Interactive Scientific Visualization of Polygonal Knots

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Abstract

This paper presents our work in the development of a scientific visualization package for interactive manipulation of gel electrophoresis simulations. The simulation is meant to explore the possible correlation between the behavior of physically polygonal knots and that of DNA loops in gel electrophoresis experiments. Of particular interest in this research is the design and implementation of a real-time interactive 3D visualization of the gel electrophoresis simulation.

Introduction

A knot is a closed curve in 3 space. You could imagine a string wrapped and coiled around itself with the two ends joined in a seamless connection. Polygonal knots are knots that use straight-line segments; much like the jump ropes with plastic segments that are often used in elementary school. Knot topology is the study of knots. This field of study was considered purely abstract until the discovery of the shape and behavior of DNA. DNA is actually a closed curve, just like the theoretical knots and exhibits some interesting geometric properties that may mirror those of polygonal knots. If knot-theoretical models can be used to predict DNA behavior, then we have a wide variety of theories, properties, and tools we can then apply to the study of DNA.

One of the fundamental properties of a knot is a measure of its compactness or tangledness. The *energy* [1] of a knot quantifies this property where higher knot energies correspond to more compact knots. A high-energy knot is comparable to a closed knotted loop of string that is crumpled into a tight ball while a low-energy knot is that same loop of string extended into as large a 3 dimensional space as possible. The image to the left in Figure 1 shows a trefoil knot in a high-energy configuration while the right-hand image shows the same knot in a low-energy configuration.

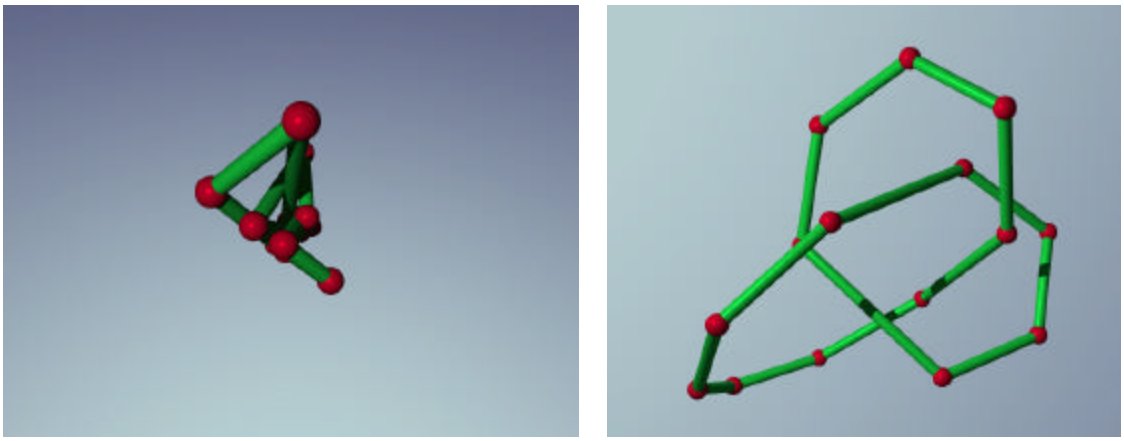

Figure 1: Low energy trefoil conformation on the left. High-energy trefoil conformation on the right.

The energy of polygonal knots of the same type is dependent upon both the number of line segments contained by the knot and the compactness of the knot. For any particular knot, however, the knot energy is solely dependent upon its compactness. A knot is said to have been relaxed if it is in a minimal energy conformation. The trajectory or behavior of the knot as it moves from a high-energy state to a low-energy state may predict DNA movement in gel electrophoresis. The intent of this research is to develop visualization tools that will allow scientists to explore this possible connection.

Background

Jonathan Simon has proposed a polygonal knot energy function [1] that is formally defined in the following paragraphs.

