

# DIMACS EDUCATIONAL MODULE SERIES

## MODULE 08-1

### Linkages as Applied to Protein Folding

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## Module Description Information

- **Title:**

**Linkages as Applied to Protein Folding**

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- **Abstract:**

A linkage consists of a set of bars or rods which are connected by joints. In this module these are represented by line segments and the points that connect them. Background, hands on experience with the pantograph linkage, and basic terms and definitions of linkages are explained. These serve as a foundation for understanding Kempe's *Universality Theorem*, modern linkages, and protein folding involving chains of links. The exercises throughout this module will help the student solidify their knowledge of the key concepts and capabilities of linkages. In addition, certain open problems are provided for students interested in doing further research in classical linkages, modern linkages, and protein folding.

- **Informal Description:**

This module consists of two parts. Part I gives an introduction to classical linkages, Kempe's *Universality Theorem*, and modern linkages. Part II gives a presentation of the conical model for protein manufacturing. The goals are to give a somewhat in depth introduction of the concepts of classical linkages, explore reachability issues associate with linkages, and apply linkages to protein folding. The entire module would take six class meetings. Part I: An Introduction to Linkages could be covered in three lecture periods; Part II: An application of Linkages: Protein Folding could also be covered in three periods. Part I could be covered alone, as could Part II by providing just the key concepts from Part I that directly apply to protein folding. Also, the module, or only Part I or only Part II, could be used by students doing independent work, devoting little or no class time to the material.

- **Target Audience:**

This module is suitable for undergraduate sophomore to senior students in mathematics.

- **Prerequisites:**

Trigonometry and Discrete Mathematics

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- **Other DIMACS modules related to this module:**  
MODULE 03-4: Planar Linkages: Robot Arms and Carpenters' Rulers

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The authors wish to thank Dr. Joseph O'Rourke, Olin Professor and Chair of Computer Science; Professor of Mathematics, Smith College, Northampton, MA, for introducing the concepts presented in this module at the DIMACS "Folding and Unfolding in Computational Geometry" workshop in July 2004.

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## **ABSTRACT**

A linkage consists of a set of bars or rods which are connected by joints. In this module these are represented by line segments and the points that connect them. Background, hands on experience with the pantograph linkage, and basic terms and definitions of linkages are explained. These serve as a foundation for understanding Kempe's *Universality Theorem*, modern linkages, and protein folding involving chains of links.

The exercises throughout this module will help students solidify their knowledge of the key concepts and capabilities of linkages. In addition, certain open problems are provided for students interested in doing further research in classical linkages, modern linkages, and protein folding.

## Part I. An Introduction to Linkages

### 1. Linkages: What They Are

#### Background

Linkages are simple structures that can be thought of as straight rigid sticks or rods hinged together at their endpoints to enable rotation with respect to each other. Linkages are important mechanisms that are widely used. Consider these familiar devices using linkages: the movement of a sewing machine needle, a windshield wiper, elevator doors, and the robotic arm used to assemble the International Space Station. Even your finger is an example of a linkage. Figure 1.1 illustrates examples of various linkages: (a) the linkage on a ladder controls the folding and unfolding of the ladder, (b) a sewing machine, (c) a windshield wiper, and (d) elevator doors. Animated linkages for (b), (c), and (d), can be found at the web reference site [1].

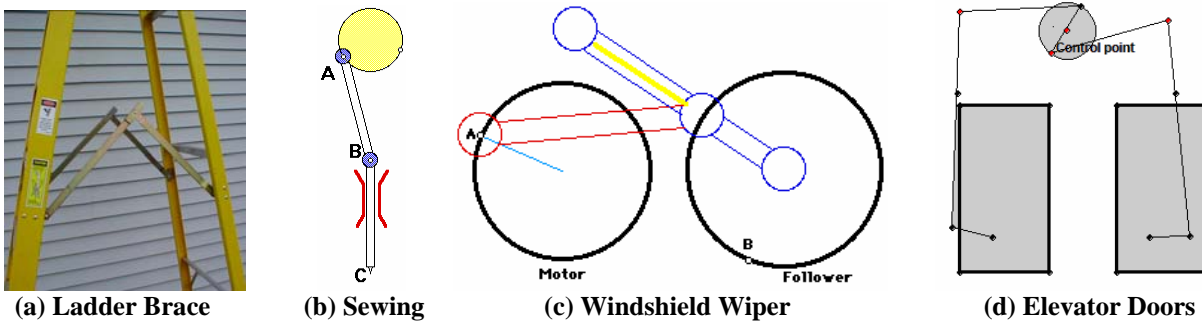


Figure 1.1 Linkages

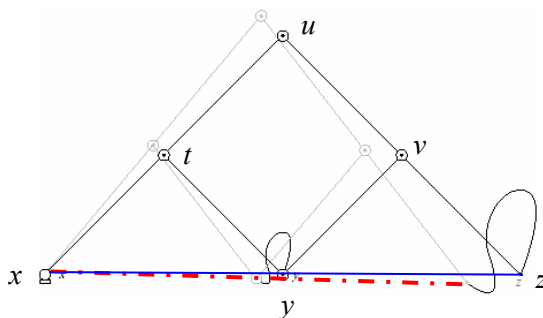
The study of linkages dates from before the time of Leonardo da Vinci through the time of James Watt to the present, including skeletal animation applied to computer games and movie special effects to give a natural movement to computer generated characters. James Watt (1784) began the modern era of mechanism in conjunction with his work on developing the steam engine. Charles-Nicolas Peaucellier (1832-1912), whose background was in engineering, developed a way to convert circular motion into true linear motion using a linkage. A major figure in investigating linkages was Alfred B. Kempe (1849-1922) who was a student of the famous mathematician Arthur Cayley and graduated in 1872 with distinction in mathematics from Trinity College, Cambridge, England. Although he chose law as his profession, Kempe formulated a very significant theorem known as the *Universality Theorem*, which states that given any algebraic curve a linkage can be constructed such that one of its joints will trace the curve. His proof was flawed but his basic ideas were sound. It was not until 2002, when the first complete and detailed proof, correcting the flaws in Kempe's theorem, was published by Kapovich and Millson [KM]. This theorem stated that if one has a planar curve described by an algebraic equation, then a linkage can be designed which will generate this plane curve. Kapovich and Millson's theoretical result that there is a planar linkage that traces out any given algebraic curve is very elegant, but unfortunately, the physical linkages suggested would be extremely complicated to realize. Because of developments in computer technology, electronic motors, and mechanical design, modern linkages which are less complex can be built [WK].

## The Pantograph

By building a linkage we can better understand how it works. Linkages can be constructed by using any number of rigid physical rods of various sizes, for example popsicle sticks, tinker-toy like components, pieces of cardboard, or graphically by using a software tool like *Cinderella* at the web reference site [8] or *The Geometer's Sketchpad* at the web reference site [9].

The *pantograph* is a particularly interesting planar linkage that can give us some insight into how linkages work. This mechanism is used for copying, reducing, or enlarging a drawing's size. Based on the principles of this device, Thomas Jefferson built a mechanism that allowed him to sign several documents at once [DO]. His signature was an exact duplicate on each document.

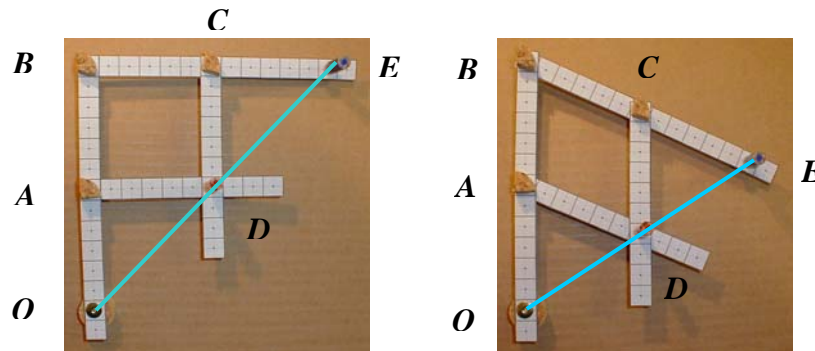
See Figure 1.2, where a duplicate drawing twice the size of a drawing (at position  $y$ ) is generated. The duplicate drawing (at position  $z$ ) has a scale factor of two. In this figure,  $x$ ,  $y$  and  $z$  are all on the same line. Line segment  $x$  to  $u$  is the same length as line segment  $u$  to  $z$ . The position  $x$  is stationary, but allows the rotation of line segment  $xu$ . The positions  $t$ ,  $u$ ,  $v$ ,  $y$  and  $z$  are not stationary but are allowed to rotate. Notice that  $t$ ,  $u$ ,  $v$ ,  $y$  form a parallelogram, i.e. a quadrilateral with opposite sides parallel. Also, note that  $t$  is half way between  $x$  and  $u$  and  $v$  is half way between  $u$  and  $z$ , where  $t$ ,  $u$ ,  $v$ , and  $y$  specifically form an equilateral parallelogram, i.e. a rhombus. By placing pencils at each position  $y$  and  $z$ , as  $y$  traces (or draws) a figure,  $z$  draws the same figure twice the size.



**Figure 1.2 A Pantograph Mechanically Doubling the Size of a Drawing.**

We will now consider how a pantograph can copy, reduce, or enlarge the size of a drawing. The pantograph in Figure 1.3, consists of four rods with hinged joints at the corner points of the parallelogram  $ABCD$ , whose angles can vary in size. The linkage is pivoted at point  $O$ , which is a fixed position. The points  $O$ ,  $D$ , and  $E$  remain collinear as the shape of the parallelogram changes. As a result, rods  $OA$  and  $BC$  are each scaled versions of rods  $OB$  and  $BE$ , respectively, by the same scale factor. If the scale factor is  $s$ , then  $s = OB/OA = BE/BC$ . Since, this scale relationship holds for any position of the pantograph, the movements of  $E$  are just  $s$ -times the movements of  $D$ . As  $D$  moves and a pencil is placed at position  $E$ , then  $E$  draws a copy of the figure that  $D$  traces. Depending on the scale factor  $s$  built into the particular linkage, the figure drawn by  $E$  is an exact copy, a reduced copy, or an enlarged copy (see Exercise 1.2).





**Figure 1.3 – A Pantograph in Two Different Positions**

**Exercise 1.1** Use an Internet applet of a pantograph to duplicate a figure.

1. To get a feel for a pantograph's movement, play with the applet at web referenced site [2].
2. Notice that the pantograph at this website draws a duplicate figure that is larger but is not twice the size of the one drawn by the red point. Why?
3. Determine the scale factor from the red drawing to the blue drawing?  
(Hint: Notice the dimensions on the pantograph at the top of the website page.)

**Exercise 1.2:** What is the condition on the value of the scale factor  $s$  for a pantograph if

- (a) an exact copy of a figure is drawn?
- (b) a reduced figure is drawn?
- (c) an enlarged figure is drawn?

**Exercise 1.3 (Hands-On Activity for Students):** Have a team of two or three students build three pantographs. One pantograph will make an exact copy of a drawing, another will reduce the drawing, and the last will enlarge the drawing.

