



We've done several combinations of the constraints of equilateralness, equiangularity, and obtusehood for 3-D chains we want to know whether can be locked. What about the others?





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The geometric (cone) model for a ribosome seems too simple. Is it actually based on some verified model from biology?

Image of surface of polypeptide exit tunnel removed due to copyright restrictions.

### [Nissen, Hansen, Ban, Moore, Steitz 2000]

**[L21]** In proving the NPhardness of the 2D HPmodel folding problem, what are the NP-hard problems used in various reductions?

### Protein Folding in the Hydrophobic-Hydrophilic (HP) Model is NP-Complete

Bonnie Berger\*

Tom Leighton<sup>†</sup>



Figures removed due to copyright restrictions. Refer to: Fig. 4-5 from Berger, B., and T. Leighton. "Protein Folding in the Hydrophobichydrophilic(HP) is NP-complete." *Proceedings of the Second Annual International Conference on Computational Molecular Biology* (1998): 30-9.

### **On the Complexity of Protein Folding**

Pierluigi Crescenzi, Deborah Goldman, Christos Papadimitriou Antonio Piccolboni, Mihalis Yannakakis

Hamiltonicity in max-degree-4 graphs

> Figure and excerpts removed due to copyright restrictions. Refer to: Fig. 2 from Crescenzi, P., D. Goldman, et al. "On the Complexity of Protein Folding." *Journal of Computational Biology* 5, no. 3 (1998): 423–65.

# Any progress on any of the open problems?



## Flattening Fixed-Angle Chains Is Strongly NP-Hard

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Problem	Linkage	Edge lengths	Angle range
Flattening	fixed-angle chain	equilateral	$[16.26^{\circ}, 180^{\circ}]$
Flattening	fixed-angle chain	$\Theta(1)$	$[60 - \varepsilon^{\circ}, 180^{\circ}]$
Flattening	fixed-angle caterpillar tree	equilateral	$\{90^{\circ}, 180^{\circ}\}$
Min flat span	fixed-angle chain	equilateral	$[16.26^{\circ}, 180^{\circ}]$
Max flat span	fixed-angle chain	equilateral	$[16.26^{\circ}, 180^{\circ}]$



[Demaine & Eisenstat 2011]



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Courtesy of Erik D. Demaine and Sarah Eisenstat. Used with permission.





### [Demaine & Eisenstat 2011]



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### [Demaine & Eisenstat 2011]

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# Advanced Problems

3763. Proposed by Paul Erdös, The University, Manchester, England.

Given any simple polygon P which is not convex, draw the smallest convex polygon P' which contains P. This convex polygon P' will contain the area Pand certain additional areas. Reflect each of these additional areas with respect to the corresponding added side, thus obtaining a new polygon  $P_1$ . If  $P_1$  is not convex, repeat the process, obtaining a polygon  $P_2$ . Prove that after a finite number of such steps a polygon  $P_n$  will be obtained which will be convex.

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Erdős 1935

Fig. 1a and 1b removed due to copyright restrictions. Refer to: Demaine, E. D., B. Gassend, J. O'Rourke, et al. "All Polygons Flip Finitely... Right?" *Contemporary Mathematics* 453 (2008): 231–55.



Fig. 2 removed due to copyright restrictions. Refer to: Demaine, E. D., B. Gassend, J. O'Rourke, et al. "All Polygons Flip Finitely... Right?" *Contemporary Mathematics* 453 (2008): 231–55.

### de Sz. Nagy 1939

Fig. 6 removed due to copyright restrictions. Refer to: Demaine, E. D., B. Gassend, J. O'Rourke, et al. "All Polygons Flip Finitely... Right?" *Contemporary Mathematics* 453 (2008): 231–55.

### Joss & Shannon 1973

Table 1 removed due to copyright restrictions. Refer to: Demaine, E. D., B. Gassend, J. O'Rourke, et al. "All Polygons Flip Finitely... Right?" *Contemporary Mathematics* 453 (2008): 231–55.

### Demaine, Gassend, O'Rourke, Toussaint 2008

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### Demaine, Gassend, O'Rourke, Toussaint 2008

Доказательство этой теоремы, данное Б. Секефальви-Надем [см. В. Sz.-Nady, Amer. Math. Monthly 46, 1939, стр. 176-177], неверно.

"The proof of this theorem, given by B. Sz. Nagy, is incorrect"

Table 1 removed due to copyright restrictions. Refer to: Demaine, E. D., B. Gassend, J. O'Rourke, et al. "All Polygons Flip Finitely... Right?" *Contemporary Mathematics* 453 (2008): 231–55.

"Bing and Kazarinoff remark that Nagy's proof is invalid, but there is no basis for this claim."

Demaine, Gassend, O'Rourke, Toussaint 2008<sub>24</sub>

#### SOLUTIONS

3763 [1935, 627]. Proposed by Paul Erdös, The University, Manchester, England.

Given any simple polygon P which is not convex, draw the smallest convex polygon P' which contains P. This convex polygon P' will contain the area Pand certain additional areas. Reflect each of these additional areas with respect to the corresponding added side, thus obtaining a new polygon  $P_1$ . If  $P_1$  is not convex, repeat the process, obtaining a polygon  $P_2$ . Prove that after a finite number of such steps a polygon  $P_n$  will be obtained which will be convex.

#### Solution by Béla de Sz. Nagy, Szeged, Hungary.

The process described in the above problem, *i.e.*, the reflection of *all* additional areas, does not always lead from a simple polygon to a simple one, as shown in the following example:



This means that the repeating of this process is not always possible.