Let **X, Y** be disjoint line segments in $\hat{\mathbf{A}}^3$. Then the minimum distance between **X** and **Y** is a positive number that we denote by **MD(X,Y).** Letting |**X**| denote the length of a segment **X**, define the *energy* **U** between line segments **X** and **Y** to be

$$U_{x,y} = \frac{|X| \bullet |Y|}{MD(X,Y)^2}$$

The disjointed property is required since the denominator becomes zero if the lines segments intersect at any point. This implies that the energy between two connecting line segments becomes infinite. The above term describes the energy contribution of a single pair of line segments to the total knot energy. The total energy of a knot **K** is the sum of all possible combinations of such disjoint line segment pairs and is defined as

$$U_K = \sum_{Non-Adjacent-Segments-X,Y} \frac{|X| \bullet |Y|}{MD(X,Y)^2}$$

Since the knot energy is inversely proportional to the square of the minimum distance between line segments, the knot segments are *self-repelling*. As knots move from high-energy to low-energy states line segments seek to remain as far from every other line segment as possible without breaking the knot. This energy function is also scale invariant, that is, the knot energy doesn't vary if the knot is scaled either up or down.

Physically based computational modeling of knots seeks to describe the behavior of a knot as it moves from a high energy conformation to a low energy conformation in the presence of external forces while following a reasonable physical interpretation of motion.

Motivation and Problem Statement

Although the study of polygonal knot energy is interesting as a purely mathematical notion there has been a great deal of work in recent years [1][3] in attempting to correlate polygonal knot behavior with that of DNA. Of particular interest in this proposal is the possible correlation between the behavior of physically real polygonal knots and that of DNA loops in gel electrophoresis experiments.

Gel electrophoresis is process that uses an enzyme to parse a strand of DNA into smaller segments. Those segments are set in gel solution. By applying electric current, the various DNA segments are moved various distances in the gel, depending on their sizes.

The laboratory utility of gel electrophoresis as a measurement tool is well known. But as we get deeper and ask, “What are the mechanisms involved in gel electrophoresis?” questions remain unanswered. Other questions include "What is the conformation of DNA in solution?" (The conformation is the geometry of the DNA segment, or how it looks.); "What are the mechanics of DNA traveling through solution?" and "Can knot-theoretical models predict DNA behavior?"

To answer these questions we are developing a computer model of gel electrophoresis using polygonal knots as a model of DNA. The gel is modeled as a series of randomly oriented sticks placed in three-space. These sticks are fixed in space and provide a coarse approximation to the physical structure of agarose gel. Knot movement through the gel is determined by the self-repelling energy function of the knot in combination with rigid-body collision handling and the application of an external applied force that moves the knot through the gel.

While this project is large in scope our research is limited to the challenge of visualizing and interacting with this dynamic computational simulation. The work includes the development of a useable graphical user interface allowing dynamic control over the simulation as well as integrated network capabilities. The following section describes our work and provides implementation decisions made along the way.

Implementation

Efficiency

First, we want the simulation to be visualized in real-time which requires a high degree of computational efficiency. The DNA is modeled as a polygonal knot to which physical attributes have been ascribed. Each edge is given a "mass" which is proportional to its length with respect to the total knot length. Force is exerted by each non-adjacent knot edge. The force is applied along the vector formed by the minimum distance between two edges, MD(X,Y), with a magnitude that is proportional to the energy exerted between the two edges. Computing the movement of the DNA through the gel then requires the following general steps:

1. Compute the applied forces between all pairs of disjoint knot edges
2. Detect any knot collisions with gel edges and adjust the applied forces accordingly.
3. Move the knot vertices along the vector defined by the applied forces by an amount proportional to the applied force

The computational demand of step 1 above is characterized by a quadratic growth rate dependent upon the number of sticks contained by the knot. Our code maintains explicit data structures representing relationships between edges that, although enhancing computational performance, results in a quadratic increase in memory requirements.

Step 2 can essentially be characterized as a search algorithm. In the brute force approach we examine all gel-edges for a collision with any knot edge. If such a collision is detected we then model the collision as a repelling spring-force that increases with the inverse of the distance between the segments. Since in a typical scenario there are on the order of 50 thousand gel segments, most of which are not in collision with the knot, there is a need to optimize the collision detection subroutine. We have chosen to use oct-trees as a convenient speed-up of this search process.

Oct-trees are a well-known way of hierarchically organizing spatial data and allow for fast regional searches. Instead of querying every gel edge for a possible collision with every knot edge we first find all gel edges within a radius $R_{collision}$ of the knot center. The radius $R_{collision}$ is determined by R_k, the distance from the geometric center of the knot to the knot vertex furthest from the center, plus R_e which is one-half the length of the longest gel edge. No gel edge can be in contact with the knot if it lies outside of this region. Figure 2 gives a simple illustration of this idea.