**I. Required Materials for a Pantograph (Figure 1.4):**

1. Four links (Made from the drawings A.1 in Appendix A)
2. A piece of small cardboard that all four links can fit on without overlap
3. Glue stick
4. Scissors
5. A piece of graph (grid) paper
6. Two thumb tacks
7. Three push pins
8. Two small sharpened pencil stubs
9. A  $\frac{1}{4}$ " diameter nail
10. A piece of cork marked at the height of the push pin base
11. A large piece of heavy cardboard for mounting the pantograph



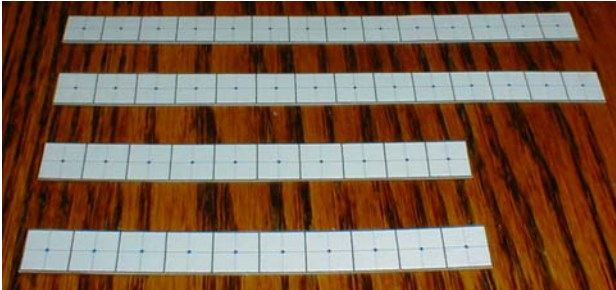
**Figure 1.4 – Required Materials for Building a Pantograph**

## **II. Instructions:**

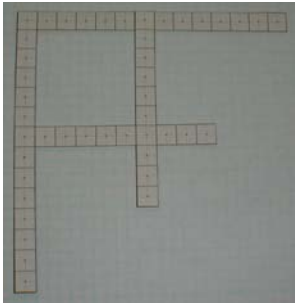
### **A. Constructing a Pantograph (Figure 1.5):**

- Step 1: Cut-out the four link strips in Figure 6.1 (Appendix A). Using the stick glue, paste the links on the small piece of cardboard. Then cut out the links.
- Step 2: Lay the linkage on the graph paper so each angle is a right angle ( $90^\circ$ ) and you satisfy your scaling factor.
- Step 3: Using one push pin (blue in Figure), attach the two largest links at one end through the point in the square at the end of each link. Make sure the pin goes through the corresponding point in each link. Using the other two push pins (red in the Figure), attach the end of each small link to each of the large links. Take care, to make sure your scaling factor is maintained. Again, make sure the pin goes through the corresponding point in each link.
- Step 4: Find two points, one on each large link, that are collinear with the intersection point of the two small links. Then use a thumb tack to make a hole at each of these three points. Make sure the tack goes through the intersection point of each small link.
- Step 5: Use the nail to enlarge the hole in the end of the large upper link and the hole at the intersection point of the two small links.
- Step 6: Cut the cork so that it is the height of the base of a push pin.
- Step 7: Reinsert all push pins through the bottom of the linkage in their respective holes. Cut three pieces from the remaining cork so that each piece has a height greater than the point of the pin sticking through. Push each piece of cork on top of the point of each pin.
- Step 8: Push a thumb tack through the large link on the left into piece of cork under the link. This cork was made in Step 6.
- Step 9: Place one pencil through the intersection point of the two small links and the other pencil through the hole in the upper large link. Make sure each pencil point extends the length of a push pin base.
- Step 10: Push the other thumb tack through the bottom of the heavy piece cardboard into the cork. This will secure the position of the pantograph and allow it to rotate.

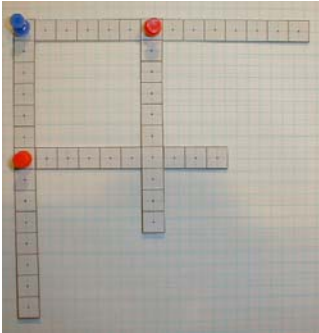
The pantograph is now complete and is ready to be used. Piece of paper can be slipped up the pantograph to draw on. It is a good idea to pin the paper to the heavy cardboard so it does not move.



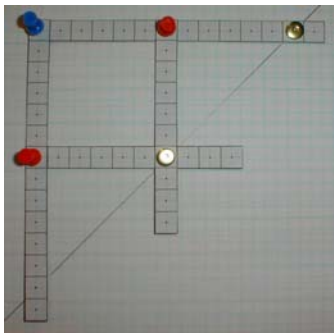
(a) Step 1



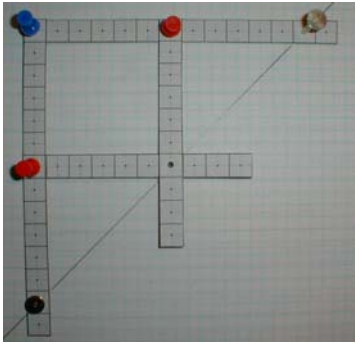
(b) Step 2



(e) Step 3



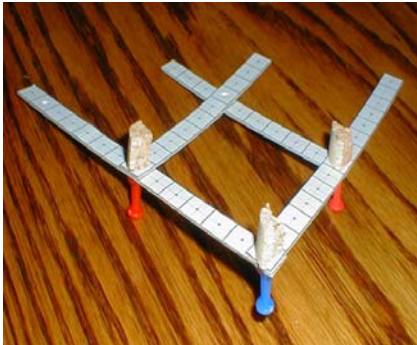
(f) Step 4



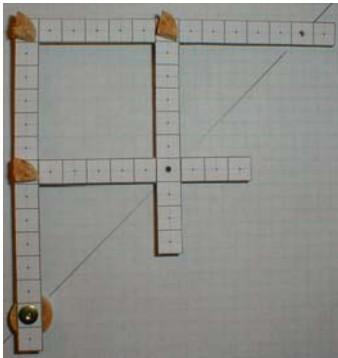
(g) Step 5



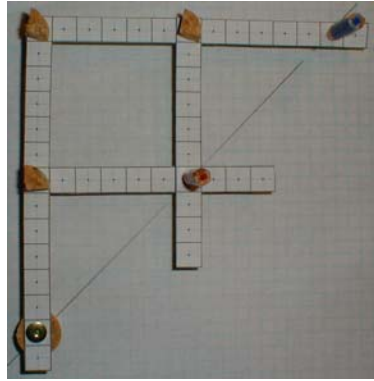
(h) Step 6



(i) Step 7



(j) Step 8



(k) Step 9



(l) Step 10

Figure 1.5 Steps to Construct a Pantograph

### III. Experiment

1. Make three different pantographs, each designed for a particular use: one to make an exact copy of a drawing, the second to enlarge a drawing by a scale factor of 1.5, and the third to reduce a drawing by a scale factor of 1/2. Explain why each works the way it does and demonstrate it. (Note: If you wish, the pantograph constructed above can be adjusted to make these three different pantographs by changing the positions of the push pins and the pencils. If you decide to use it in this way, to avoid extra adjustments, do both experiment 1 and 2 for on pantograph before converting it to a different use.)
2. Now let us use each pantograph in a different way. For each of the three pantographs interchange the use of the two pencils (Figure 1.5, Step 10). Trace the drawing with pencil 2 and draw the duplicate drawing with pencil 1. In each case, what is the scale factor of the duplicate drawing relative to the traced drawing? Why is this true?

## 2. Terminology for Linkages

### Basic Terms and Definitions

A few concepts from graph theory will be useful in the following discussion. A **graph** is a set of points called **vertices** connected by line segments called **edges**. A **path** in a graph is a sequence of  $n$  vertices  $v_1, v_2, v_3, \dots, v_n$ , such that  $[v_1, v_2], [v_2, v_3], \dots, [v_{n-1}, v_n]$  are edges in the graph. A graph is **connected** if there is a path between every pair of vertices. A path is called a **simple path**, if there are no repeated vertices in the path. A **cycle** is a path that begins and ends at the same vertex. A **tree** is a connected graph with no cycles. Figure 2.1, illustrates the above concepts, (a) is a graph that is a single cycle a, b, c, a, where  $[a, b], [b, c], [c, a]$  are edges, (b) is a tree containing the simple path a, d, h, where  $[a, d], [d, h]$  are edges, and (c) is a general graph.

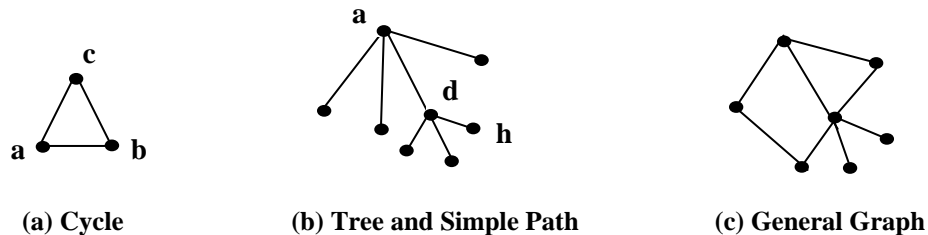


Figure 2.1

A **link**, **bar**, or **edge** is a fixed-length one-dimensional segment. The endpoint of a link is referred to as a **vertex**. As an example of a link and its endpoints see Figure 2.1 (a), having vertices a and b. If a particular vertex is fixed in a location it is referred to as **pinned**. A **linkage** is a set of links joined at their endpoints forming a graph. For an example, see Figure 2.2 (b), consisting of two links. Linkages can be classified in three ways: their graph structure (i.e. general graph, a tree, single cycle, or simple path), the dimension (i.e. 2D-space, 3D-Space, etc.) in which they reside, and if they intersect themselves or obstacles in their space.

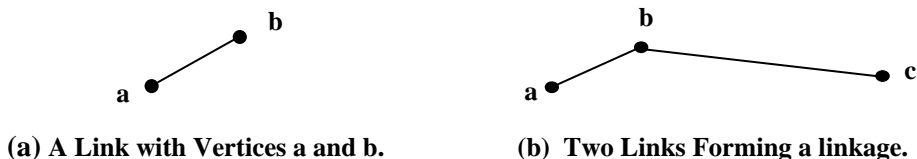


Figure 2.2

When two links share a common endpoint, this vertex is often referred to as a **joint**. The type of joint affects the movement of the linkage. A **universal joint** is a joint that allows two adjacent links to rotate at any angle relative to each other depending only on the dimension in which they are defined. For example in 2D-space, each link can pivot between  $0^\circ$  and  $360^\circ$  in a planar circle about the universal joint. As an example see Figure 2.3(a). In 3D-space, each link can pivot about a sphere centered at the universal joint. As an example, see Figure 2.3(b), where one link is seen pivoting about a great circle, i.e. the intersection of a plane (passing through the universal joint) and the sphere.

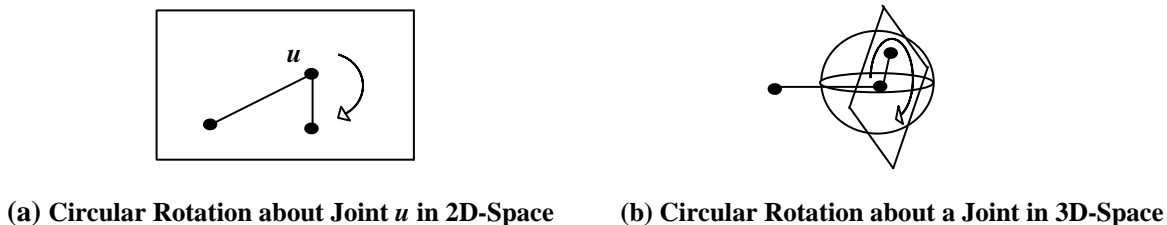


Figure 2.3

A **fixed-angle linkage** has a fixed angle at the joint between each pair of incident links (The fixed angle at different joints can differ.). As an example see Figure 2.4(a). Also, notice in a pantograph, Figure 2.4(b), that each pair of adjacent links,  $\{[x, t], [t, u]\}$  and  $\{[u, v], [v, z]\}$ , has a fixed angle of  $180^\circ$ , but this is not a fixed-angle linkage because all joints are not assigned a fixed angle. Some joints are allowed to vary in angle. Fixed-angle chains are of particular interest as models for proteins.

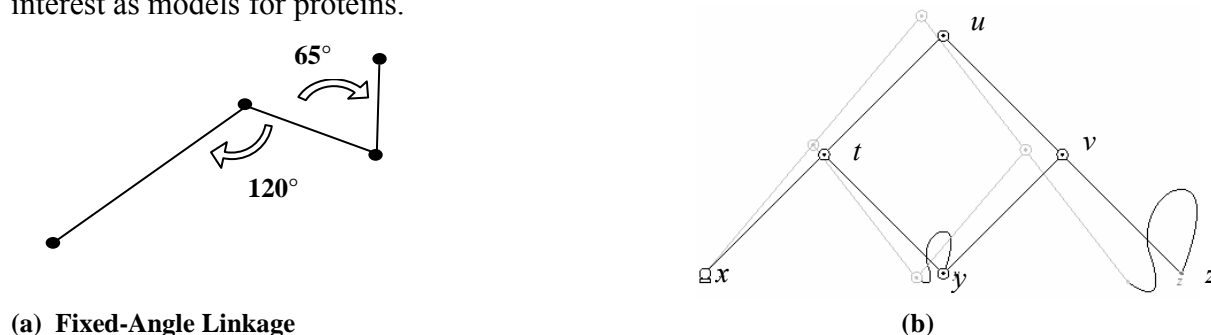


Figure 2.4

## Open and Closed Chains

Note throughout this text, graph theory language is used but it is important to keep in mind that linkages are really metric objects in that the links have specific fixed lengths.

