Protein Folding: Planar Configuration Spaces of Disc Arrangements and Hinged Polygons: *Protein Folding in Flatland*

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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 [1]

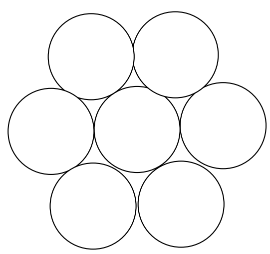

Figure 1: A locked 7 ball configuration

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 [**?**, 4, 3].

2.1 Linkages

Definition 2.1 (Linkage)**.** A collection of fixed-length 1D segments joined at their endpoints to form a graph.

Definition 2.2 (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 2.3 (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.[2]

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, $\mathcal{A}$ and $\mathcal{B}$ of a linkage L, $\mathcal{A}$ can be continuously reconfigured to $\mathcal{B}$ 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.

2.2 Circle Packing

Definition 2.6 (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. [**?**]

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. [4]*

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.

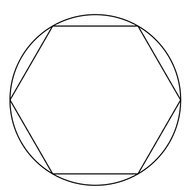

Figure 2: A circumbscribed hexagon

2.2.2 Hinged Polygons

Definition 2.7 (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. [**?**]

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 [**?**, **?**].

Consider the locked configuration of figure 3. We can configure the hexagons to be locked by placing hing points as follows: To prove that it is a locked configuration:

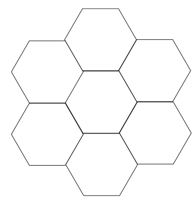

Figure 3: A locked 7 hexagonal configuration. (needs to modify picture by placing red points for hing points.)

(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. [**?**]*

The Shapes Figure 4 is a locking shape: Figure 4 shall reside in the boundary of a lattice and have

`Sgraphics/lockingShape.pdf`

Figure 4: This is the shapte that resides in boundary of the lattice.

a hinge 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 6.

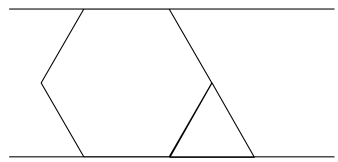

Figure 5: A locking shape in the lattice boundary's channel.

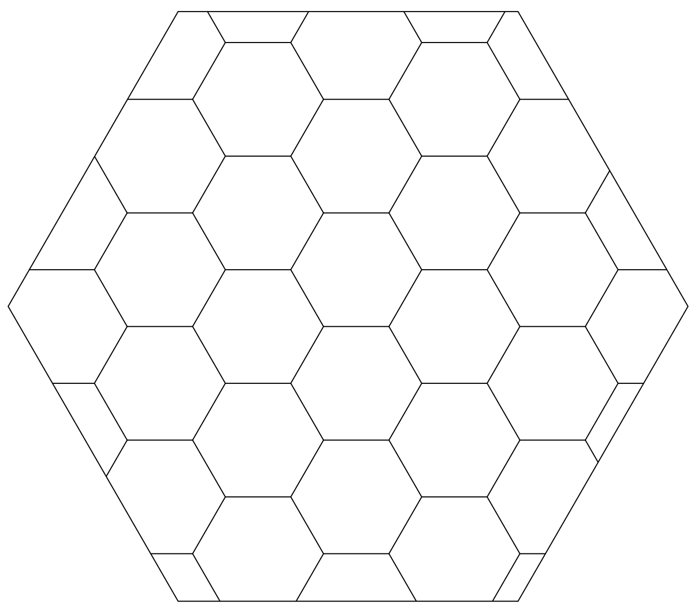

Figure 6: A portion of a hexagonal lattice.

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. [3]

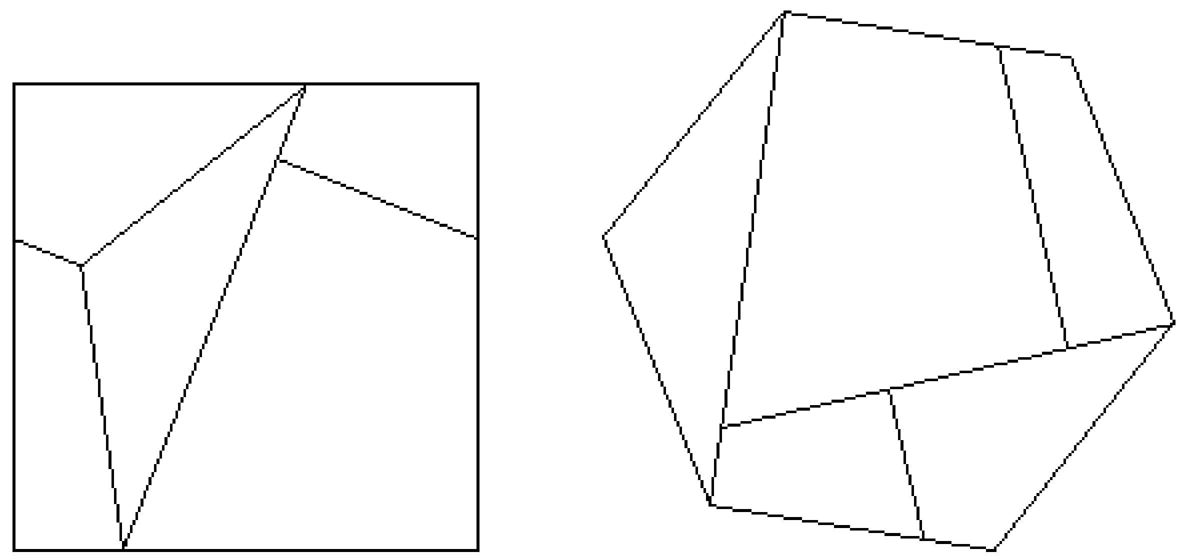

Figure 7: An axample of two polygons of equal area that can be rearranged into the other by the given partition.[?]

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.:

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

[?]

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

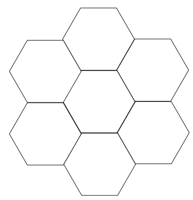

Figure 8: 7 hexagonal configuration

5 Conclusion

We conclude...

References

[1] Heinz Breu and David G. Kirkpatrick. Unit disk graph recognition is np-hard. *Computational Geometry*, 9(12):3 – 24, 1998. Special Issue on Geometric Representations of Graphs.

[2] E.D. Demaine and J. O'Rourke. *Geometric Folding Algorithms: Linkages, Origami, Polyhedra*. Cambridge University Press, 2008.

[3] G.N. Frederickson. *Dissections: Plane and Fancy*. Cambridge University Press, 1997.

[4] K. Stephenson. *Introduction to Circle Packing: The Theory of Discrete Analytic Functions*. Cambridge University Press, 2005.