SOAR Research Proposal – Summer 2013

Project Information

Title: Locked and Unlocked Chains in 3-Space
Student: Alicia Altemose
Faculty mentor: Kevin Hartshorn, Associate Professor
Department: Mathematics and Computer Science

Start date: May 28, 2013
Duration: 10 weeks

1 Description of Project

We will examine a geometric model of protein folding. Long chains of proteins can be modeled as chains of line segments in 3-dimensional space. One fundamental— and still open — question is whether a given path of line segments can be "straightened". There are known examples of chains that are "locked," or stuck in a knotted form. There are also known conditions upon which a chain can always be straightened. Open questions are essentially of two types: *Under what conditions can we guarantee a chain is (un)locked?* and *What is the computational difficulty of deciding whether a chain is lockable?*

For our project, we will focus on finding conditions under which a chain can be straightened (or proven to be locked). Specifically, we will look the following questions.

1. Can an equilateral chain (that is, a chain for which all segments are the same length) be locked?
   A protein chain can be approximated by a chain of segments all of which are the same length (or the same length up to some error factor). While there are examples of locked chains, it is not known whether there exists such an equilateral chain of segments that is locked in 3-space, although any locked chain is known to require at least 6 segments [1].

2. Can a fixed angle chain (that is, a chain that fixes the angle between segments, but allows adjacent segments to pivot around one another) be straightened (in this case, meaning that the chain can be flattened into a planar configuration)?
   Just as the segments modeling a protein chain will likely be the same length, the bonds between molecules often have a fixed angle. Thus we will also look at examples of chains with restricted angles between segments, in order to model the fact that molecular bonds can be bent slightly, but have a preferred angle. Demaine and et al. [4] have developed a notion of *producability* that is equivalent (under certain conditions) to the notion of straightenability. This producability — essentially a notion of building the chain by a virtual machine — provides an interesting technique for us to explore examples of chains having restricted angles.

Our work will focus on developing examples to better understand the mechanics of locked chains. Through our examples, we plan to develop some conjectures on conditions that determine whether or not a chain can be straightened. These will be pulled together into an article by the end of the summer that will be presented to an journal of undergraduate mathematical research (such as the Rose-Hulman Undergraduate Mathematics Journal).

2 Roles and Responsibilities

This is a topic that is new to me. While I have done research on folding algorithms, I have not specially looked at folding 1-dimensional models (i.e.: chains). However, my interest in questions on computational origami together with Alicia's interest in both mathematics and chemistry should provide an excellent groundwork for our summer project. Further, this project grows out of an expository paper that Alicia wrote for my Computational Origami course — a special topics course taught in the Fall of 2012.

Initially, we will be reviewing research on the topic, working together through several papers that demonstrate the techniques used in proofs of known theorems. I will lend my expertise to help fill in needed background in algebra and geometry to understand and work with the given papers.

After some initial reading, we will begin to develop examples in order to address the open questions in the project description. Alicia's role will be to develop new examples, begin to think about conjectures based on our examples, and write the results of our work. My role will be to help put the examples in the context of the current research, work with Alicia to develop proofs of our conjectures, and to aid in the editing/revision of the written results.

2.1 Time-frame for project

- **2–3 weeks:** Initial review of the literature. We have an initial selection of articles (see citation list) to work through based on Alicia's work in my special topics course in the Fall of 2012. See section 3 for more information about Alicia's previous work on the topic.
- **4–6 weeks:** Development of examples and conjectures. This will form the bulk of our research work, trying to make a positive statement on the potential for straightening given chains.
- **1–2 weeks:** Writing and checking our results. While we will be recording our observations throughout the summer, this time will be needed to put together an article and revise for accuracy and readability.

3 Engaging the student in scholarly research

With her mixed interest in both chemistry and mathematics, this topic appeals very specifically to Alicia. In a special topics course Computational Origami in the fall of 2012, Alicia conducted independent research on the topic of polygonal protein chains. By the end of the semester, she put together an excellent expository essay on the topic of 1-dimensional chains. It is largely through her work on that project that she developed an interest in conducting more substantial research on the topic.

Her ability to conduct independent research was quite evident in her fall research project. She was able to track down very relevant papers on the topic and worked hard to understand the techniques and methods laid out in those papers. The summer SOAR project would be an excellent opportunity for her to focus on these techniques with more direct help from me. We are optimistic that we can use our time over the summer to do more than simply work through the latest research — our time this summer will provide her the opportunity to develop her own examples and theorems, generating her own knowledge on the topic.