An *open chain* or *arc* is a linkage whose underlying graph is a simple path that is not a cycle. The canonical (i.e. standard) form of an open chain is called a *straight configuration* if it can be reconfigured into a linkage where each adjacent link is connected by a joint with an angle of  $180^\circ$ . Figure 2.5 shows two open chains on the far left and right that have been reconfigured into a straight configuration for an open chain.

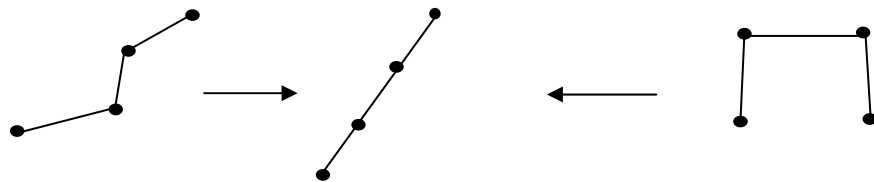


Figure 2.5 Straight Configuration for an Open Chain

A *closed chain* is a linkage whose graph is a simple cycle. A cycle is *convex* if every line segment drawn between two points on or in the cycle has no point outside the cycle. Another way to describe a convex cycle is that all interior angles are less than or equal to  $180^\circ$ . The canonical form of a closed chain is called a *convex configuration* if it can be reconfigured into a linkage that is a convex simple cycle. Figure 2.6 shows two non-convex closed chains, on the far left and right, that have been reconfigured into a convex configuration.

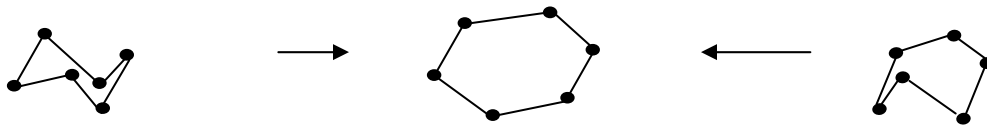
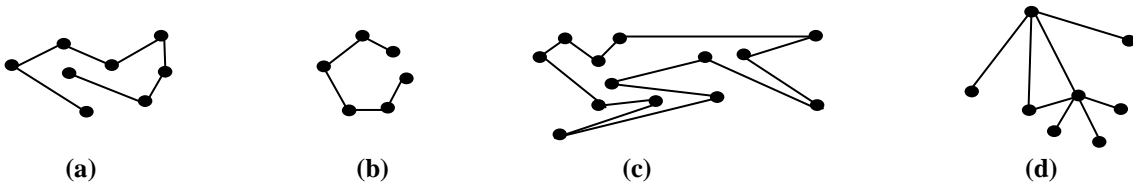


Figure 2.6 Convex Configuration for a Closed Chain

**Exercise 2.1** If possible, reconfigure each linkage into a canonical form for a chain.



An *orthogonal chain* is one in which all angles between adjacent links are  $90^\circ$ . For an example, see Figure 2.7.

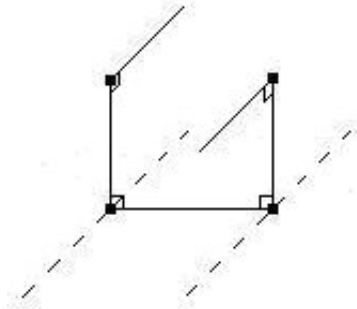


Figure 2.7 An Orthogonal Chain

### Configuration and Configuration Space

The *configuration* or *placement* of a linkage is a particular specification of all link endpoints of a linkage, including link orientations and joint angles. A *reconfiguration* occurs if a linkage can be continuously moved, satisfying its defining constraints, from an initial configuration to a final configuration. In a reconfiguration of a linkage all link lengths must remain the same, stay within their defining space, and not violate any imposed intersection conditions. As an example see Figure 2.8, a replication of Figure 1.1, which shows both the initial and final configurations occurring through the reconfiguration of a pantograph.

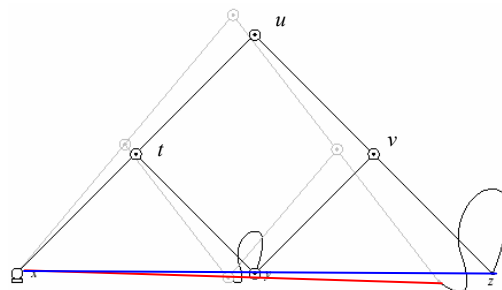


Figure 2.8 Two Configurations of a Pantograph

The *configuration space* of a linkage is the set of all possible reconfigurations of the linkage. An example, Figure 2.9 shows all possible reconfigurations of the linkage as the circle is generated by a complete rotation ( $0 \leq \theta \leq 2\pi$ ) of a single link, pinned at the universal joint  $x$ . The point  $P$  can “reach” any point on the circle centered at  $x$  with a radius of the length of the link. The configuration space consists of the disk swept by the link centered at  $x$ .

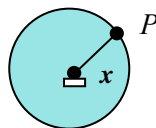


Figure 2.9 – Configuration Space of a Pinned Link

### Self-intersection

The *self-intersection of a chain* occurs whenever two non-adjacent links of the chain share a point. Although a time physical chain would not allow self-intersection, for mathematical simplicity we will let this to occur unless stated otherwise. As an example, see Figure 2.10.

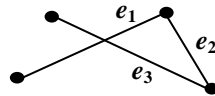


Figure 2.10 Link  $e_3$  Intersects Link  $e_1$

### Flattenable

A chain is called a *flattenable chain* if it can be folded (without self-intersection) to lie entirely on a plane. For an example, see Figure 2.11.

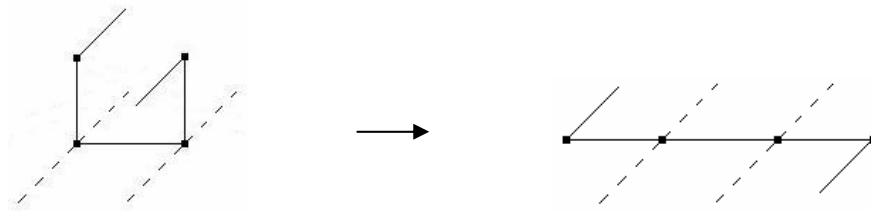


Figure 2.11 A Flattenable Chain

Demaine, Connelly, and Rote have proven in [DCR] that all 2-D chains, and therefore all flattenable chains, can be straightened, i.e. moved to a linear configuration.

**Open Problems:** There are many unsolved problems involving linkages. One of these is: Can all motions be performed without linkages crossing themselves? (cf. [DO])

## 3. Reachability, Linear Motion, and Kempe's Universality Theorem

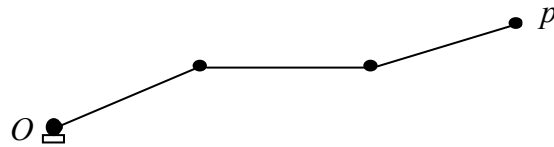
### Reachability

The *reachability* of a linkage refers to whether a particular point (usually a link endpoint) of a linkage can reach a given point in a given space. It is often important to determine all the points that a particular link can reach. For example, in Figure 2.9 the circle illustrates all the points which that single link can reach. An internal joint  $v_i$ ,  $i = 1, \dots, n - 1$  is said to be *kinked* if its two incident links  $e_i$  and  $e_{i+1}$  are not collinear, i.e., the angle between them is not  $0$  or  $180^\circ$  (or a multiple of  $180^\circ$ ). A linkage that is pinned is called an *arm*. For example, a pantograph is an arm, since it is pinned at one of its endpoints and the single link in Figure 2.9 is an arm. The *median*



**link** of an arm is the link  $e_m$  that includes the midpoint of the arm when all links are stretched out straight in a line (or either link incident to the midpoint if it falls at a joint).

The *Two-Kinks Theorem* states if an  $n$ -link arm  $C$  can reach a point  $p$ , it can reach  $p$  with at most two internal joints kinked. The two kinked joints may be chosen to be at either end of the median link. Figure 3.1 is an example of 3-link arm pinned at  $O$  where the median link is the middle link.



**Figure 3.1 3-Link Arm Pinned at  $O$**

**Exercise 3.1** Experiment with how far a 2-arm linkage can reach.

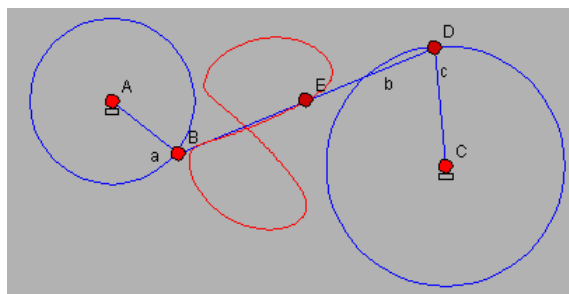
Given a 2-arm linkage where one vertex is free, the middle joint is universal, and the other vertex is pinned, but edge of the pinned vertex is allowed to move in any angle. What is the reachability of the free vertex for this linkage, i.e. the set of points that it sweeps out, given that the link with the pinned joint has:

- (a) a longer length than the other link?
- (b) the same length as the other link?
- (c) a shorter length than the other link?

### Approximate and True Linear Motion

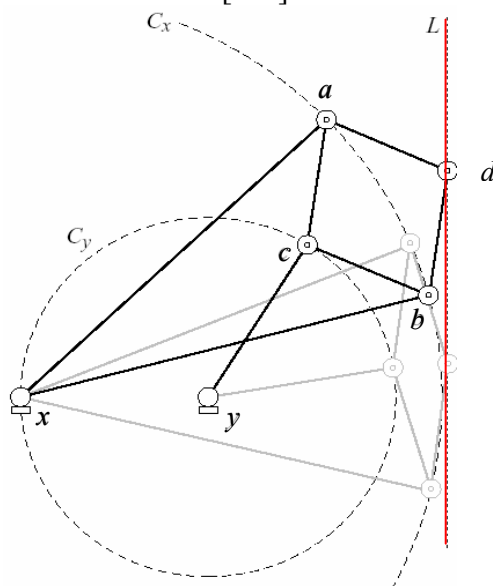
Some of the earliest work done in the study of linkages tracing curves began with James Watt in 1784 when he developed a linkage that nearly traced out a straight line. In 1864, Charles-Nicholas Peaucellier developed a linkage that traced a straight line by converting circular motion into true linear motion. Independently, Lippman Lipkin developed the same linkage and published a detailed solution in 1871. In 1875, A. B. Kempe published a proof of a theorem known as the *Universality Theorem*. Some important results in the development of useful linkages are *Watt Parallel Motion*, the *Peaucellier Linkage*, *Kempe's Linkage Parallelogram*, the *Contraparallelogram*, and *Kempe's Multiplier*. These linkages lead to *Kempe's Universality Theorem*, which stated that any algebraic curve can be traced by a linkage. We will now review these earlier developments to gain some knowledge of how these linkages work.

The **Watt Parallel Motion** (Figure 3.2) converts circular motion to nearly linear motion. Note joints A and C are pinned, the joints B and D are free to move, and joint E, the mid-point of BD, is a joint whose incident links are fixed at  $180^\circ$ . As B and D move on their respective circles, E traces the locus of points which looks like a figure eight. Notice part of the figure eight is nearly straight compared to the line segment BD. For more careful examination, an animation of this motion can be found at the web reference site [3].



**Figure 3.2 Watt Parallel Motion**

The *Peaucellier linkage* (Figure 3.3) converts circular motion to true straight line motion. It was the first straight-line mechanism to be discovered. Note joints  $x$  and  $y$  are pinned, the joints  $a$ ,  $b$ , and  $c$  are free to move, and joint  $d$  draws the straight line  $L$ . An animation showing the movement of this linkage can be found at the web reference site [4]. For a proof that the Peaucellier linkage is exactly linear motion see [DO].



**Figure 3.3 The Peaucellier Linkage**

### **Kempe's Linkages and Universality Theorem**

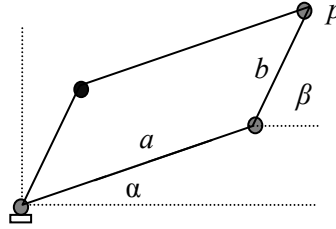
A. B. Kempe's *Universality Theorem* is one of the most significant results in the study of linkages.