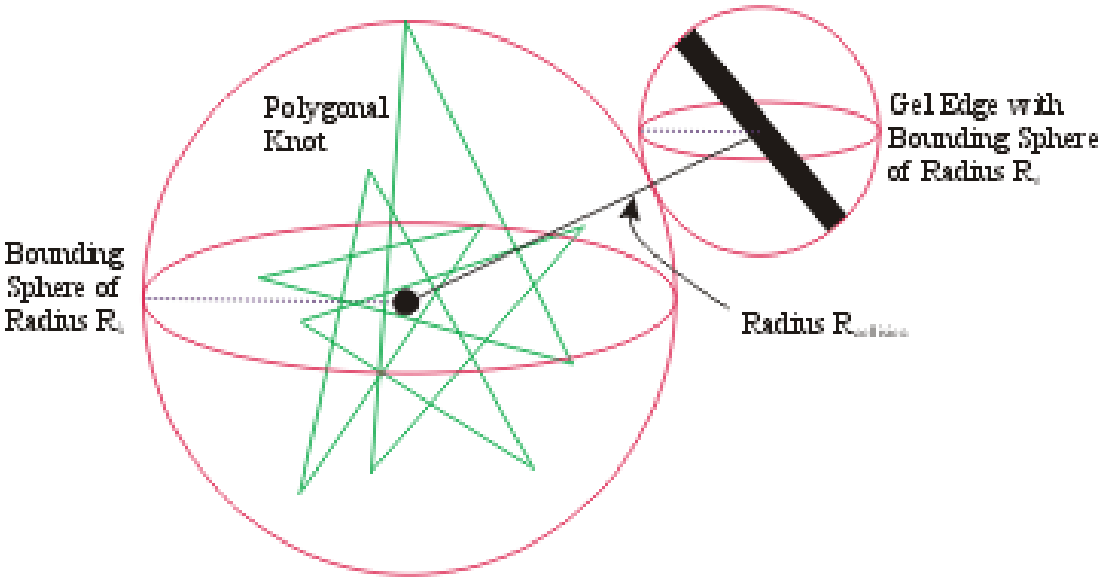

Figure 2: Finding gel edges that may be colliding with the polygonal knot

The set of all gel edges within radius $R_{collision}$ of the knot center is much smaller than the set of all gel edges within the simulation. Finding this set of gel edges is efficiently performed via oct-tree searches and the algorithm proceeds by determining if any gel edge within this regional set is in contact with the knot.

Finding the set of all gel edges that fall within a radius R of the knot center takes time proportional to the log of the number of edges in the simulation. This dramatically reduces the computational time required for collision detection. Other, faster collision detection schemes exist but incur a much greater implementation cost. Our method is comparatively easy to implement and provides adequate real-time results.

Visualization and User Interface Design

We want our visualization to be in real-time, 3 dimensions. We've chosen to implement our application in Java3D. Java3D is a standardized add-in to the Java programming language and is meant for developing real-time interactive 3D graphical applications. This package works seamlessly with the standard Swing components and, in addition to leveraging Java's excellent GUI packages, the use of Java3D also allows us to benefit
-in support for networking and synchronization.

We also wish to have interactive control of the simulation. We want the ability to stop the simulation in progress, add or subtract features or change parameters, and then continue with the simulation. We need a well-designed GUI – Graphical User Interface – with buttons and windows to make these modifications.

Figure 3 is a screenshot of our application and gives an overview of the type of control that users can exert over the simulation. The panel shown on the left is used to control

the appearance (colors, material, and lighting) of various simulation entities including the knot edges and vertices, gel edges, and background color.

The panel shown on the right allows users to control much of the appearance of the application as well as controlling various parameters of the simulation as it progresses. Gel edges, knot edges, bounding spheres, applied force vertices, and other visualizations can be dynamically enabled and disabled. These components utilize standard Java Swing components and seamlessly integrate with the Java3D visualization package.

