CALIFORNIA STATE UNIVERSITY, NORTHRIDGE

PROTEIN FOLDING: PLANAR CONFIGURATION SPACES OF DISC ARRANGEMENTS AND HINGED POLYGONS: PROTEIN FOLDING IN FLATLAND

A thesis submitted in partial fulfillment of the requirements
For the degree of Master of Science in Mathematics

By

Clinton Bowen

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The thesis of Clinton Bowen is approved:

Dr. John Dye | Date

Dr. Silvia Fernandez | Date

Dr. Bernardo Abrego | Date

Dr. Csaba Toth, Chair | Date

California State University, Northridge

DEDICATIONS

ACKNOWLEDGEMENTS

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ABSTRACT

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Insert Abstract here

Abstract

We look into the decidability of whether a hinged configuration locks.

1 Introduction

We look into the decidability of continuity on planar configuration space using regular, unitary hexagonal polygons. These polygons can also represent unit disk configurations [4]

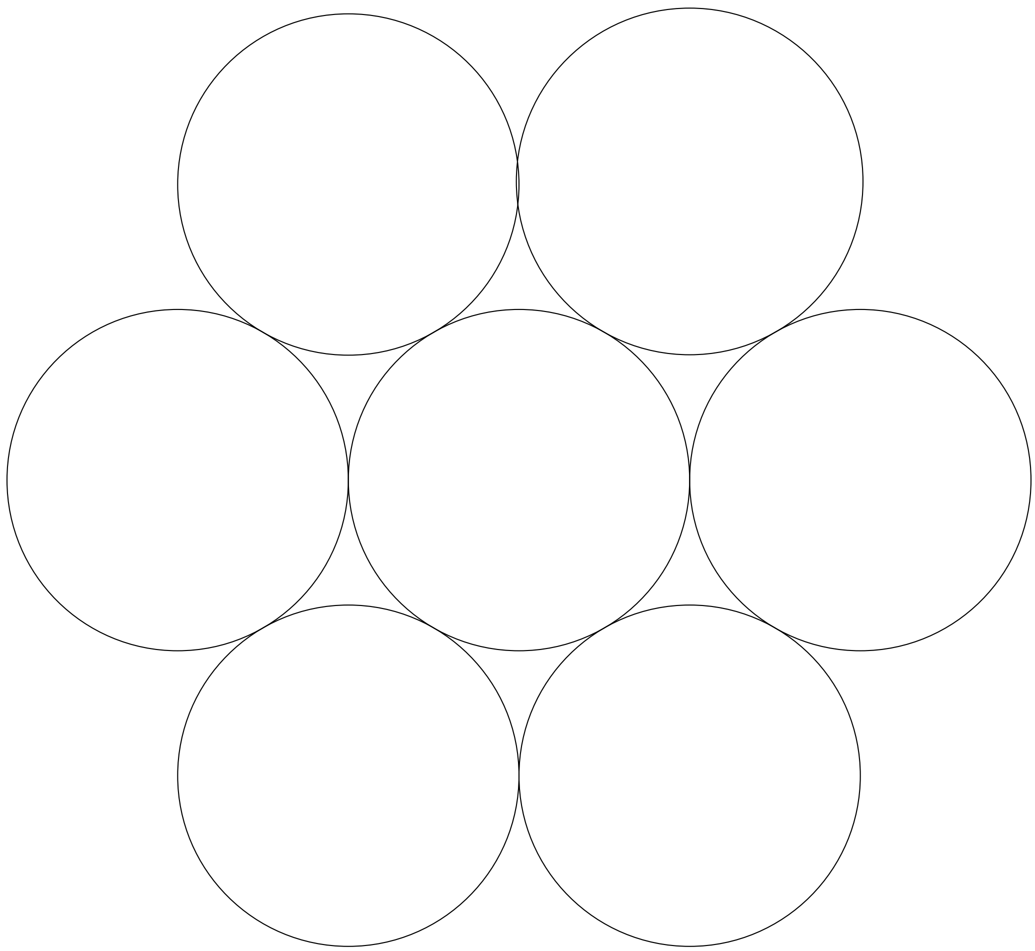

Figure 1: A locked 7 ball configuration

Motivation Protein folding, graphite, crystalline structures in metallurgy; disc packing; hexagonal configurations; Determine whether chemical structures are realizable.

Outline Section 2 covers the necessary mathematical concepts to understanding the problem. Section 3 explains the problem, Section 4 covers the results and findings about the problem. Section 5, the conclusion, offers final remarks on the problem.

2 Background

Here we review some of the necessary mathematics behind the problem. The definitions found in this chapter are those found in [9, 11, 8].

2.1 Linkages

Definition 2.1 (Graph)**.** An ordered pair $G = (V, E)$ comprising a set V of vertices or nodes together with a set E of edges or lines

Definition 2.2 (Linkage)**.** A collection of fixed-length 1D segments joined at their endpoints to form a graph.