*Kempe's Universality Theorem* [KM]

Let  $C$  be a bounded portion of an algebraic curve in the plane. Then there exists a planar linkage such that the orbit of one joint is precisely  $C$ .

An algebraic curve, over the real or complex numbers, is an equation of the form  $f(x, y) = 0$ , where  $f(x, y)$  is a polynomial in  $x$  and  $y$  with real or complex coefficients. The following are examples of algebraic curves:  $x^2 + 3x + 1 = 0$ ,  $xy^2 = 0$ ,  $x^2y + 3xy + (2 + 3i)y + 5i = 0$ .

The phrase “orbit of one joint” refers to the curve traced by the movement of the joint. We saw this type of tracing earlier when using the pantograph. The *parallelogram* linkage (Figure 3.4) developed by Kempe is fundamental to the proof of his theorem. This linkage uses joint  $p$  to draw an algebraic curve. An animation motion of this linkage can be found at the web reference site [5].



**Figure 3.4 The Linkage Parallelogram**

The following reasoning explains how the parallelogram can be used to draw an algebraic curve [DO]. Let the algebraic curve be defined by the polynomial equation  $A(x, y) = 0$  and traced out by the joint  $p$ , which is located on the parallelogram as shown in Figure 3.4. Note that the coordinates of  $p = (x, y)$  can be represented in terms of the cosines of angles:

$$\begin{aligned} x &= a \cos \alpha + b \cos \beta \\ y &= a \cos (\alpha - 90^\circ) + b \cos (\beta - 90^\circ) \end{aligned} \quad (3.1)$$

Substituting (3.1) into  $A(x, y)$  and repeatedly applying the trigonometric identity

$$\cos \theta \cos \Psi = \frac{1}{2}[\cos(\theta + \Psi) + \cos(\theta - \Psi)] \quad (3.2)$$

converts powers and products of  $x$  and  $y$  into cosines of the sums of angles, resulting in the following general form for the polynomial  $A(x, y)$ :

$$A(x, y) = c + \sum_i c_i \cos(r_i \alpha + s_i \beta + \delta_i) \quad (3.3)$$

where  $c$  and  $c_i$  are constants,  $r_i$  and  $s_i$  are integers, and  $\delta_i$  is 0,  $-90^\circ$ , or  $90^\circ$ . The  $i$ -term in the summation in Equation 3.3 is achieved by a link of length  $c_i$  at a suitable angle. The summation across all  $i$  is then shifted by the value  $c$ . Thus the problem reduces to constructing an angle of the form  $r_i \alpha + s_i \beta + \delta_i$  from  $\alpha$  and  $\beta$ .

As an example, the term  $xy^2$  in  $A(x, y) = 3 + xy^2$  expands and reduces to

$$\begin{aligned} \frac{1}{4} [(a^3 + 2ab^2) \cos \alpha - a^3 \cos(3\alpha) + ab^2 \cos(\alpha - 2\beta) + a^2b \cos(2\alpha - \beta) + \\ (2a^2b + b^3) \cos \beta - b^3 \cos(3\beta) - 3a^2b \cos(2\alpha + \beta) - 3ab^2 \cos(\alpha + 2\beta)] \end{aligned} \quad (3.4)$$

Therefore,

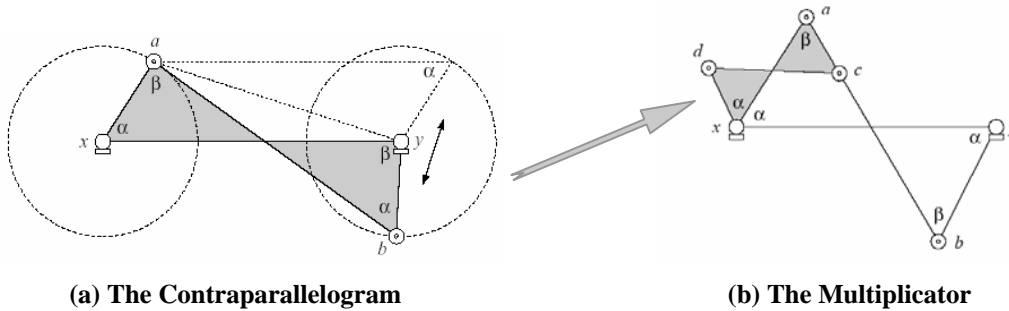
$$\begin{aligned} A(x, y) &= 3 + xy^2 \\ &= 3 + \frac{1}{4} [(a^3 + 2ab^2) \cos \alpha - a^3 \cos(3\alpha) + ab^2 \cos(\alpha - 2\beta) + a^2b \cos(2\alpha - \beta) + \\ &\quad (2a^2b + b^3) \cos \beta - b^3 \cos(3\beta) - 3a^2b \cos(2\alpha + \beta) - 3ab^2 \cos(\alpha + 2\beta)] \end{aligned}$$

**Exercise 3.2** Understanding the general form of the polynomial  $A(x, y)$ .

- (a) Use trigonometry to show that the equations in (3.1) are correct.
- (b) Determine the specific values in Equation 3.3, where  $A(x, y) = -2 + xy^2$ . (Use Expression (3.4) to find the value  $c$ , the range of  $i$ , and the corresponding values  $c_i$ ,  $r_i$ , and  $s_i$ .)

Kempe showed that the planar linkage in the *Universality Theorem* can be constructed with three linkages: a *multiplicator* for multiplying an angle by a positive integer; an *additor* for adding any two angles; and a *translator* for translating a motion.

The first linkage to be examined will be the *multiplicator*. This linkage depends on the *contraparallelogram* linkage, Figure 3.5(a), which is a four-bar linkage formed by flipping two adjacent sides of a parallelogram across the diagonal they determine. Note there is no joint at the point at which the links  $xy$  and  $ab$  cross. The *contraparallelogram* is an example of a self-intersecting linkage. An animation of the *contraparallelogram* motion can be found at the web referenced site [6]. The *multiplicator*, Figure 3.5(b), was created by Kempe when he joined two similar *contraparallelograms* sharing the same angle  $\beta$  at joint  $a$ , effectively multiplying the angle  $\alpha$  by 2. An animation of the motion of a two-angle *multiplicator* and a three-angle *multiplicator* can be found at the web reference site [7].



**Figure 3.5**

Now examine the *additor* and the *translator*. The *additor* linkage, which adds two angles together, relies on the *multiplicator*, but only in its times-2 version. The details of the additor construction can be found in [DO]. The *translator* is the simplest linkage. Its purpose is to copy a link to a different location maintaining the same orientation. Basically, the *translator* is the action of a pantograph, discussed in Section 1. The details of the translator construction can be found in [DO]. Note that Kempe’s version of the translator had a flaw in its design which was later corrected by Kapovich and Millson [KM].

The overall design can be understood in terms of Equation 3.3, which is repeated below:

$$A(x, y) = c + \sum_i c_i \cos(r_i \alpha + s_i \beta + \delta_i)$$

By the *multiplicator* any angle can be multiplied by an integer  $r_i$ . Angles can be added by using the *additor*. Terms in the sum are combined by the *translator*. Applying these linkages in an appropriate structure yields a joint  $p'$  that remains a distance  $A(x, y) - c$  from the  $y$ -axis. The joint  $p'$  is forced, using a Peaucellier linkage, to stay on the vertical line  $x + c = 0$ . This in turn forces  $p$

to stay on the curve  $A(x, y) = 0$ . Thus, this complex linkage has the joint  $p$  follow the equation  $A(x, y) = 0$  within the range of  $x$ -values provided by the parallelogram linkage in Figure 3.4. See Figure 3.6 which shows how the pieces fit together. Note, in this figure all joints labeled  $O$  are the same.

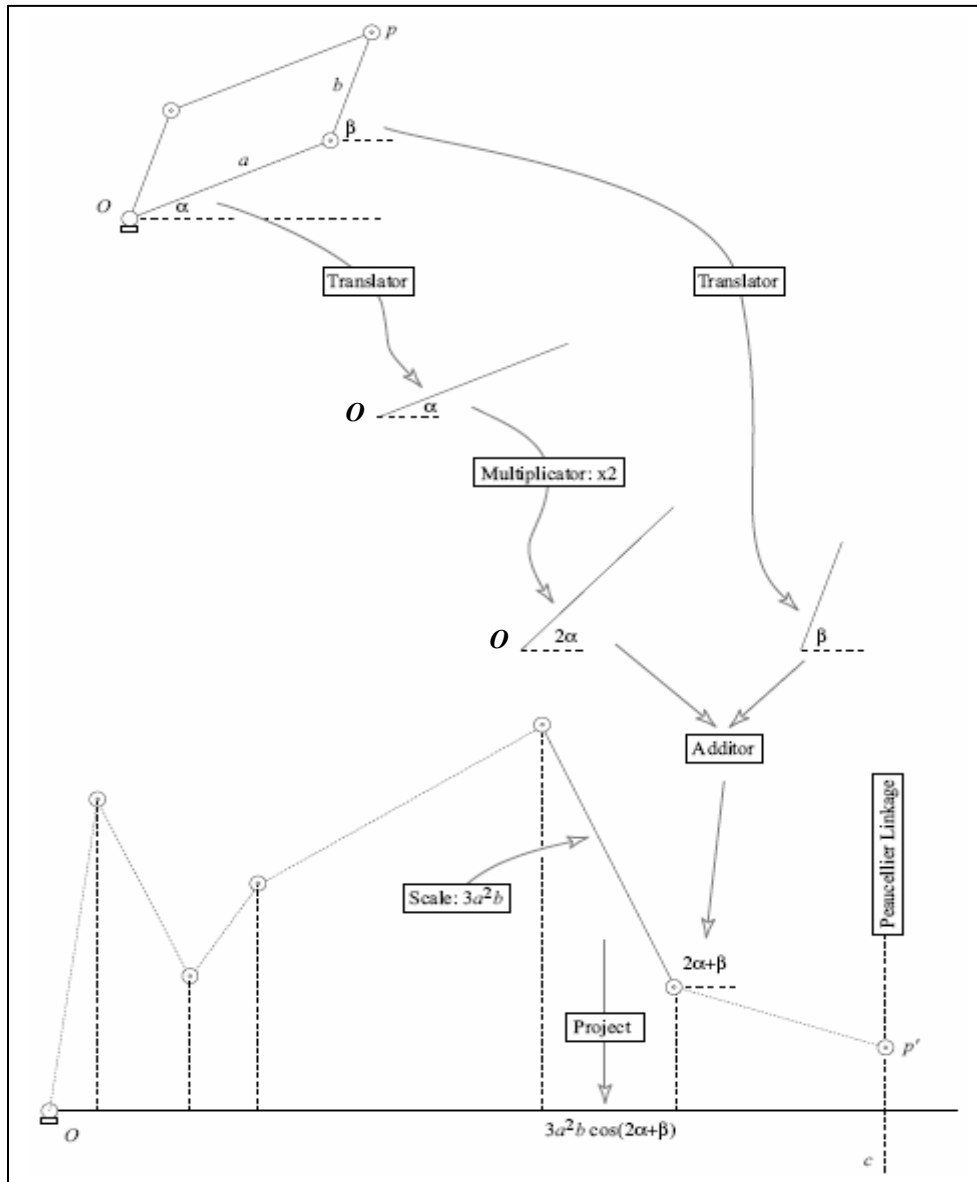


Figure 3.6 The Design of Kempe's Construction

Kempe's basic ideas were correct, but there were some flaws in his proof. As mentioned in the introduction, Kapovich and Millson [KM], in 2002, published the first complete and detailed proof correcting the flaws. Their proof follows the spirit of Kempe's theorem but employs modified versions of many of Kempe's linkages, and avoids his *multiplicator* in favor of a more complex linkage for multiplication. This linkage incorporates three *translators*, a *pantograph*,

three *inversors* (which are modified Peaucellier linkages), and a modified *additor*. The properties of this last linkage are more easily controlled than was Kempe's *multiplicator*.