4 Contribution to the discipline

As mentioned in the description of the topic, there are still interesting open questions in 1-dimensional chains. By developing new examples we plan to begin addressing some of these questions.

Alicia will be able to present her work over the summer in several venues. In addition to Scholar's Day, Alicia will likely present her findings at the Moravian Student Mathematics Conference and at the EPaDel section meeting of the Mathematical Association of America. We also plan to submit our findings to one of several outlets for undergraduate writing in mathematics (such as the Rose-Hulman Undergraduate Mathematics Journal).

5 Budget Items

The only costs we project for materials are incidental copying costs (printing documents from Interlibrary Loans, copying chapters from books, etc.). Thus we are not asking for any additional money for supplies or travel.

References

[1] Therese Biedl, Erik Demain, Martin Demaine, Sylvain Lazard, Anna Lubiw, Joseph O'Rourke, Mark Overmars, Steve Robbins, Ileana Streinu, Godfried Toussaint, and Sue Whitesides. Locked and unlocked polygonal chains in three dimensions. *Discrete Computational Geometry*, 26(3):269–282, 2001.

[2] Jason Cantarella and Heather Johnston. Nontrivial embeddings of polygonal intervals and unknots in 3-space. *Journal of Knot Theory and its Ramifications*, 7:1027–1039, 1998.

[3] Thomas Creighton, editor. *Protein Folding*. W. H. Freeman & Co, June 1992.

[4] Erick Demain, Joseph O'Rourke, and Stefan Langerman. Geometric restrictions on polygonal protein chain production. *Algorithmica*, 44(2):167–181, February 2006.

[5] Eric Demaine and Joseph O'Rourke. *Geometric Folding Algorithms: Linkages, Origami, Polyhedra*. Cambridge University Press, 2007.

Title of Project: Locked and Unlocked Chains in 3-Space

Name: Alicia Altemose

Major: Mathematics, Chemistry

Date of Graduation: May 2014

Faculty Mentor: Dr. Kevin Hartshorn

Requesting On-Campus Housing: Yes

My Rationale:

I wish to participate in this project for many reasons. In Fall 2012, I was a member of Dr. Hartshorn's Computational Origami class when I first learned of linkages and locked chains, a series of links that can't be straightened. I was fascinated with the topic and spoke with Dr. Hartshorn about working with locked linkages in further detail. I have little experience with large scale research, especially in mathematics, and I would like to enhance my studies in this kind of professional atmosphere. In addition to my hopes of learning about performing academic research alongside an experienced faculty member, I have further interest in the applications of this topic. While locked linkages and chains are interesting, applying their characteristics and properties to protein folding appeals to both of my majors and interests.

In my initial research of chains and linkages as a student in Dr. Hartshorn's Computational Origami class, I learned of the similarities between protein structure and fixed angle chains: linkages that have the same rigid angle at each joint. As a mathematics and chemistry major, I was instantly intrigued. While I hope that this summer research project provides a geometric basis for and mathematical models of general linkages and chains that I can later apply to the kinetics of protein folding in my potential future Honor's project, I understand that this project will have its own individuality and merits. There are many open questions in the field of locked chains and linkages, and Dr. Hartshorn and I hope to scratch the surface of one of the most popular questions, dealing with whether or not chains with certain numbers of links can become locked. This question is important to the field of linkages and planar geometry in general, and our hopeful contribution to the field would consist of finding examples to demonstrate different types of the unlocked chains and develop basic proofs on our examples.

Expected Outcomes

On a general level, I expect to learn professional research collaboration techniques and how mathematicians perform and document their research. I also expect to learn more about giving professional presentations of my progress, both written and oral. In terms of the specifics of the project, Dr. Hartshorn and I expect to test multiple examples of different length or angled chains for locking capabilities, research other mathematicians' progress on the topic, and prove some theorems related to classes of chains that are or are not locked. We hope to add to the compilation of tested examples as a part of solving this open question in planar geometry by developing conjectures based on our general examples and then proving these conjectures in order to write basic theorems. Overall, we expect to learn from current researchers' methods and possibly develop our own methods for testing examples in hopes of contributing to the answering of this question.

Finally, my own personal expectation for this project is to use it as a mathematical foundation for my potential Honors project which will combine these geometrical ideas and properties of chains with the kinetics and computational simulations of protein folding. Overall, I really hope to use this project as a learning experience in professional research and presentation, regardless of my decision to pursue an Honors project or not.