CALIFORNIA STATE UNIVERSITY, NORTHRIDGE

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

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By

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DEDICATIONS

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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 [3]

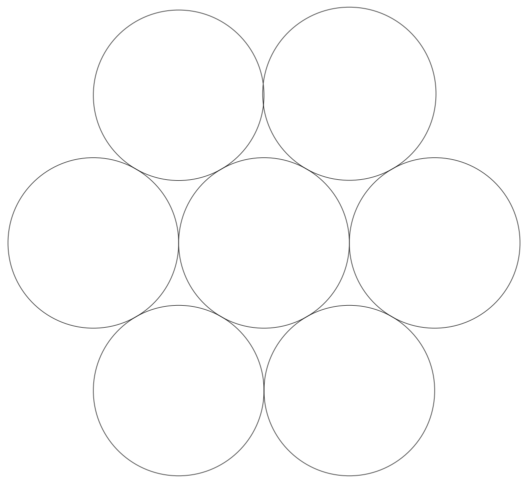


Figure 1: A locked 7 ball configuration

**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 [7, 10, 6].

## 2.1 Linkages

Given a *graph*, an ordered pair $G = (V,E)$, comprising of a set $V$ of vertices or nodes together with a set $E$ of edges or lines, then a linkage of $G$ is the realization (or embedding) of $G$ in $\mathbb{R}^2$. For this paper, we focus on linkages that are simple planar graphs, i.e.:

(i) does not have edges that cross,

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

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

We may visit special cases in which we look at planar graphs that satisfy the last two conditions but not the first.

### 2.1.1 Configuration Spaces of Linkages

To describe the types of motion that we are interested in linkages we must define the graph isomorphism. Two graphs $G = (V_1, E_1)$ and $\Gamma = (V_2, E_2)$, a bijection $f : V_1 \mapsto V_2$ such that for any two vertices $u, v \in V_1$ that are adjacent, i.e. $(u, v) \in E_1$, if and only if $(f(u), f(v)) \in E_2$.

| Graph | Vertices | Edges |
| --- | --- | --- |
| $G$ | $\{a,b,c,d,e\}$ | $\{(a,b),(b,c),(c,d),(d,e),(e,a)\}$ |
| $\Gamma$ | $\{1,2,3,4,5\}$ | $\{(1,2),(2,3),(3,4),(4,5),(5,1)\}$ |

Table 1: Two graphs that are isomorphic with the alphabetical isomorphism $f(a) = 1$, $f(b) = 2$, $f(c) = 3$, $f(d) = 4$, $f(e) = 5$.

Next we add restrictions to our graph isomorphisms to narrow our focus:

(i) We focus on isomorphisms for planar graphs, simple planar graphs, and

(ii) the isomorphism preserves edge lengths, e.g. $d(u, v) = d(f(u), f(v))$.

With these restrictions of our isomorphisms, we can begin to describe a range of motion to transform a linkage. That range of motion is said to be the configuration space of that linkage. To expand on this concept, for given linkage, $L = (V, E)$, and for a given vertex $v \in V$, the set of points in which $v$ can be realized in the plane would be the configuration space for that vertex, $C_v$. Defining some order of the vertices in $L$, i.e. $V = \{v_n\}_{i=1}^{n}$, then the *configuration space* for $L$ is said to be the cartesion product of the configuration space of vertices:

$$C(L) = C_{v_1} \times C_{v_2} \times \cdots \times C_{v_n} \tag{1}$$

Some food for thought on configuration spaces and motions on linkages:

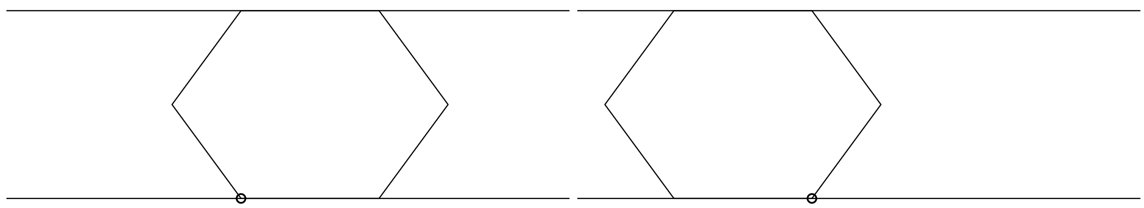
(i) A configuration space is said to be *connected* if there is a continuous mapping for any two planar realizations (linkages) of a graph in the plane. Otherwise it is said to be *disconnected*.

(ii) If the configuration space of a vertex, $C_v$, is a singleton set, then the vertex is said to be *pinned*. Otherwise it is said to be *free*.

(iii) The types of motions (mappings) that we refrain from using on linkages are translations.

