Eric, I have added some editorial changes in red in the text. I think it is pretty complete but, imagining myself as a reviewer, I find myself looking for specific conjectures to be proved. Granted that there are some in the text…perhaps they should be more visible. In the section about our work you might include some statements of things we hope to be able to show based on the statistical analysis you are doing. By the way, I was able to print the graphs. I have not tired to put the data in an excel file. What is the Connection between excel and SPSS? Have not yet had time to look closely at the graphs. Want to get this in the email tonight, well early tomorrow morning. Good luck getting all this done. Ken

Project Description

The object of this research is to find relationships between several measures of knot complexity and the structure of polygonal knot space. Recent research [Stasiak] uses polygonal knots as a model for knotted DNA to predict different DNA knots' relative velocities in gel electrophoresis. Results would provide mathematicians with insight into the structure of knot space and let scientists test the existing model and develop new models for similar macromolecules.

This grant has been split into three sections, each of which describes a particular project. In the first project, Ken Millett and I will study the relationship between knot space, polygonal rope-length [Rawdon], MD-energy [Simon], knot probability [Millett], and other spatial measures of polygonal knots [Millett]. In the second project, I will analyze relationships between two different measures of polygonal thickness [Rawdon, Stasiak] and the MD-energy [Simon]. In the third section, we will present projects that will be completed by undergraduates related to the goals of sections 1 and 2.

Knot Energies and Knot Space

For a fixed n, let Geo(n) be the space of based oriented n-sided polygonal knots and Equ(n) be the space of based oriented n-sided equilateral polygonal knots. Geo(n) and Equ(n) can be naturally embedded in $\sum^{3n}$ by simply listing the 3-dimensional coordinates of the vertex points in the order determined by the basepoint and orientation. The connected components of the two spaces consist of knots of the same topological knot type and define the respective geometric knot type. However, Calvo [Calvo] has shown that there are more connected components than there are topological knot types for the cases of n=6 and n=7. For example, there are two connected components of right-handed trefoils in Geo(6) and two connected components of figure-eight knots in Geo(7). Cantarella [Jason] and ??? [???] have found a non-equilateral topological unknot that cannot be deformed to a planar unknot without changing edge lengths. The spaces of geometric knots have a structure that is much different than the structure of smooth topological knot space. Scientists [Stasiak][others???] are using polygonal knots to model the behavior of knotted DNA and polymers. To large extent, knots on the cubic lattice have provided insight into local and global knotting of polygons, in particular into the probability of knotting as the length of the knot increases without bound. However, the spaces Geo(n), Equ(n), and others spaces of polygons created by restricting the vertex angles, restricting the ratios of edge lengths, or restricting the distance between non-consecutive edges provide a more realistic model of these macromolecules. Points in these conformation spaces, i.e. knots, are the solutions to algebraic equations and inequalities involving the vertex coordinates. As a result, these spaces are manifolds and algebraic varieties. Because of the sheer number equations and inequalities needed to describe the spaces for even for small n, it is improbable that the connected components of the spaces can be described using the traditional topological analysis of homologies and cohomologies. However, Monte Carlo and numerical analyses of polygonal knot energies and other spatial quantities provide an alternate path to unerstanding the structure of these spaces.

To determine the actions of enzymes, such as topoisomerases, on DNA, it is necessary to know what knot types are "near", that is require a few small scale crossing changes to connect each other in knot space. Endowing the conformation spaces mentioned above with the sup norm, we can create conformational metric spaces. This provides us with a finer definition of being "near." The question remains focused on determining which knots are close in the conformation space. Given an n-sided polygonal knot K , what is the shortest distance to a knot of a different knot type? In other words, what knots lie in the intersection of the conformation space and spheres of different radii centered at K? For example, suppose that K is a regular 100-gon with edge lengths of 1 in Geo(100). The first singular knots occur at a distance of 1 from K. However, since the knots at this distance correspond to Reidemeister I moves, the knot type has not yet changed. As the radius increases, one encounters "small trefoils", "small" figure-eight knots, etc. On the other hand, if K' is an equilateral 100-gon twisted to look nearly like an 8 (which would be singular), the first singular knots one encounters actually have a different type of crossing change. Along similar lines, suppose that K is a trefoil in a fairly standard 3-dimensional conformation. At the distance that the first singular knots are encountered, the knots will still be of an equivalent knot type corresponding to a Reidemeister I move. However, if K' is a trefoil which has been distorted to have two of its "foils" very close to each other, one encounters unknots at small distances from K'. Therefore, the knot types that are nearby to K are a function of both the edge lengths of the knot and a self-distance of the knot, that is the distance between distal (with respect to arc length) pairs of edges. In [Rawdon], we define the thickness of a polygonal knot as the minimum of this self-distance and a quantity that measures the bending that occurs at the vertices. In this project, we will analyze the knots that are encountered as the radius increases.