A linkage can be thought of as a type of path-connected graph, i.e. the segments of a linkage are the edges of a graph, and the endpoints of the segments are the vertices. For this paper, we restrict our self to linkages that are simple planar graphs, i.e. a linkage that:

(i) does not have multiple edges between any pair of vertices,

(ii) does not have edges that cross, or

(iii) have loops (i.e. $(v, v) \in E$).

Definition 2.3 (Cycle)**.** A closed walk with no repetitions of vertices or edges allowed, other than the repetition of the starting and ending vertex

Definition 2.4 (Configuration)**.** A specification of the location of all the link endpoints, link orientations and joint angles.[6]

Definition 2.5 (Configuration Space)**.** The space of all configurations of a linkage.

A configurations space is said to be continuous if for any two configurations, $\mathscr{A}$ and $\mathscr{B}$ of a linkage L, $\mathscr{A}$ can be continuously reconfigured to $\mathscr{B}$ such that, the reconfigurations reside in the configuration domain, L remains rigid throughout reconfiguration (i.e. all links' lengths are preserved), and no violations of linkage intersection conditions.

Definition 2.6 (Pinned Joint)**.** A vertex of a graph (or linkage) that is fixed to a position in a plane.

Definition 2.7 (Free Joint)**.** A vertex of a graph (or linkage) that is not fixed to a position in a plane.

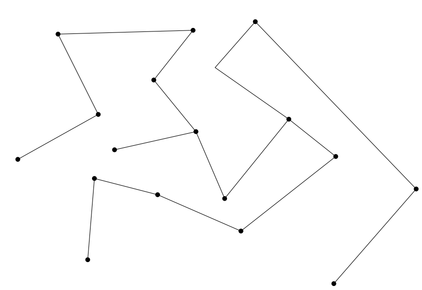

Figure 2: A linkage with joints.

For illustrations in the remainder of this paper, free joints will be represented as crosses and pinned joints will be represented as disks.

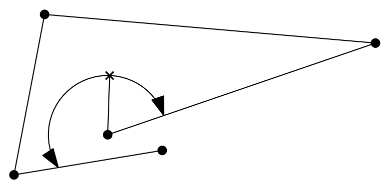

Figure 3: The cross represents a free joint; the pinned joints are denoted as disks. The range of motion shown by the arc describes the continous configuration space of the linkage.

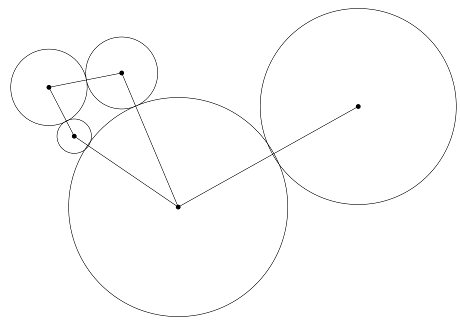

Figure 4: This figure is an example of a circle packing for the given simple planar graph.

2.2 Circle Packing

Definition 2.8 (Circle Packing)**.** *P of a planar graph G is a set of of circles with disjoint interiors $\{C_v\}_{v \in G}$ such that two circles are tangent if and only if the corresponding vertices form an edge.* [2]

Theorem 2.1 (Circle Packing Theorem)**.** *For every connected simple planar graph G there is a circle packing in the plane whose intersection graph is (isomorphic to) G.*

A proof of Theorem 2.1 is found in [11].

2.2.1 Circle Packings and Polygonal Linkages

Given a circle of radius r and its center point, (x, y), we establish the isomorphism to a hexagon by circumscribing the vertices of the regular hexagon.

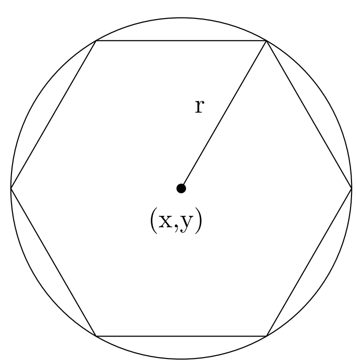

Figure 5: A circumbscribed hexagon

2.2.2 Hinged Polygons

Definition 2.9 (Polygonal Chain)**.** A polygonal chain $P = (v_0, v_1, \ldots, v_{n-1})$ is a sequence of consecutively joined segments (or edges) $e_i = v_i v_{i+1}$ of fixed lengths $l_i = |e_i|$, in a plane. [3]

A chain is said to be closed if $v_{n-1} = v_1$, otherwise it is said to be open. Hinged polygons have been researched for decades and related to linkage problems [3, 5].

Consider the locked configuration of figure 6. We can configure the hexagons to be locked by placing hinged points as follows:

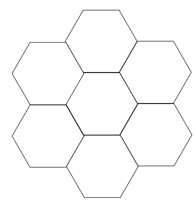

Figure 6: A locked 7 hexagonal configuration. (needs to modify picture by placing red points for hing points.)