In the 1970's William Thurston (U. California, Davis) investigated Kempe's ideas and suggested that: *One can design a linkage that will sign your name!* The idea was that as long as the signature is the union of continuous curves, one can approximate the pieces by algebraic equations and then use Kempe's approach to realize these pieces with a linkage. Although this is theoretically possible, no one has built such a complicated linkage to do this. In fact, by using the new linkages introduced by Kapovich and Millson the situation became even more complicated. But, in geometric modeling there do exist certain spline curves, called B-splines, that can draw a person's signature. These spline curves have structural definitions that are strikingly similar to links. To begin investigating this similarity, we will now examine a modified linkage that will give us more flexibility and allow us to draw a certain class of curves known as Bézier curves, which are a special case of the B-spline class of curves. In G. Farin's book listed in the Further Reading section below, one can find more information on splines and Bézier curves.

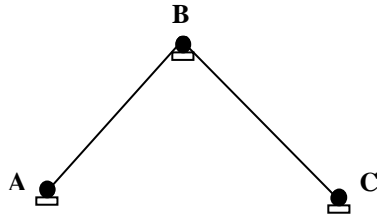
#### **4. Designing a Modern Linkage: Relaxing Constraints on the Linkage**

##### **A Modern Linkage**

So far we have seen examples using the joint of a linkage to draw a curve. The links in these "classical" linkages must always remain the same length and each joint remains at the endpoint of a link through all movements. Classical linkages have been based on a single force, like a crank, with all links mechanically coordinated by the linkage design. Now we will modify these linkage constraints by allowing *telescoping links* and *sliding joints*. *Telescoping links* are rigid links that can continuously change from one length to another within a finite range. *Sliding joints* are joints that are allowed to move along a link from one end to the other. This type of linkage will be referred to as a *modern linkage*. Modern linkages are possible because of modern developments in computer technology, electronic motors, and mechanical design [WK]. Movements of a modern linkage are often coordinated electronically. A modern linkage will allow us to simplify the drawing mechanism, reducing the complexity of the linkage used by Kempe, Kapovich, and Millson in the proof of the *Universality Theorem*.

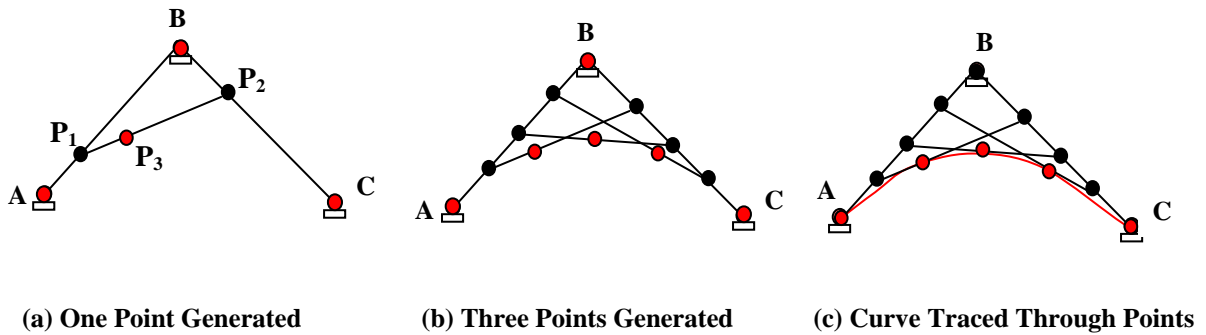
The following constraints will be applied to the modern linkage construction of an  $n^{\text{th}}$  degree Bézier curve defined by  $n + 1$  points, where  $n > 0$ . This construction follows the de Casteljau algorithm for constructing a Bézier curve [PW]. Each step of the construction will be illustrated by the development of a 2<sup>nd</sup> degree (quadratic) Bézier curve.

1. Choose any  $n + 1$  distinct points,  $n > 0$ . Through these points connect  $n$  distinct line segments to form a simple path where each point is shared by one or at most two line segments. These given points correspond to the pinned joints and the line segments joining them correspond to the links. Together these joints and links form the frame which is by itself a fixed-angle linkage. For a quadratic Bézier curve, let  $n = 3$ , where the initial three points (pinned joints) are A, B, and C and the line segments (links) are AB and BC. See Figure 4.1.



**Figure 4.1 Frame for Quadratic Bézier Curve Construction**

2. Following the de Casteljau algorithm, the overall construction process generates one point at a time on the curve. To begin this construction, let a point be placed at a specific position on each initial line segment. The location depends on the length of each of the  $n$  segments and a common ratio  $r$  times the segment's length, giving the distance of that point from the start of the link. Point placement will always be from the relative start position, going from left to right, of each segment along the path. After each new point is placed on the  $n$  segments, lines are drawn between each consecutive pair of new points on each pair of consecutive lines, creating a new set of  $n-1$  line segments. Again the common ratio  $r$  is used to place new points in each of these newly generated lines, a process that is repeated until the final line segment is drawn and the final point is placed on that segment maintaining the same common ratio  $r$  of distance along its length. The final point placed is a point on the curve. This entire process is then repeated for as many ratios  $0 \leq r \leq 1$  as necessary to determine the shape of the curve. See Figure 4.2 (a), where points  $P_1$  and  $P_2$  are placed at a distance satisfying the common ratio of  $r = \frac{1}{4} = \frac{|AP_1|}{|AB|} = \frac{|BP_2|}{|BC|}$ , line  $P_1P_2$  is drawn, and then the point  $P_3$  is placed  $\frac{1}{4}$  the distance along  $P_1P_2$ , satisfying  $r = \frac{1}{4} = \frac{|P_1P_3|}{|P_1P_2|}$ . Consequently, the point  $P_3$  is on the Bézier curve.



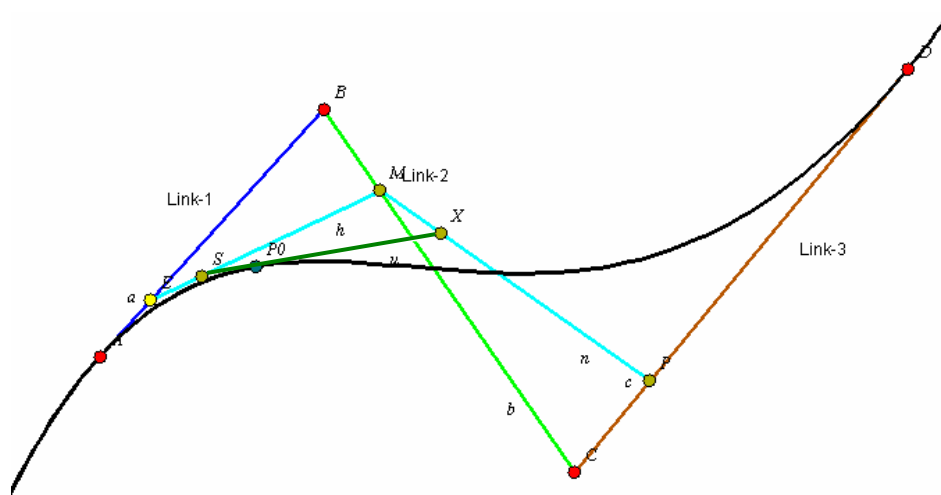
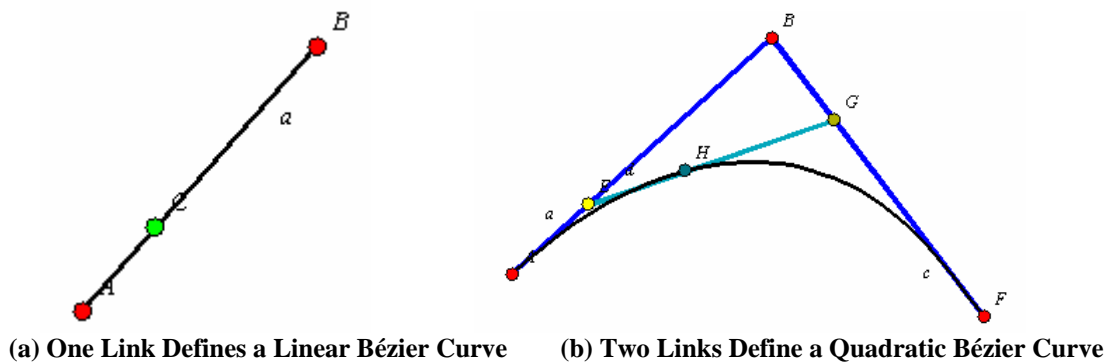
**Figure 4.2 Generating Points on a Quadratic Bézier Curve**

Following the same process a different common ratio is used to generate another set of new lines, resulting in another point being placed on the curve. In this way, as many points as desired can be constructed on the curve. See Figure 4.2 (b) where two additional point are placed on the quadratic curve for different ratios  $r = \frac{1}{2}$  and  $r = \frac{3}{4}$ . After enough points are drawn, a smooth curve is traced through the points forming the line. The curve would look similar to the one in Figure 4.2 (c).

3. Note all the line segments constructed to generate points on the curve are of a fixed length. Unfortunately, there would need to be an uncountable number of these corresponding to an uncountable number of ratios between 0 and 1 in order to generate every point on the continuous curve. To avoid this impossible process, we can use

$n(n - 1)/2$  telescoping links and  $n(n + 1)/2$  sliding joints to create a linkage to draw the curve [Fact05b]. To see how this works in this modern linkage, first place a sliding joint at the beginning of each of the  $(n + 1)(n + 2)/2$  links generated by Step 1 and the first application of the process in step 2. In general, the construction will allow the corresponding sliding joint  $P_i$  to move from the start to end on each link  $L_i$ , always maintaining the same ratio  $r$  on all links  $L_i$  as  $r$  varies continuously from 0 to 1. As an example consider the quadratic Bézier curve in Figure 4.2 (a), where the fixed-length link AB has length  $|AB|$ , the fixed-length link BC has length  $|BC|$ , and  $P_1P_2$  is a telescoping link.  $P_1$  is a sliding joint on AB,  $P_2$  is a sliding joint on BC, and  $P_3$  is a sliding joint on  $P_1P_2$ . For all links  $r = |AP_1|/|AB| = |BP_2|/|BC| = |P_1P_3|/|P_1P_2|$  as  $r$  varies continuously from 0 to 1.

4. The final sliding joint placed on the final telescoping link in the construction traces the curve as the joint moves from start to end on the link, while  $r$  varies continuously from 0 to 1. See the following examples in Figure 4.3 constructed with the *Cinderella* software [8]. In Figure 4.3, all the red dots are pinned joints, (a) is a 1<sup>st</sup> degree (linear) Bézier curve, (b) is a 2<sup>nd</sup> degree (quadratic) Bézier curve, and (c) is a 3<sup>rd</sup> degree (cubic) Bézier curve with a point of inflection.



(c) Three Links Define a Cubic Bézier Curve

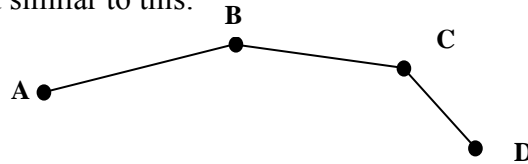
Figure 4.3 Linkages Tracing Bézier Curves



This modern linkage construction can be applied to trace any  $n^{\text{th}}$ -degree Bézier curve in two or three dimensional space. The mathematical details for constructing this modern linkage are given in [Fact05a].

**Exercise 4.1** Understanding the construction of the modern and classical linkages.

(a) Using the de Casteljau algorithm, construct eight points on a cubic Bézier curve defined by three points and four links positioned similar to this:



(b) Based on the curve constructed in (a), draw the modern linkage at the specific ratio  $r = \frac{1}{2}$  and identify the pinned joints, the fixed-length links, the telescoping links, the sliding joints, and the joint that traces the curve. Do the links in this modern linkage cross? Explain your answer.

(b) In Figure 4.3 (c), do the links cross in this modern linkage of a cubic Bézier curve? Explain your answer.

(c) Create a linkage that can trace only one letter in the alphabet or a number.

(d) Create a linkage that can draw one geometric figure.

(For (c) and (d), build a physical model or use a software tool like *Cinderella* at the web reference site [8] or *Geometer's Sketchpad* at the web reference site [9] to make the linkages.)

**Open Problems:** Here are some interesting unsolved problems involving both classical and modern linkages.

1. Can you create a classical linkage that will
  - a. draw a 1<sup>st</sup> degree Bezier curve? (This one is solved.)
  - b. draw a 2<sup>st</sup> degree Bezier curve?
2. Can a modern linkage, based on the B-Spline underlying structure, be constructed to write a person's name?