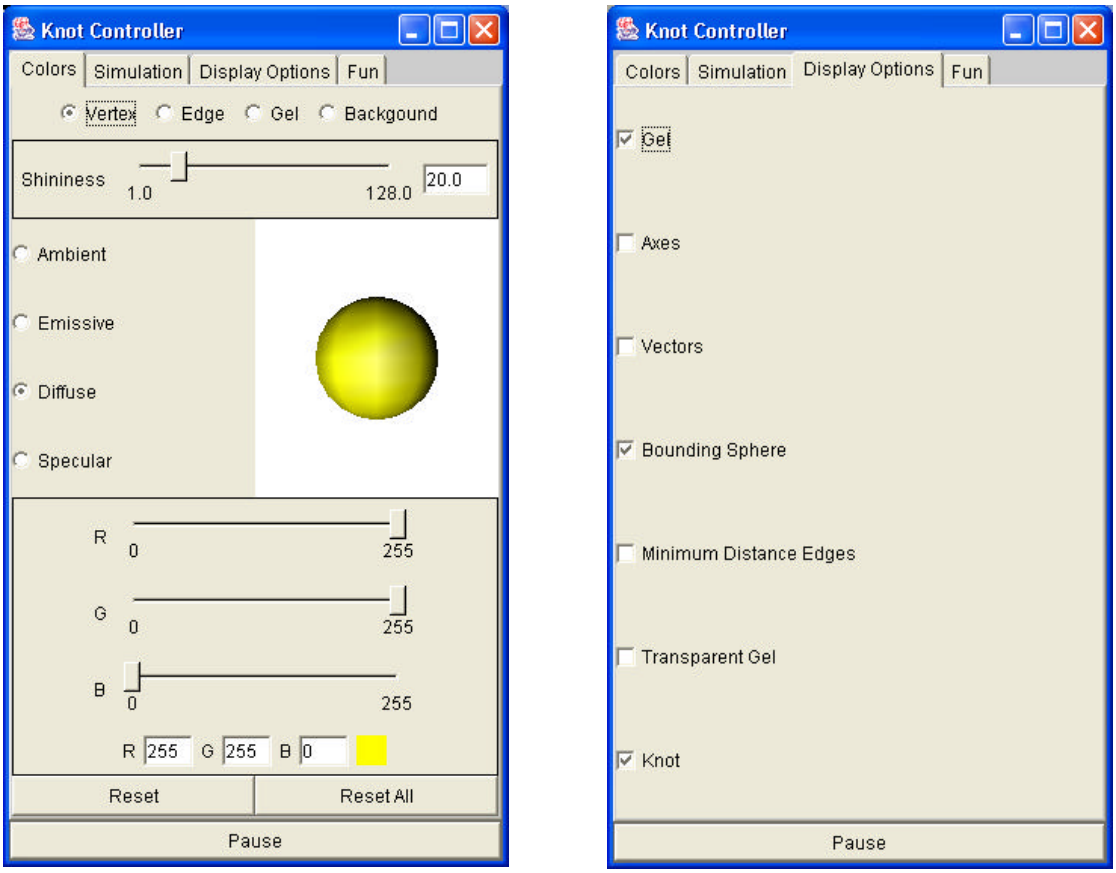

Figure 3: Screenshot of the main control panels. The panel on the left is used to adjust colors of the knot vertices and edges, the gel edges, and the background. The panel on the right is used to either display or hide various entities of the simulation.

Figure 4 shows a large screenshot of our primary visualization window. It depicts a DNA strand, modeled as a polygonal knot, embedded in a field of gel obstructions. The knot is always centered in this window but left-clicking and dragging the mouse within the window can dynamically change the viewpoint. The view can also be zoomed by alt-left clicking and dragging within the window. The knot edges are blue with yellow vertices; the gel edges are red and the knots bounding sphere is also drawn to aid in understanding the perspective of the various entities.