### 2.1.2 Confining Linkages to a Restricted Space Within a Configuration Space

So we've covered the idea of linkages within a plane; now let's constrain the plane to a strip and have a linkage that is a *polygon*, i.e. a linkage that forms a closed chain (e.g. Table **??**), hugging the boundaries of the strip: So here we have a linkage whose conifguration space is limited to just two realizations. With just

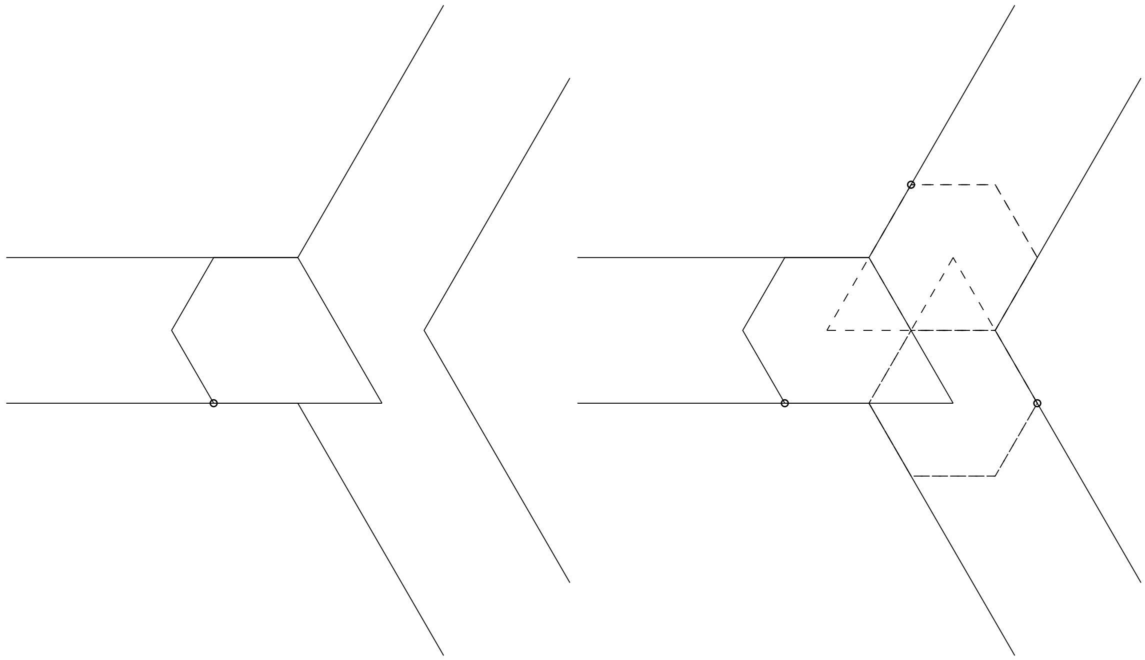


(a) A bounded hexagon that resides in a channel with a pinned vertex

(b) The second realization of the hexagon residing in a channel with a pinned vertex.

Figure 2: Due to the strip in the plane that the hexagon is bounded within the configuration space is limited to just two realizations.

two realizations, we can assign a binary value to them and have the linkage act as a boolean variable. We will revisit this concept when we cover satisfiability problems later on in the paper.



(a) A pentagon that is pinned in a channel junction that is formed by the sides of 3 large regular hexagons. It has two possible configurations, much like that of 2

(b) A pinned pentagon residing in a channel junction that is formed by the sides of 3 large regular hexagons with 2 dashed pentagons intersecting it.

Figure 3: Suppose the channel formed is a junction of three regular hexagons. The polygon partially residing in the junction is a regular hexagon with an equalateral triangle appended at an edge. This polygon would prevent other polygons (i.e. the dashed polygons) of the same shape residing in the center of the channel without intersection. This demonstrates that a the configuration space within a multichannel environment can have concurrency issues, i.e. some configurations cannot be realizable.

Expanding upon the ideo of 2, forming channels with junctions as shown in Figure **??** can be formed as such by evenly spacing the edges of a hexagonal lattice. Visually, it is shown that only one of three possible pentagons can reside in the channel at one time. By asserting certain conditions on the lattice, and extending the problem to a greater region of a hexagonal lattice, we will be able to pose a realizability problem of whether a configuration $\mathscr{A}$ can be reconfigured to $\mathscr{B}$ by switching pentagons without violating overlapped polygon conditions.

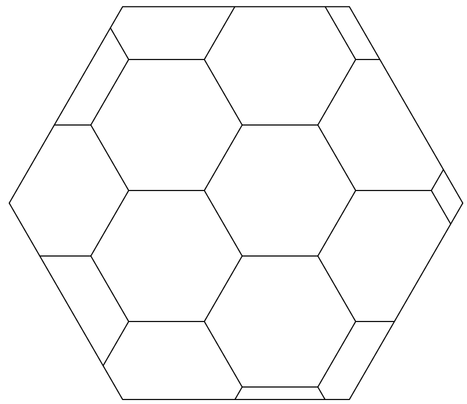


Figure 4: A hexagonal lattice contained in a hexagon.

#### 2.1.3 Realizability of Linkages

Suppose we had two configurations of a linkage, $\mathscr{A}$ and $\mathscr{B}$. A question that can be posed is can we reconfigure $\mathscr{A}$ to $\mathscr{B}$ continuously while respecting simple planar graph conditions? The answer to this question is a yes or no. It has been shown that this problem can be posed as a planar satisfiability problem [3, 8] (Later on in this paper we'll cover satisfiability problems). This is the type of problem that we face in this paper. We will continue to explore this in a different manner, with circle packings.