2.2.3 Hinged Hexagons of Fixed Size

The Shapes Figure 7 is a locking shape: Figure 7 shall reside in the boundary of a lattice and have a hinge

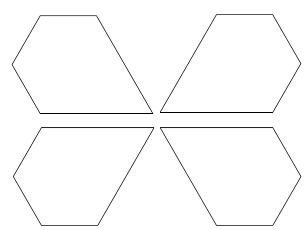

Figure 7: A locking shape in the lattice boundary's channel.

point at one vertex where the locking shape and boundary meet.

Junctions We define junctions to be the point three hexagons meet in a hexagonal lattice, e.g. Figure 8.

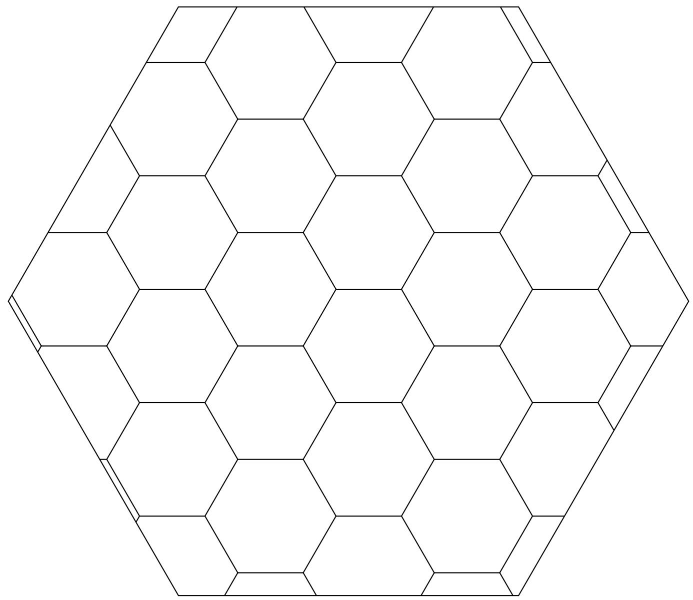

Figure 8: A portion of a hexagonal lattice.

Central Scaling

Junctions in Conjunctive Normal Form Explain the configurations we're interested in.

3 Configuration Spaces of Polygonal Chains

3.1 Polygonal Linkages

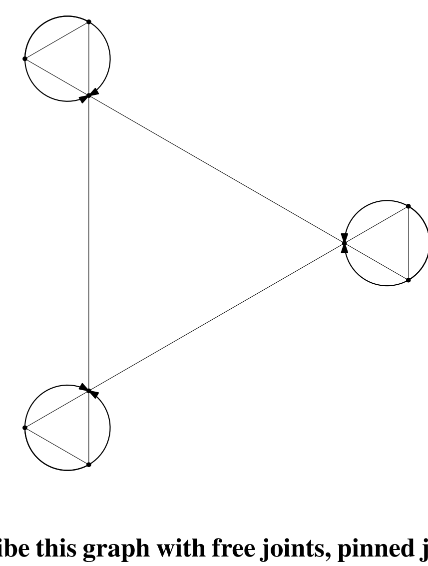

Figure 9: **Not sure how to describe this graph with free joints, pinned joints. Do I need to define another joint(i.e. axis of rotation joint)?**

3.1.1 Configurations and Locked Configurations

3.2 Dissections

Problem 3.1 (Polygonal Dissection). Given two polygons of equal area, P_1 and P_2, partition P_1 into smaller pieces,$\{P_{1,i}\}_{i=1}^{n}$, rearrange the pieces to form P_2. [8]

Theorem 3.1. *Any finite collection of polygons of equal area has a common hinged dissection. [1]*

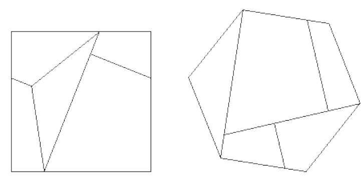

Figure 10: An axample of two polygons of equal area that can be rearranged into the other by the given partition.[7]

3.3 SAT Problems

Problem 3.2 (Satisfiability Problem). Let $\{x_i\}_{i=1}^{n}$ be boolean variables, and $t_i \in \{x_i\}_{i=1}^{n} \cup \{\bar{x}_i\}_{i=1}^{n}$. A *clause* is is said to be a disjuction of distinct terms:

$$t_1 \vee \cdots \vee t_{j_k} = C_k$$

Then the *satisfiability problem* is the decidability of a conjuction of a set of clauses, i.e.:

$$\wedge_{i=1}^{m} C_i$$

[10]

3.3.1 3-SAT Problems

A 3-SAT problem is a SAT problem with all clauses having only three boolean variables.

4 Problem

4.1 Problem Statement

text

4.2 Decidability of Problem

test

4.3 Hexagonal Locked Configuration

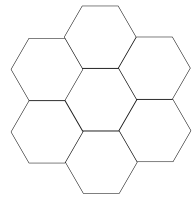

Figure 11: 7 hexagonal configuration

5 Conclusion

We conclude. . .

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