting configuration is no longer self-avoiding [8].

In addition to a per-β sampling approach, the Wang–Landau sampling method [8] runs once and consequently allows us to estimate the average energy for any given β. Wang–Landau sampling would involve

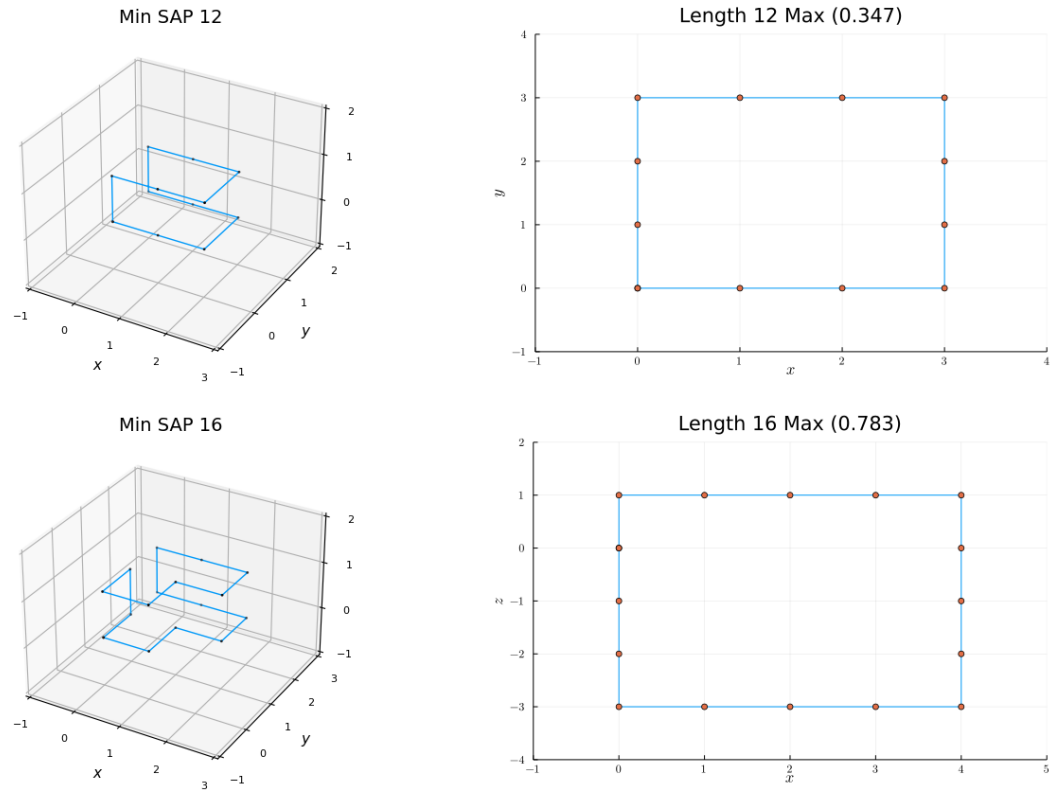

FIGURE 2. Minimum and maximum energy configurations for SAPs of length 12 and 16.

approximating the density of a given energy $g_N(E)$. More specifically, if $\{x_1, x_2, \ldots, x_n\}$ is the set of all length N SAPs, $g_N(E)$ is defined as the cardinality of the set $\{x_i | E(x_i) = E\}$ [8].

6. Finding Minimum Energies, Maximum Energies, and Average Energies

The number of SAPs of length N grows at an exponential rate relative to N, however there are less than seven-million of length sixteen [3]. So for shorter length SAPs, we completely enumerate and calculate exact minimum, maximum, and average energies across different values of β.

Figure 2 illustrates minimum and maximum energy configurations for SAPs of lengths 12 and 16. As can be seen and as follows for other lengths between 4 and 16, the minimum configurations are more condensed and balled up than the maximum configurations while the maximum configurations are squares of side length 3 and 4 respectively.

Figure 3 displays the curves for exact average energies of length N SAPs at β ranging from 100 to -100 with intervals of 0.5. As was hinted at before, higher β values result in higher probability of low energy configurations, and lower β values result in higher probability of high energy configurations. On each end of the curves, the energy values approach the maximum and minimum energy values. The length 4 plot is flat because the only possible SAP of length 4 is a square with side lengths 1.

7. Goals

As was mentioned earlier, we wish to replicate some of the results in [1] in their work of studying average, minimum, and maximum energies of vortices modeled as SAWs, but in the context of SAPs instead. Our first goal is to implement the set of transformations described in [**?**] and analyze their effectiveness in achieving the minimum and maximum configuration SAPs when β is set to a large and small value respectively. As

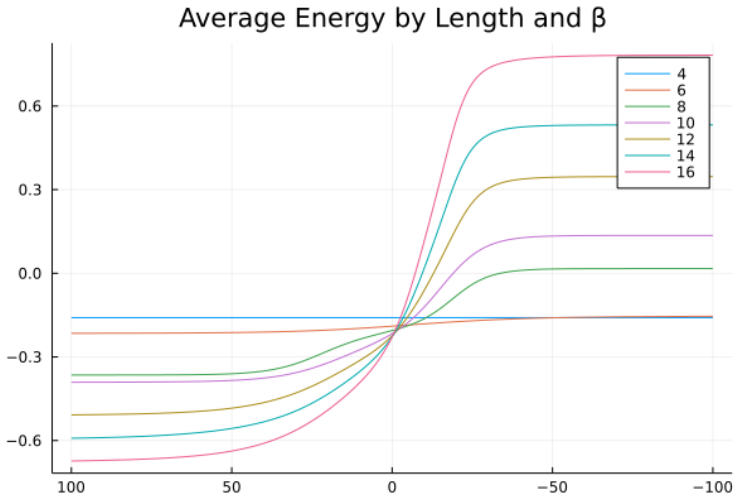

FIGURE 3. Exact average energies for SAPs of length 4 through 16 with β from 100 to -100.

is visualized in Figure 3, we should approach the minimum and maximum energies on both ends of the spectrum if the set of transformations allow us to properly investigate the space of length N SAPs.

Along the way, we wish to study the pattern of minimum and maximum energy configurations to see if they follow a pattern similar to the former work on SAWs [1].

Our first Monte-Carlo approach involves beginning with a high energy SAP x_0, say a square, and a large β value. Then after a series of burn-in transformations, we will run the transformations, accepting or rejecting at each step by the Metropolis-Hastings algorithm, for a set number of iterations recording the average energies. We then reduce β and repeat the process until we reach some minimum β value [1]. We are interested in looking at the curve of average energy versus β as is shown in Figure 3, and also recording the maximum and minimum energy configurations along the way.

An effective Monte-Carlo sampling technique will likely depend largely on the set of transformations used. We also wish to study and implement the pull and bond-rebridging moves described by Wüst and Landau to compare their effectiveness against the first moves mentioned. Specifically, we believe that the pull moves and bond rebridging moves could be used to find better approximations for the minimal and maximal configurations. Since pull moves have the property of possibly displacing one end of a SAW, we will need to investigate how they can be implemented for SAPs and if they still follow ergodicity. Similar questions may need to be asked for bond-rebridging moves.

We also mentioned the Wang–Landau method for approximating the energy density of a distribution, and we are interested in exploring how that method does at approximating average energy per β as it is more flexible in the sense that if it has run properly, it could calculate average energy for any β [8].

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