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

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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]

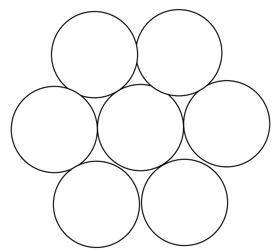

Figure 1: A locked 7 ball configuration

**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.

**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.

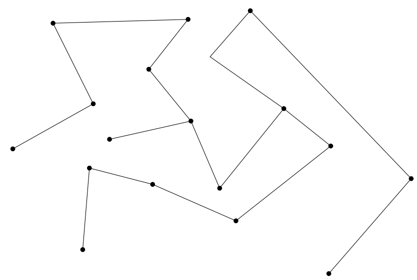

Figure 2: A linkage with joints.

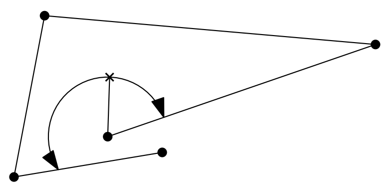

Figure 3: The cross represents a free joint; the pinned joints are denoted as disks. The range of motion shown by the arc describes the continous configuration space of the linkage.

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

## 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.*

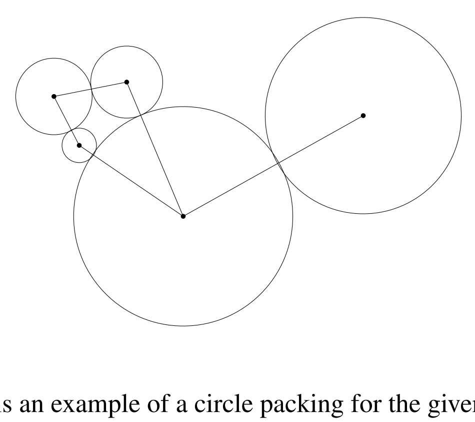

Figure 4: This figure is an example of a circle packing for the given simple planar graph.

**Are all linkages simple planar graphs?** A proof of Theorem 2.1 is found in [11].

### 2.2.1 Circle Packings and Polygonal Linkages

Given a circle of radius $r$, we establish the isomorphism to a hexagon by circumscribing the vertices of the regular hexagon.

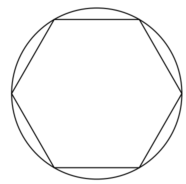

Figure 5: A circumbscribed hexagon

### 2.2.2 Hinged Polygons

**Definition 2.9** (Polygonal Chain)**.** A polygonal chain $P = (v_0, v_1, \dots, v_{n-1})$ 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: To prove that it is a locked configuration:

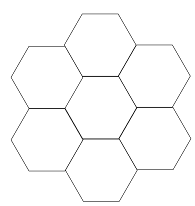

Figure 6: A locked 7 hexagonal configuration. (needs to modify picture by placing red points for hing points.)

(i)

(ii)

(iii)

(iv)

(v)

(vi)

(vii)

(viii)

(ix)

(x)

### 2.2.3 Hinged Hexagons

**Theorem 2.2.** *Any finite collection of polygons of equal area has a common hinged dissection. [1]*

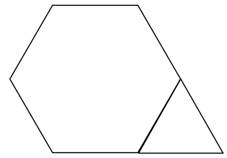

Figure 7: This is the shape that resides in boundary of the lattice.

**The Shapes** Figure 7 is a locking shape: Figure 7 shall reside in the boundary of a lattice and have a hinge point at one vertex where the locking shape and boundary meet.

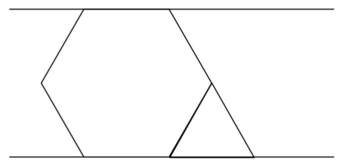

Figure 8: A locking shape in the lattice boundary's channel.