## ***Part II. An Application of Linkages: Protein Folding***

### **5. Protein Folding**

#### **Introduction**

Dubbed ‘Nature’s Robots<sup>1</sup>’, proteins are the building blocks of cells and organs. They act as biological workhorses to perform many of our body’s vital tasks, from contracting muscles to pumping salts through membranes. They also play the more heroic role of antibodies, fighting off disease that may attack our body. On the other hand, we have recently seen that proteins can also be villainous by assuming a different shape to become *prions* (pronounced pree-ahns), which attack brain cells. One such disease, dubbed bovine spongiform encephalopathy (BSE), was first observed in cows raised in England and has become more widely known as ‘mad cow’s disease’<sup>2</sup>.

The fact that proteins by themselves can cause disease came as quite a shock to the scientific community. This is because proteins were never thought to be infectious on their own, unlike larger agents such as viruses or bacteria, which *are* composed of proteins. According to R. L. Guyer [10], ‘Prions enter cells and apparently convert normal proteins found within the cells into prions just like themselves. The normal cell proteins have all the same "parts" as the prions--specifically the same amino acid building blocks--but they fold differently’. This is because a protein, acting like a chain, normally folds into a tight helical shape and the final form determines its function, but a prion on the other hand maintains a more open structure. And the process of how a healthy protein refolds into a prion is unclear. However, what is clear is the need to accurately understand protein folding.

#### **Structure of Proteins**

A protein is a large polymeric molecule consisting of a peptide chain of amino acids (monomers) linked together by amide (carbon-nitrogen) bonds and folded into a tight organized structure (Figure 5.1). The final structure depends on amino acid interactions with water, intra-molecular hydrogen bonds and salt links. The amino acids involved and their linear sequence largely determine the structure and thus function of the protein.

Proteins are produced by ribosomes, which are tiny granules that translate messenger RNA molecules into amino acid chains (see the web reference site [11]). Once a protein chain completely exits the ribosome, it begins to coil into a state that minimizes the energy of interaction with water, which may be either hydrophilic (attractive) or hydrophobic (repulsive). Minimization of intra-molecular hydrogen bonds between neighboring or distant amino acids is also a major consideration. However, no algorithm exists for describing this folding.

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<sup>1</sup> *Nature’s Robots*, Charles Tanford and Jacqueline Reynolds

<sup>2</sup> <http://www.pbs.org/wnet/nature/holycow/madcow.html>

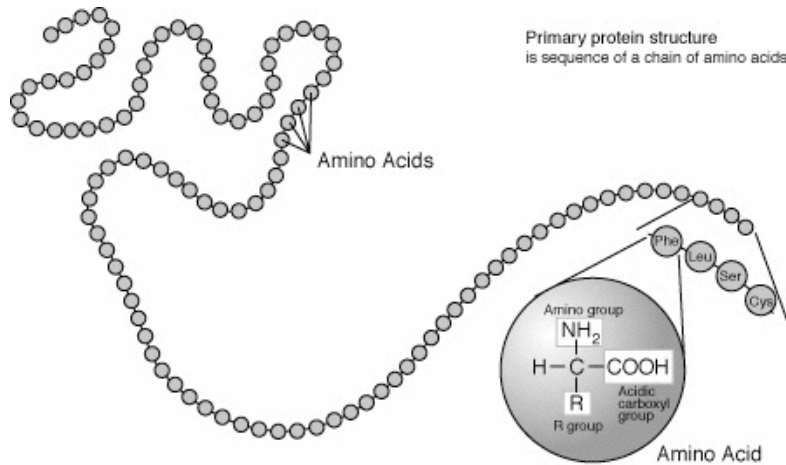


Figure 5.1

The fact that such protein chains are never knotted has led O'Rourke et al (cf. [DO]) to develop a corresponding mathematical model for describing protein production involving two symmetric cones, known as the *conical* model (Figure 5.2). Here, the region where proteins are manufactured is modeled by the interior of a cone  $C_\alpha$  with conical angle  $\alpha$  and radius  $r$ . Each amino acid link is assumed to emerge one by one out through the tip of  $C_\alpha$  and into the interior of its inversion, i.e. a cone  $B_\alpha$  symmetric to and having the same conical angle and radius as  $C_\alpha$ . The exiting of a single link  $v_0v_1$  is described in the series of illustrations in Figure 5.3. In the first frame vertex  $v_0$  makes its exit through the tip of the cone at initial time  $t_0$ . The second frame represents the exiting of the link  $v_0v_1$  during  $t_0 < t < t_1$  and the third frame shows the completion of this process in which  $v_1$  exits at final time  $t_1$ . The process then repeats for the next adjacent link  $v_1v_2$ . Since it is assumed that during this transition that links  $v_0v_1$  and  $v_1v_2$  are confined to the cones  $B_\alpha$  and  $C_\alpha$ , respectively, it follows that every dihedral angle between adjacent links must be at least  $180 - 2\alpha$  degrees.

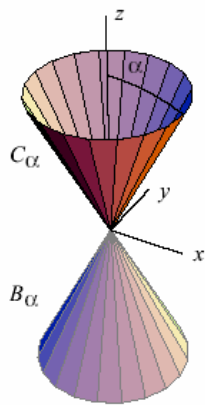


Figure 5.2

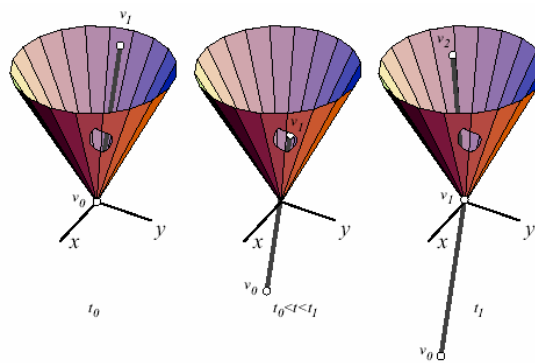


Figure 5.3

Chains constructed from the conical model are called  $\alpha$ -*producible* chains. The fact that the conical angle cannot exceed  $90^\circ$  restricts the kinds of proteins chains that can be manufactured.

In particular, it has been established that  $\alpha$ -producible chains can always be *flattened* (cf. [DO], [DLO]), i.e. they always permit a flat (planar) reconfiguration, meaning that one can reposition them (without self-intersection) to lie flat along a plane. This is because every  $\alpha$ -producible chain configuration can be moved to a canonical (helical)  $\alpha$ -CCC configuration and therefore to any other  $\alpha$ -producible configuration (cf. [DO]). To visualize a  $\alpha$ -CCC configuration, we reconsider the manufacture of a protein using the conical model but now assume the cones  $C_\alpha$  and  $B_\alpha$  to be confined inside a square column having sides of width  $2r$  and infinite length in both directions (Figure 5.4). As a result, only protein chains whose links are positioned in an open helical configuration will fit inside the square column as it exits cone  $B_\alpha$  (Figure 5.5). If a link produced in cone  $C_\alpha$  (say  $v_1v_2$  in Figure 5.3) does not allow this fitting, then it can be reconfigured to permit this by pivoting itself about  $v_1$ . This intuitively reveals why every  $\alpha$ -producible chain configuration can be moved to a  $\alpha$ -CCC configuration. Moreover, from this  $\alpha$ -CCC configuration it is then possible to straighten, and therefore flatten, the chain by simply pulling the ends along opposite directions.

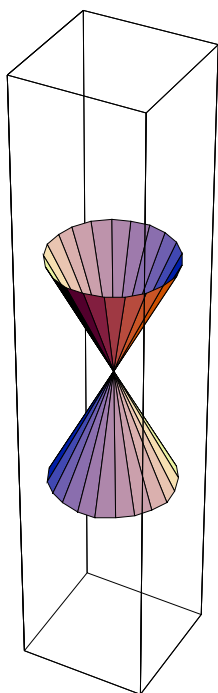


Figure 5.4

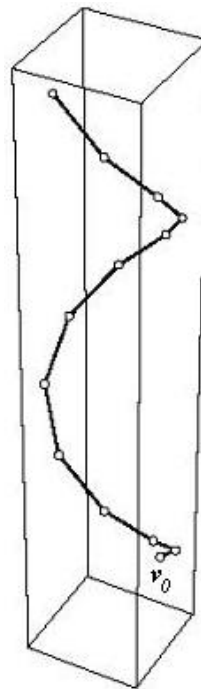


Figure 5.5  $\alpha$ -CCC Configuration

A chain that *cannot* be flattened is said to be a *locked* chain. Therefore,  $\alpha$ -producible chains based on the conical model can never lock, a property shared by proteins. However, it is not known if the conical model provides an accurate description of protein production as instructed by Nature.

In general however not all chains are flattenable. The classic example is the ‘knitting needles’ chain, a 5-chain that is locked in space, as illustrated in Figure 5.6.

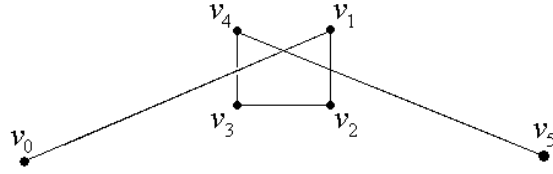


Figure 5.6

Any attempt to unlock the chain  $v_0v_1v_2v_3v_4v_5$  will require straightening the three middle links as far as possible. However, their combined length, denoted by  $r = v_1v_2 + v_2v_3 + v_3v_4$ , is shorter than either of the end links,  $v_0v_1$  and  $v_4v_5$ . This is demonstrated in Figure 5.7, which shows both end links extending past the circle of radius  $r$  centered at  $v_1$ . It follows that neither of these end links can be pulled back completely through the knot to untie the chain. As a result, the chain cannot be flattened since it cannot even be unknotted.

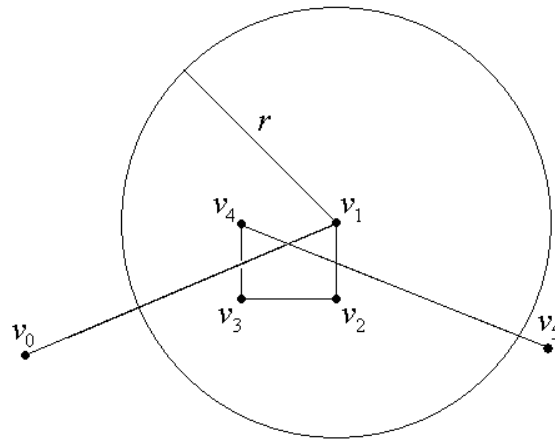


Figure 5.7

Chains can also lock if their links are restricted to dihedral motions, i.e. each link is forced to pivot at a fixed-angle about a joint. For example, if the 2-chain in Figure 5.8 is a fixed-angle chain, then edge  $v_1v_2$  is restricted to pivoting about vertex  $v_1$  at angle  $\alpha$  (its full motion is represented by the circle centered at  $v_0$  shown in the same figure).

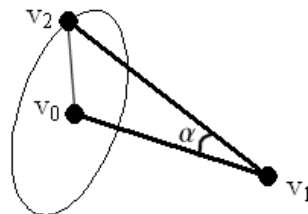


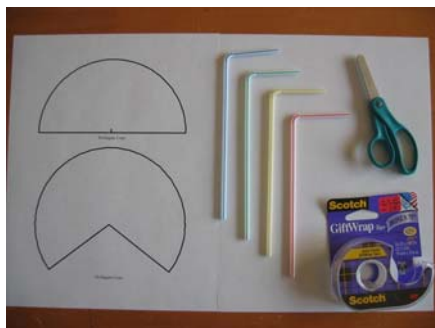
Figure 5.8

**Note:** Recall from Section 2, Part I, that a 2-D chain *without* fixed angles can always be straightened (and hence can never lock) (cf. [DCR], [DO]). Some results concerning the straightening of 3-D chains appear in [B et al]. Some interesting animations of chains being unlocked can be found in [12].

**Exercise 5.1 (Hands-On Activity For Students):** Students can build their own models of protein molecules and ‘manufacture’ them based on the conical model. Teams of 2-3 students should be formed.