### 2.2 Circle Packing

It turns out the circle packings are an equivalent way to to represent linkages and their corresponding problems. Before we establish the relation, we will cover some fundamental concepts of circle packings. A *circle packing*, $P$, embedded in a plane is a set of circles with disjoint interiors $\{C_i\}_{i=1}^n$ such that for any circle $C \in \{C_i\}_{i=1}^n$, $C$ is tangent to a different circle of $\{C_i\}_{i=1}^n$.

Any circle embedded in a plane has a given center point and radius. This information of planar embedded circle packings allows us to establish the relationship to linkages with the following construction:

(i) let the centerpoints of the circle packing be a set of vertices $V$;

(ii) if two circles in a circle packing are tangent, we define an edge between their centerpoints. The distance of this edge is the sum the radii of the two tangent circles.

This construction establishes a relationship between linkages and circle packings. It begs questioning as to whether every connected simple planar graph has a circle packing. The question is answered in the following theorem.

**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 chapter 7 of [10]. Theorem 2.1 also gives us the ability to establish an equivalent definition of configuration spaces on circle packings and allows us to pose the same realizability problems found with simple planar graphs. To narrow the focus of the types of circle packing realizabilty problems that we are interested in, we add the following restriction: all circles in a circle packing have unit diameter.

#### 2.2.1 Realizability Problems in Unit Disk Packings

In [3], it was shown that unit disk graph recognition is NP-Hard.

## 2.3 Area Packing Problem

### 2.3.1 Hinged Polygons

**Definition 2.1** (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. [2]

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 [2, 4].

Consider the locked configuration of figure 5. We can configure the hexagons to be locked by placing hinged points as follows:

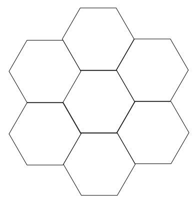


Figure 5: A locked 7 hexagonal configuration. (needs to modify picture by placing red points for hing points.)

### 2.3.2 Hinged Hexagons of Fixed Size

**The Shapes** Figure 6 is a locking shape: Figure 6 shall reside in the boundary of a lattice and have a hinge

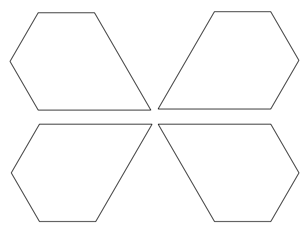


Figure 6: A locking shape in the lattice boundary's channel.

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 7.

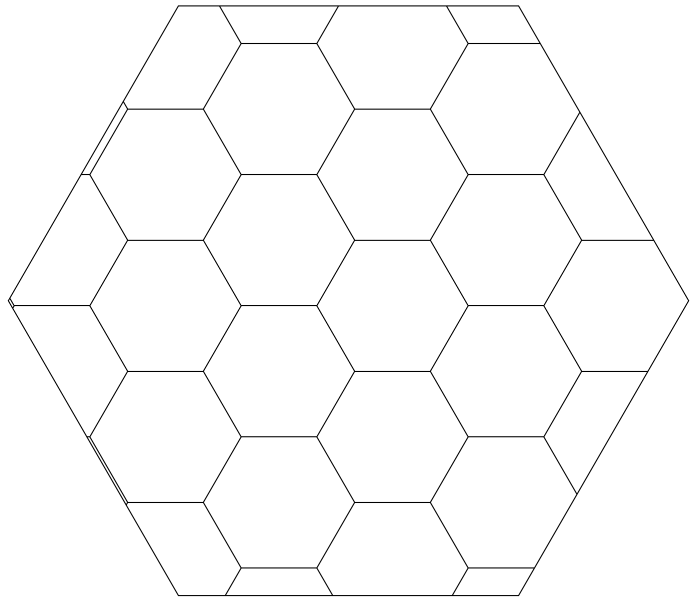


Figure 7: A portion of a hexagonal lattice.

**Central Scaling**

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

# 3 Configuration Spaces of Polygonal Chains

## 3.1 SAT Problems

*Problem* 3.1 (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.:

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

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

**Definition 3.1** (Planar 3-SAT Problem)**.** Given a boolean 3-SAT formula $B$, define the associated graph of $B$ as follows:

$$G(B) = (\{\, v_x \,|v_x \text{ represents a variable in } B\,\} \cup \{\, v_C \,|v_C \text{ represent a clause in } B\,\}, \{\,(v_x, v_C)\,|x \in C \text{ or } \bar{x} \in C\,\}) \tag{2}$$

If $G(B)$ in equation (2) is planar, then $B$ is said to be a *Planar 3-SAT Problem* [8].

# 4 Problem

## 4.1 Problem Statement

text

## 4.2 Decidability of Problem

test

## 4.3 Hexagonal Locked Configuration

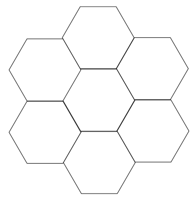


Figure 8: 7 hexagonal configuration

## 5 Conclusion

We conclude...

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