**Junctions** We define junctions to be the point three hexagons meet in a hexagonal lattice, e.g. Figure 9.

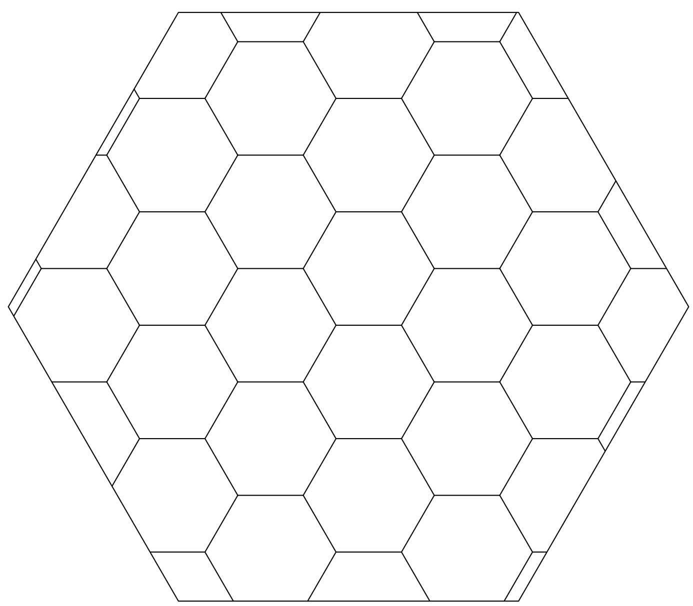

Figure 9: A portion of a hexagonal lattice.

**Central Scaling**

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

# 3 Configuration Spaces of Polygonal Chains

#### 3.0.4 Configurations and Locked Configurations

## 3.1 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]

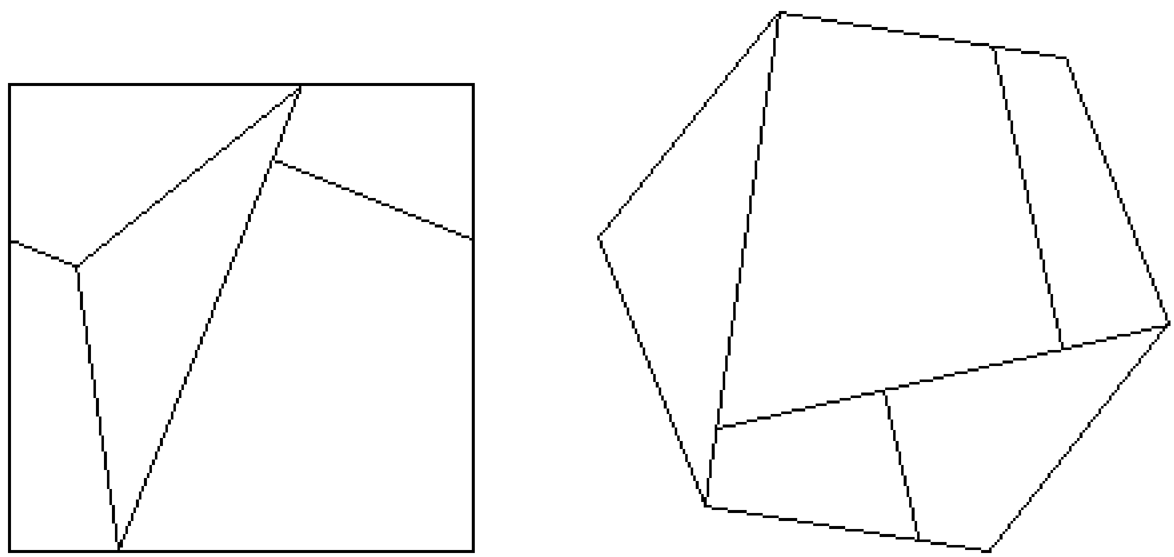

Figure 10: An axample of two polygons of equal area that can be rearranged into the other by the given partition.[7]

## 3.2 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]

#### 3.2.1 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

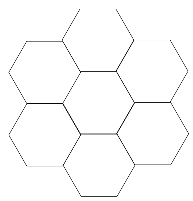

Figure 11: 7 hexagonal configuration

# 5 Conclusion

We conclude…

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