From the above examples, we see that nearby knots can exhibit "additional" knotting in the form of connect sums with "small" trefoils or more large-scale changes in the knotting. Our first question to answer is, what can we say about knots at distance r from K in terms of n, the knot's thickness, and the lengths of the edges? For what r do we see local knotting in the form of connect sums? For what r do we see local knotting in the form of satellite knots that are not connect sums? When do we see more large-scale changes in knotting? The asymptotic behavior of knot probabilities in relation to small and large-scale knotting on the cubic lattice have been studied extensively [Stu and the Gang, Nardo]. However, the small and large-scale knotting changes that occur as a result of perturbations of a particular conformation is yet unstudied. Monte Carlo analysis for random and biased perturbations will be employed to study the probability of the knotting changes at sufficiently large distances from a given knot. In this project, we will restrict our attention to Geo(n) and Equ(n) for n=6, 7, 8, 16, 32, and 64. Millett and Bruce Ewing's [Knotscape] program for computing the HOMFLY polynomial of polygonal knots will be the tool used to determine the knot type, to the extent that this polynomial distinguishes the knot type, of the knots realized at the different distances. For a fixed n and knot type K, we have also conjectured that a thickness-maximized polygonal knot is the conformation in K that is the largest distance from the large-scale changes in knotting. In other words, a thickness-maximized knot is in the "middle" of the "widest" part of its connected component and, as such, is an "average" of the knots in that component. This would provide a convincing argument for the nearly linear relationship that Stasiak, et al [Stasiak] exhibited numerically between the writhe of randomly generated knots and the writhe of the thickness-maximized conformation.

One important application of this exploration of the local structure of knot space is the study of type II topoisomerases which catalyze strand passages between DNA segments, modeled as polygonal knots, to change the global topology of the molecules. Global changes in the DNA's topology result from enzyme reactions on a small scale. By understanding the consequences of random perturbations to polygons, we will determine to what extent these changes are possible.

Theoretical Relationships between Polygonal Energies

While the first knot energy [Fukahara] was defined for polygonal knots, most recent theoretical work has been related to energy functions for smooth knots. The polygonal energies have been responsible for the computational results that inspire further research in Physical Knot Theory, although little has been studied in relation to the polygonal energies themselves. Theorems which bound one energy as a function of other energies provide information about the interplay between the different quantities [Buck, conformal]. However, no such theorems exist for their polygonal counterparts. Since many of the insights that spur that theorems for smooth knots lie in the computations performed on polygonal knots, it is natural to ask if the same bounds hold for the polygonal energies. Of particular interest in the field are the conformal energy, a variation on the idea of electrostatic force [O'hara 1-4, Ideal, Freedman 1-2], and the rope-length energy. The conformal energy of K is $\iint_{K\times K} \frac{1}{|x-y|^2} - \frac{1}{arc(x,y)^2}$, where $arc(x,y)$ is the minimal arclength between *x* and *y*. The rope-length [lsdr] energy is best understood by first defining the thickness of a knot. For a unit-length knot K, the thickness of K is the supremum of the radii such that no two disks of the given radius normal to the knot intersect. In other words, the supremum of radii such that a non-self-intersecting tube of that radius can be placed about the knot. The thickness of a non-unit-length knot is the ratio of this supremum to the knot's arclength. The rope-length energy of a knot is the multiplicative inverse of its thickness and measures the amount of arclength needed to tie the conformation with a non-intersecting tube of radius one about the knot. The rope-length energy was defined to model the length of one-inch radius rope needed to tie the knot. Rope-length defined in this and other similar fashions have been studied extensively for the smooth case [lsdr,lsdr2, buck nature, maddocks, devr1-3] and for the polygonal case [me,me,me,maddocks,Stasiak,poland]. In particular, the minimal rope-length energy of the knot type (and the average crossing number of that conformation) was shown to be almost linearly related to the relative velocities of DNA knots in gel electorphoresis [Stasiak 1-4] for a small set of knots. Later research indicates that the relationship is more complicated [Buck, Jason]. In [Buck], the symmetric and normal energies, variations on the idea of heat radiating from a tube about the knot, of a knot conformation was shown to be bounded by 11 times the rope-length energy to the 4/3 power. In [conformal], the conformal energy was shown to be bounded by 5 times the rope-length energy to the 4/3 power using an improved argument along the same lines. Discretizations of these energy functions should have similar bounds. The discretizations that will be studied are the minimum-distance energy [Simon] for the conformal energy and the polygonal rope-length function defined by myself [Rawdon]. The arguments used to prove these results rest on fixing a point on the knot and analyzing what length of the knot can lie in spheres of varying radii centered at the point. The smooth rope-length energy guarantees an impenetrable tube about the knot that uses up the volume in these spheres. However, in the polygonal case, cylinders about near-neighboring edges are allowed to intersect. In fact, in the case of a regular n-gon, for large n, the cylinder about one edge will intersect half of the cylinders about other edges. The first task for this project will be to prove that a 4/3 argument does work for these polygonal energies.