**I. Required Materials (Figure 5.9):**

11. Paper cones (available from cut-out drawings of 30-degree and 45-degree cones appearing in A.2 of the Appendix or use drinking cones located at water fountains in your school if available)
12. Plastic straws with flexible joints
13. Scissors
14. Tape



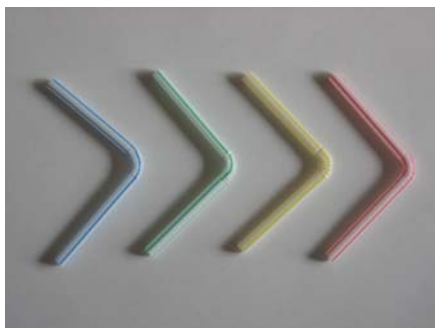
**Figure 5.9**

**II. Instructions:**

B. Constructing a Protein Chain (Figure 5.10):

- Step 1: Taper the long end of each straw to create a symmetric joint
- Step 2: Make a half-inch slit at one end of each straw
- Step 3: Slide the non-slit end of one joint into the slit end of another joint
- Step 4: Tape the two joined ends to form a chain (Figure 5.11)

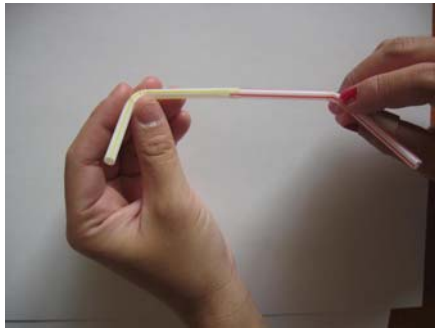
To make a longer chain with additional links, repeat steps 1-4 (Figure 5.12).



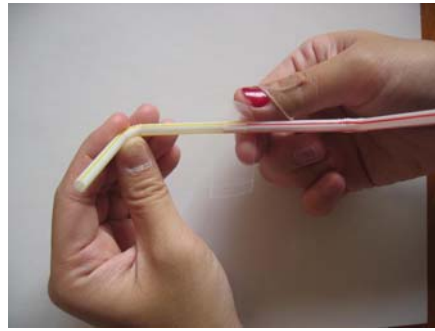
**(a) Step 1**



**(b) Step 2**



(c) Step 3



(d) Step 4

Figure 5.10



Figure 5.11

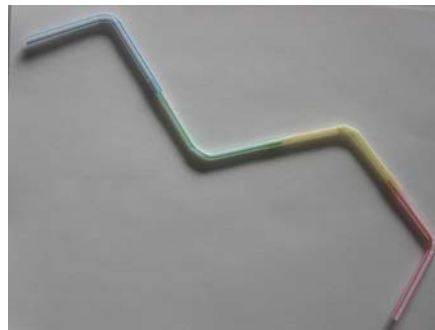


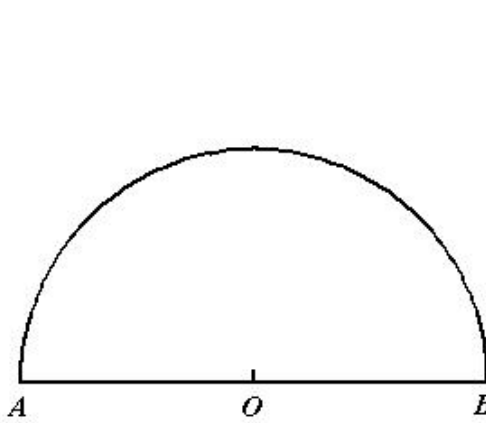
Figure 5.12

B. Constructing a Cone (Figure 5.13)

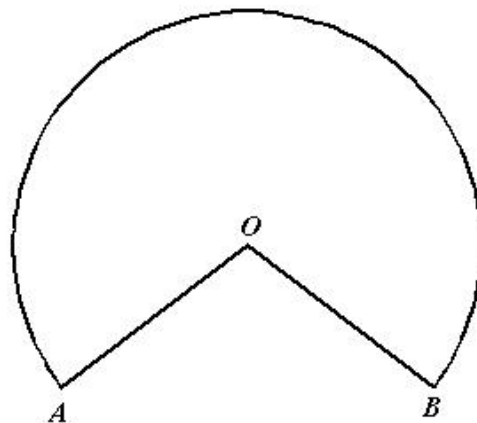
Step 1: Cut out drawings of 30-degree and 45-degree cones (Figure 5.13)

Step 2: For each drawing align edge AO with edge BO and tape them together to form a cone resembling those in Figure 5.14.

Step 3: Cut off the tip of each cone to form a 1/4-inch exit hole (Figure 5.15).



(a) 30-Degree Cone



(b) 45-Degree Cone

Figure 5.13

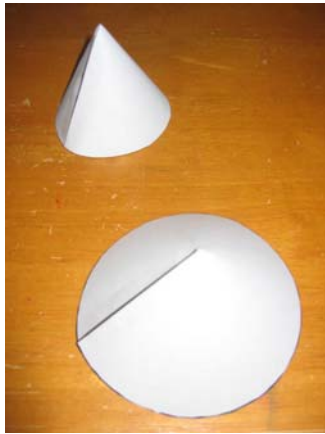


Figure 5.14



Figure 5.15

### III. Experiment

3. Manufacture two different types of chains: one where every dihedral angle between adjacent links is greater than  $180 - 2\alpha$  ( $\alpha$  is the conical angle, i.e. either 30 or 45 degrees) and a second where at least one dihedral angle is less than  $180 - 2\alpha$  (Figure 5.16)
4. Try feeding each chain link by link through the exit hole as illustrated in Figure 5.17 and record which chain meets obstruction (do not force the chain through). Note: Be sure to keep all dihedral angles fixed at their original values.
5. Which chains are producible, i.e. are able to pass through the exit hole entirely without obstruction? Make a report of your results.



(a) Producible Chain



(b) Non-Producible Chain

Figure 5.16



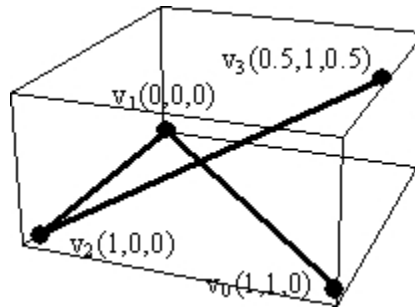


Figure 5.17

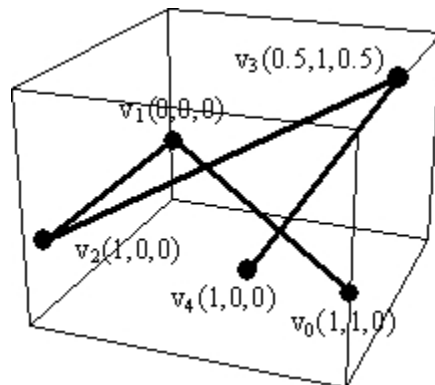
**Exercise 5.2:** Determine whether or not the following 3-D chains with universal joints can be flattened without self-intersection, i.e. links are not allowed to cross each other during and after the unfolding. If so, then describe the unfolding. If not, then explain why not.

**Note:** Each chain illustrated below is drawn inside a box that is delineated to provide the viewer with some perspective. Large black dots indicate nodes (with  $(x, y, z)$ -coordinates listed) and bold line segments connecting them indicate edges of the chain.

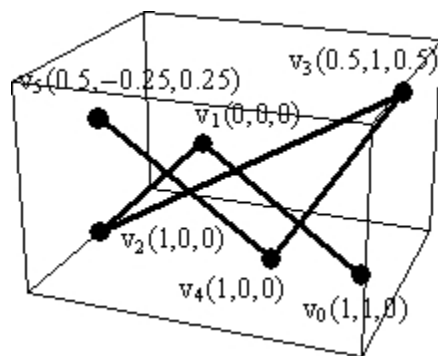
(a) 3-chain  $v_0v_1v_2v_3$



(b) 4-chain  $v_0v_1v_2v_3v_4$



(c) 5-chain  $v_0v_1v_2v_3v_4v_5$



**Exercise 5.3:** Assume now that the three chains in Exercise 5.2 above are fixed-angle so that each link is only allowed to pivot at a fixed angle (as determined by the drawn positions) about a joint. Determine whether or not each of these chains can still be flattened. If so, determine its flat (planar) configuration state by specifying the positions of each node. If not, then explain why not.

**Exercise 5.4:**

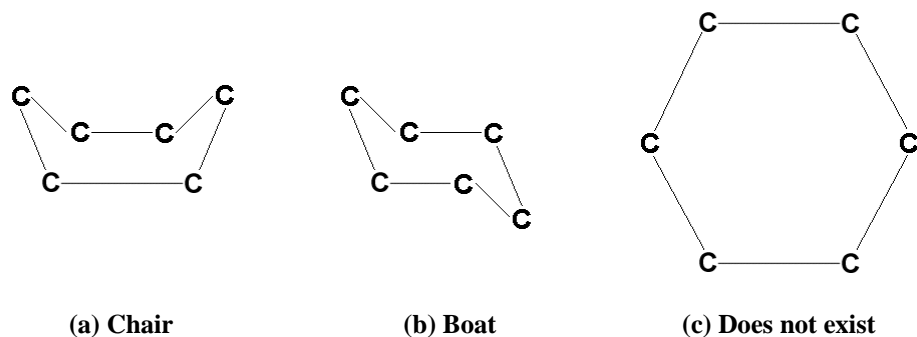
- Is every 4-chain in 3-D with universal joints flattenable?
- Is every orthogonal 4-chain in 3-D flattenable? (Note: Recall that an orthogonal chain is one in which all of its dihedral angles are  $90^\circ$ .)
- Is every orthogonal 5-chain in 3-D flattenable?

**Open Problems:** There are some interesting open problems relating to whether or not equilateral chains, i.e. those with equal link lengths, can lock (cf. [DO]).

- Can all 3D equilateral chains be straightened?
- Locked Length Ratio:* What is the smallest value of  $L \geq 1$  for which there exists a locked open polygonal chain in 3D, all of whose link lengths are in the interval  $[1, L]$ ? The value  $L$  is called the *length ratio* of the chain. Note: The knitting needles example shows that  $L$  is no bigger than 3.
- Locked Fixed-Angle Chains:* For which triples  $(\alpha, n, L)$  does there exist a fixed-angle  $\alpha$ -chain of  $n$  links and length ratio  $L$ ?

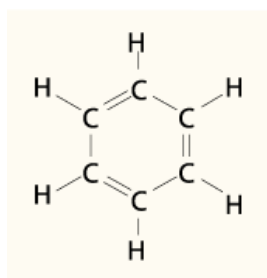
## 6. Molecule Rings

Many organic molecules are known to form interesting ring configurations of carbon atoms, which can be modeled as closed fixed-angle chains. Due to their confined energy levels, any two adjacent bonds (edges) between carbon atoms must all have the same fixed angle of approximately 109.5 degrees, called the *tetrahedral* angle; however, each bond is free to rotate. These tetrahedral angles obviously limit the number of distinct closed fixed-angle equilateral chains that can exist and explains why nature only exhibits certain kinds of molecule rings. For example, cyclohexane molecules (rings of six carbon atoms with all single bonds) are known to possess two non-planar configurations, referred to as the *boat* and *chair* forms (Figures 6.1(a) and 6.1(b), respectively).



**Figure 6.1**

Surprisingly, the simple hexagonal planar configuration shown in Figure 5.1(c) does not exist in nature. This again is due to the inherent property of single carbon-carbon bonds to form tetrahedral angles as explained by the theory of hybrid orbitals. On the other hand, alternating double bonds between carbon atoms allow the planar hexagonal configuration found in benzene molecules where all dihedral (interior) angles are  $60^\circ$  (Figure 6.2).



**Figure 6.2**

**Exercise 6.1:** A *closing* of an open chain is a reconfiguration without self-intersection where the end nodes are connected to form a closed chain. An *orthogonal* chain is a fixed-angle chain with all dihedral angles equal to  $90^\circ$ . Is it possible to close an orthogonal 3-chain? 4-chain? 5-chain? How many different closings are possible?