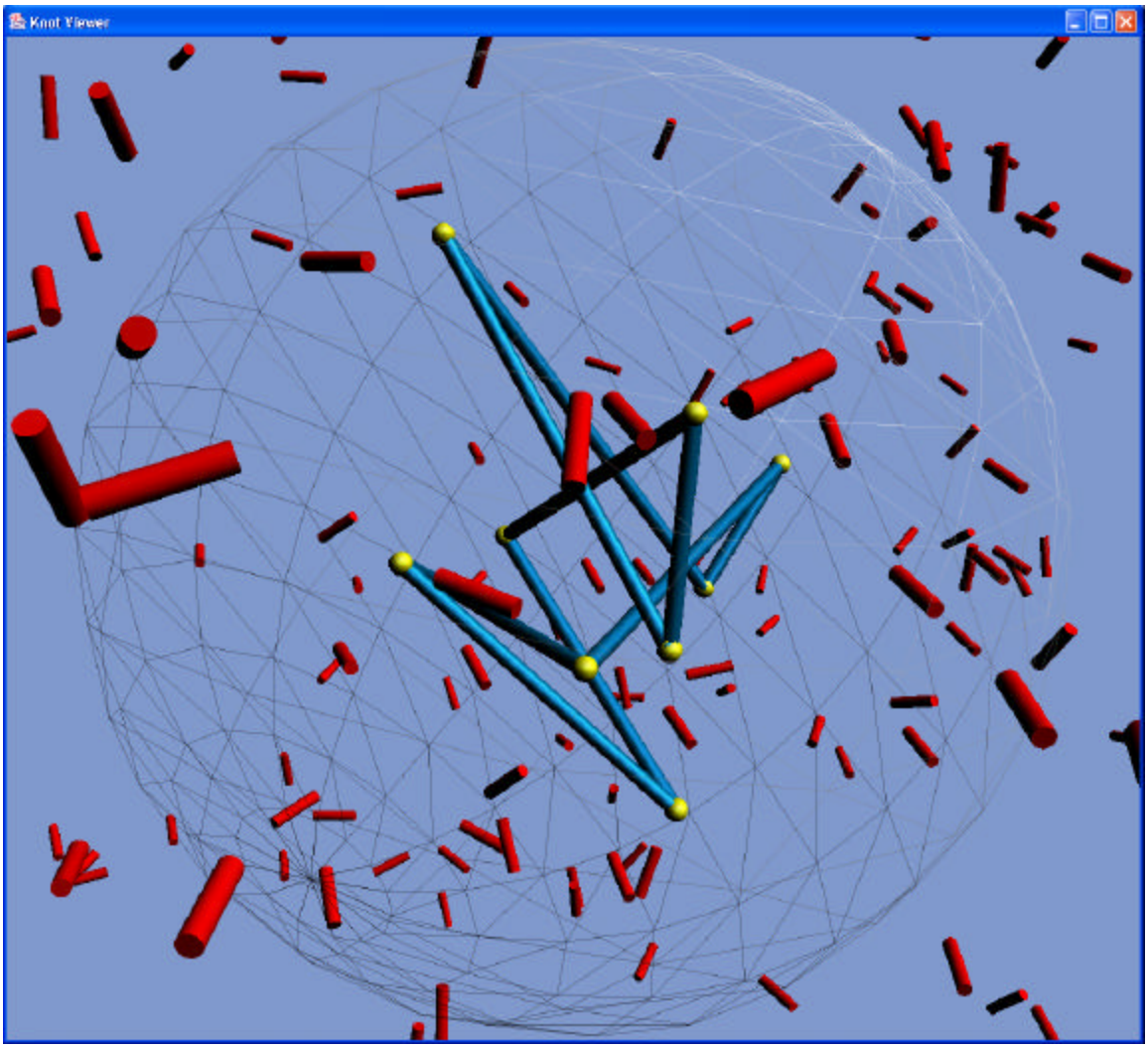

Figure 4: Screenshot of the primary visualization window. The "DNA" is modeled as a polygonal knot and rendered with blue edges and yellow vertices. The red sticks represent gel and the knots bounding sphere is enabled.

Remote interaction

Fourth, we want to have remote interaction with the simulation. Because the simulation model is so computationally expensive, desktop PC's do not have the power to perform a real-time simulation with large data sets. We envision that the computation will take place on a central high-powered compute server and for the visualization and interaction to take place on a remote client. This feature has not yet been developed and is a good area for future research.

Conclusion

Our research is a work in progress. We have developed visualization and control software for a computationally demanding scientific simulation of DNA strands in gel electrophoresis.

We anticipate splitting the software into a client-server architecture that will allow large simulations to be executed via a compute-server and controlled and viewed with a remote client on a stand-alone PC. We also anticipate interesting work in correlating real-world gel electrophoresis experiments with our simulated runs in an attempt to discover whether knot-theory can be applied in any way to DNA behavior.

References

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