An alternate definition of polygonal rope-length is used in [Stasiak12] to provide a wealth of interesting numerical observations related to physical behavior. The cylinder thickness of a unit-length knot is the supremum over all radii such that the cylinders of that radius about any two non-consecutive edges do not intersect and the cylinder rope-length is its multiplicative inverse. The SONO algorithm, an efficient deterministic algorithm for finding rope-length minimizing conformations, was developed to provide data for subsequent studies [Stasiak3-5]. While the cylinder rope-length energy has been used extensively, it has not been the object of any intrinsic study. The polygonal rope-length energy from [me,me,me] was shown to approximate the rope-length of a smooth curve in [me,me]. Still, many of the standard theorems about polygonal energies have not yet been proven. The second task of this project is to prove several theorems about the cylinder rope-length energy and the polygonal rope-length. Namely, that there are only finitely many knot types with rope-length less than any fixed value, any sequence of polygons converging to a singular knot (which is not a single point) has unbounded cylinder rope-lengths, and that cylinder rope-length is bounded below by a function of the crossing number. The polygonal rope-length from [me] can also be generalized to a one-parameter family of rope-length energies by varying the contribution of the "curvature" occurring at the vertices. The third task of the project is to find the relationship between the one-parameter family and the cylinder rope-length.

Student Contributions to this Research

There are several projects related to the research explained that are accessible to undergraduate students and where their work will make a significant contribution to towards the goals of this project.

Project 1: Exploring the changes in the minimizing conformations for various parameter values of the family of rope-length energies.
A student will use existing software [toros] to explore the effect of changing the value of the parameter. In particular, for a fixed n and a fixed knot type K, how does the value of the parameter change the knot conformation. Using various measures of the spatial attributes from the first portion of this grant, how do the conformations compare to each other? Further, the student will compare the data obtained with data produced from the above studies. The student may have the opportunity to create conjectures and prove theorems related to their observations.

Project 2: Writing software that integrates the use of all of the polygonal energies.
Algorithms exist and software is available to compute the different energies and to find energy minimizing conformations. For example, the minimum distance energy [simon] is integrated in Ming [ming], written for SGI workstations. TOROS, KnotPlot, and Evolver can be used to determine several other knot energies, but no one piece of software is available that can find energy-minimizing conformations for all of the different energies. In particular, to find rope-length and energy minima for equilateral knots in [millett], simulated annealing is used with random crankshaft rotations. This program will make this technique available for all of the energies.

Project 3: Parallelizing of existing code.
To make use of today's supercomputing power, code must be parallelized. Some or all of the code from the above project will be parallelized and tested at the Pittsburgh Supercomputing Center. Further experiments related to energy minimization can then be scheduled.

Project 4: Physical experiments on knots.
This year, two senior mathematics majors at Chatham are collaborating with me on physical experiments on models of polygonal knots. Knots were created by string together 32 thin 7/8 inch long copper jewelry beads to simulate a 32-edged polygonal knot. Our goal is to create a simplified simulation of gel electrophosesis. First, we are going to drop the knots through a 3 foot long tube filled with sugar water and time their descents. Next, we will do the same experiment except we will add a bubbler at the bottom of the tube to create some turbulence. Then we will construct a pegboard and time the descents for several different slopes of the board. When we get the information, it will be compared to the data from [millett]. There are several questions that other experiments can address. How does the bubbling rate affect the descent? How does the slope affect the rate of descent? If we change the materials, how does this affect the results? How do the experiments compare if one uses rope to model a smooth knot? How can we do similar experiments for knots with restricted vertex angles or sides with varying lengths? This year, we will attempt to find one set of experimental parameters that give us some data. Subsequent studies will find relationships between the parameters.

Longer Terms Goals

The ultimate goal of this research is to better understand the knotting and tangling that occurs in natural systems. At this time, we do not have all of the tools necessary for understanding small and large-scale changes that result from rather small perturbations to a knot. This project is a first step towards understanding the relationship between physically measurable knotting and more the mathematical models that are used to model the behavior. This is a difficult mathematical problem that is pertinent to simple scientific understanding.