**Exercise 6.2:** A *perfect* closing of an orthogonal chain is one in which the resulting closed chain has all dihedral angles equal to  $90^\circ$ . Which orthogonal  $n$ -chains have perfect closings? For which integers  $n$ ?

### Concluding Remarks

Linkages are important structures with diverse physical applications. As man-made mechanisms they have produced many useful devices ranging historical from pantographs to steam engines and more modern tools such as windshield wipers and robotic arms. As natural mechanisms they take on the form of limbs and protein molecular chains. Mathematically, linkages are essentially graphs with many interesting properties. For example, the Two-Kinks Theorem states that any point reached by a given linkage can also be reached with at most two internal joints kinked. The most significant result is Kempe's *Universality Theorem*, which guarantees that every

algebraic planar curve can be traced by one joint of a suitable linkage. The difficulty of constructing such linkages is simplified through modern linkages. On the other hand, there are questions involving the locking, flattening, and straightening of 3-D chains that are still open, some with crucial ramifications towards the folding and unfolding of proteins and their manufacture based on the conical model. The authors do hope that readers will be fascinated enough with linkages to tackle some of the elementary open problems. Also, for the student interested in further reading and other open problems, we provide the following list. Good hunting!

### Further Reading

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[Fact05a] Factor, James D, "Designing Modern Linkages to Trace Bezier Curves". Proceedings of the 17<sup>th</sup> Canadian Conference on Computational Geometry, Windsor, Ontario Canada, August 10 -12, 2005.

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[WK] J. K. Waldron and G. L. Kinzel, *Kinematics, Dynamics, and the Design of Machinery*, John Wiley & Sons, Inc., 2004.

### **Web References Sited**

[1] [http://mathforum.org/sketchpad/java\\_linkages.html](http://mathforum.org/sketchpad/java_linkages.html)

[2] <http://www.ies.co.jp/math/java/geo/panta/panta.html>

[3] <http://www.fucg.org/PartI/applets/cinderella/412Watt.html>

[4] <http://www.fucg.org/PartI/applets/cinderella/413Peaucellier.html>  
or <http://carol.wins.uva.nl/~leo/cinderella/peaucellier1.html>

[5] <http://www.fucg.org/PartI/applets/cinderella/42Parallelogram.html>

[6] <http://www.fucg.org/PartI/applets/cinderella/42Contraparallelogram.html>

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[10] Ruth Levy Guyer, Prions: Puzzling Infectious Proteins (Research in the News),  
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<http://www.stanford.edu/group/pandegroup/folding/science.html>

[12] Eric Demaine's Web Site: <http://theory.lcs.mit.edu/~edemaine/linkage/animations/>

### Source of Certain Figures

Figure 1.1(b, c, d) (with copyright permission): Mechanical Linkages in Java:  
[http://mathforum.org/sketchpad/java\\_linkages.html](http://mathforum.org/sketchpad/java_linkages.html)

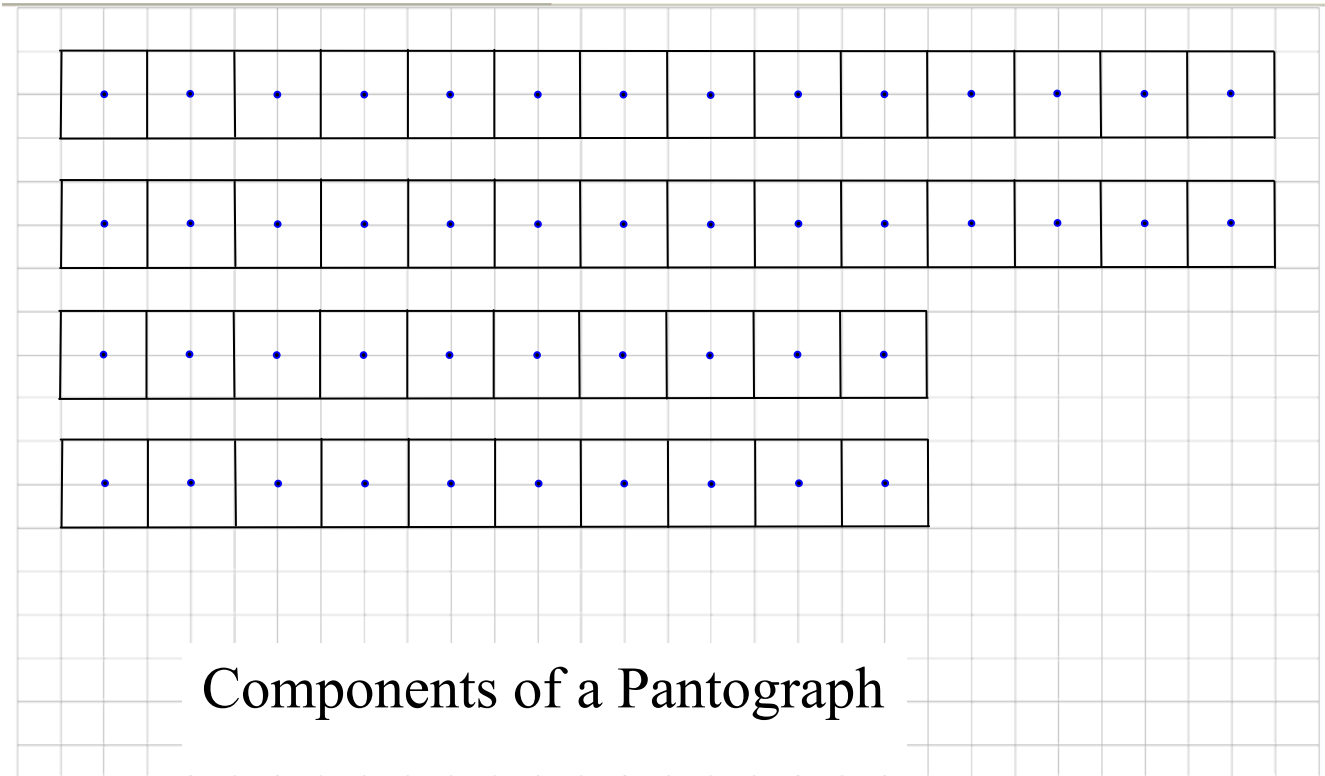
Figures 1.2, 2.4 (b), 2.7, 2.8, 2.12, 3.2, 3.5 (a,b), 3.6, 5.2-5.7 (with copyright permission):  
Demaine, Erik D. and O'Rourke, Joseph, *Folding and Unfolding in Computational Geometry*,  
Cambridge University Press, 2006. Available at: [www.fucg.org](http://www.fucg.org)

Figure 5.1: National Human Genome Research Institute:  
[http://www.genome.gov/Pages/Hyperion/DIR/VIP/Glossary/Illustration/amino\\_acid.cfm?key=amino%20acids](http://www.genome.gov/Pages/Hyperion/DIR/VIP/Glossary/Illustration/amino_acid.cfm?key=amino%20acids) (with copyright permission: <http://www.genome.gov/10003803>)

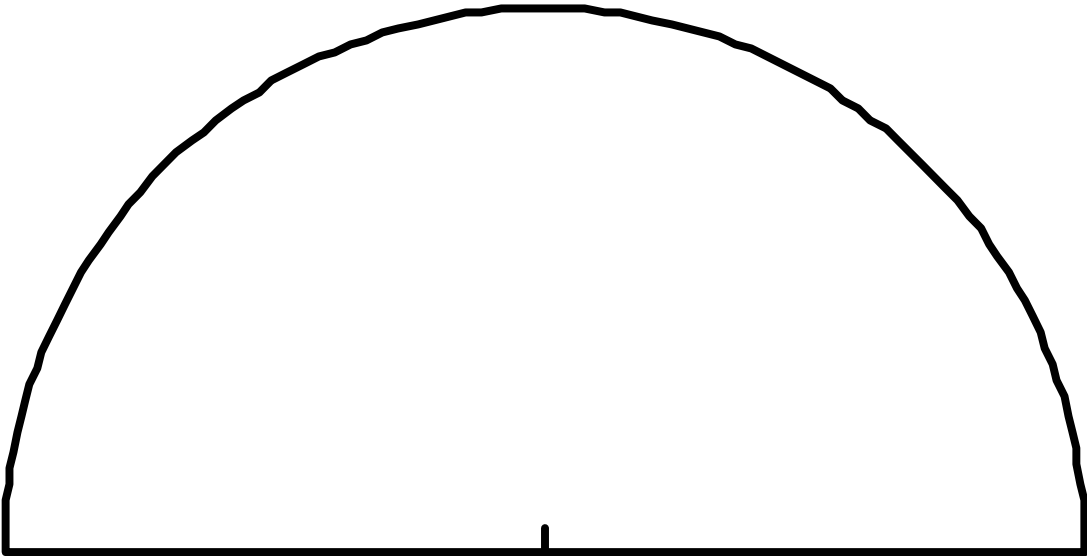
Figure 6.2 (with copyright permission): Wikipedia:  
<http://commons.wikimedia.org/wiki/Image:Benz1.png>

Appendix A

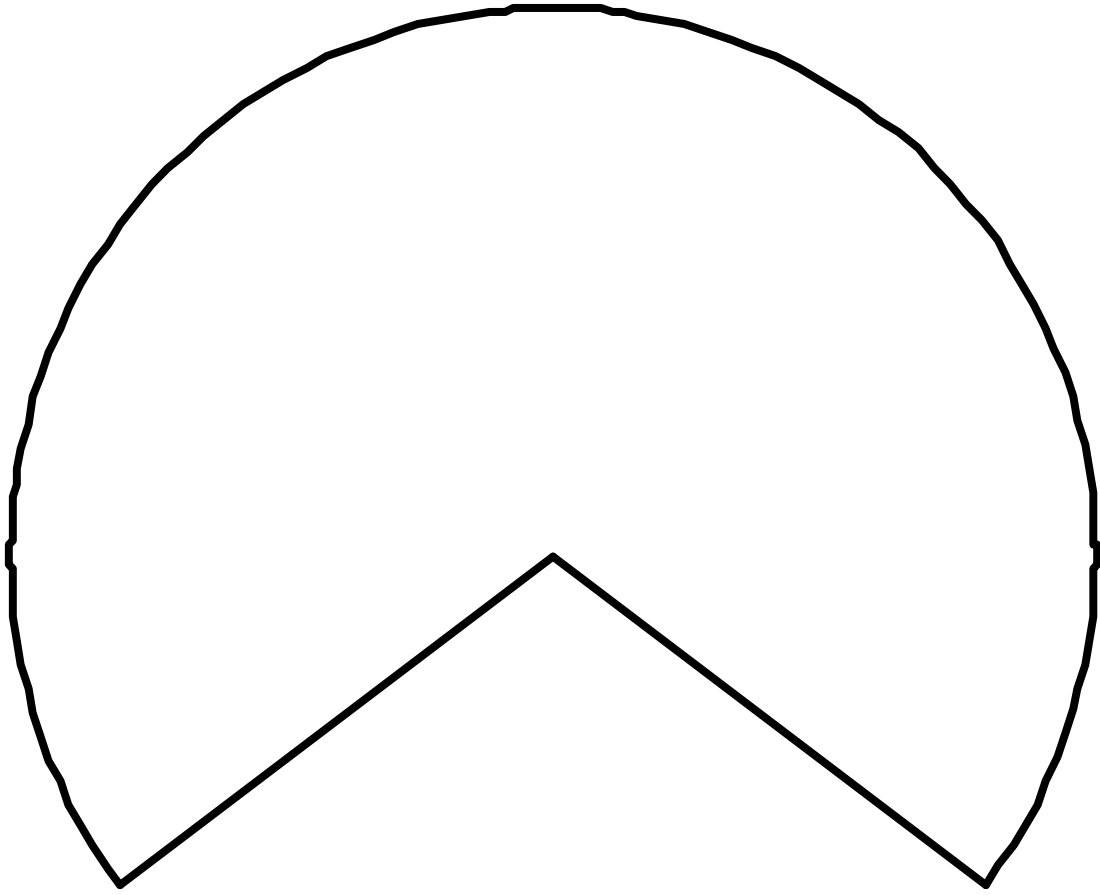
A.1 Cut-Out Drawings for a Pantograph



A.2 Cut-Out Drawings of Cones



(a) 30-Degree Cone



**(b) 45-Degree Cone**