In order to avoid this difficulty we modify the process in the following way. Instead of reflecting *all* additional areas mentioned in the problem we reflect *only one* of them, so obtaining obviously always a simple polygon again. We agree to define the process also for convex polygons as the process of leaving them invariant.

Let  $A_1^{0}, A_2^{0}, \dots, A_r^{0}$  be the vertices of the given simple polygon  $P^{0}$ . Applying the process *n* times leads to a polygon  $P^{n}$ , the points  $A_r^{0}$  ( $r=1, 2, \dots, \sigma$ ) being carried thereby into the points  $A_r^{n}$ . Let us denote by  $C^{n}$  the least convex polygon containing  $P^{n}$  in its interior. Each polygon in the sequence  $P^{0}, C^{0}, P^{1}, C^{1}, P^{2}, C^{2}, \dots$  contains obviously the foregoing ones in its interior. The lengths of all polygons  $P^{n}$  being plainly the same, there is a circle containing all  $P^{n}$ 's in its interior. This implies that the sequence of the points  $A_r^{n}$  ( $n=0, 1, 2, \dots$ ) has at least one point of accumulation.

It follows readily from the nature of the above process that if B is a point on, or inside of,  $P^m$ , then dist  $(B, A_r^n) \leq \text{dist} (B, A_r^{n+1})$  for  $n \geq m$ . Especially we have: dist  $(A_r^m, A_r^n) \leq \text{dist} (A_r^m, A_r^{n+1})$  for  $n \geq m$ . From this it follows that the sequence of the points  $A_r^n$   $(n=0, 1, 2, \cdots)$  may have only a single point of accumulation. It is thus convergent:  $A_r^n \to A_r$  for  $n \to \infty$ .

The polygon  $P = (\overline{A_1A_2}, \overline{A_2A_3}, \cdots, \overline{A_{\sigma-1}A_{\sigma}}, \overline{A_{\sigma}A_1})$ , being the limit of the sequence  $P^n$ , is also the limit of the sequence  $C^n$  and is therefore convex.

Denote by  $c_r(r)$  the interior of the circle of radius r drawn around  $A_r$  as center.

Let  $A_{\mu}$  be a convexity-point of P (i.e., such that  $A_{\mu-1}$ ,  $A_{\mu}$ ,  $A_{\mu+1}$  do not lie on the same straight line;  $A_{\tau}$  being denoted also as  $A_0$ ,  $A_1$  as  $A_{\tau+1}$ ). We may find then obviously a straight line L and a positive number  $\rho$  such that  $c_{\mu}(\rho)$  lies wholly on one side of L while all  $c_{\lambda}(\rho)$  ( $\lambda \neq \mu$ ) lie on the other side. For  $n \geq n_0(\mu)$ we shall certainly have:  $A_{\mu}^{n} \in c_{\rho}(\rho)$  for  $\nu = 1, 2, \cdots, \sigma$ . L separates thus  $A_{\mu}^{n}$  from the other points  $A_{\lambda}^{n}$  ( $\lambda \neq \mu$ ). Hence  $A_{\mu}^{n}$  is a convexity-point of  $P^{n}$ . It must be therefore invariant:  $A_{\mu}^{n+1} = A_{\mu}^{n}$ . This implies that for  $n \geq n_0(\mu) : A_{\mu}n_0(\mu) = A_{\mu}^{n}$ . So is  $A_{\mu}^{n} = A_{\mu}$  for  $n \geq n_0(\mu)$ .

Let now  $A_{\mu_1}, A_{\mu_1}, \cdots, A_{\mu_s}$  be all the convexity-points of P. We have then  $A_{\mu_r}^{N} = A_{\mu_r} (r = 1, 2, \cdots, s)$  for  $N = \max(n_0(\mu_1), n_0(\mu_2), \cdots, n_0(\mu_s))$ .

This involves that  $C^n = P$  and therefore also that  $P^n = P$  for  $n \ge N$ . We thus obtain after a finite number of steps a convex polygon indeed.

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polygon containing  $P^n$  in its interior. Each polygon in the sequence  $P^0$ ,  $C^0$ ,  $P^1$ ,  $C^1$ ,  $P^2$ ,  $C^2$ ,  $\cdots$  contains obviously the foregoing ones in its interior. The lengths

#### them invariant.

Let  $A_1^o, A_2^o, \dots, A_e^o$  be the vertices of the given simple polygon  $P^o$ . Applying the process *n* times leads to a polygon  $P^n$ , the points  $A_2^o$  ( $\nu = 1, 2, \dots, \sigma$ ) being carried thereby into the points  $A_2^o$ . Let us denote by  $C^n$  the least convex polygon containing  $P^n$  in its interior. Each polygon in the sequence  $P^0, C^0, P^1, C^1, P^2, C^2, \dots$  contains obviously the foregoing ones in its interior. The lengths of all polygons  $P^n$  being plainly the same, there is a circle containing all  $P^n$ 's in its interior. This implies that the sequence of the points  $A_2^o$  ( $n = 0, 1, 2, \dots$ ) has at least one point of accumulation.

It follows readily from the nature of the above process that if B is a point on, or inside of,  $P^m$ , then dist  $(B, A_i^n) \leq \text{dist} (B, A_i^{n+1})$  for  $n \geq m$ . Especially we have: dist  $(A_i^m, A_i^n) \leq \text{dist} (A_i^m, A_i^{n+1})$  for  $n \geq m$ . From this it follows that the sequence of the points  $A_i^n$   $(n=0, 1, 2, \cdots)$  may have only a single point of accumulation. It is thus convergent:  $A_i^n \to A_i$  for  $n \to \infty$ .

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### Demaine, Gassend, O'Rourke, Toussaint 2008



Fevens, Hernandez, Mesa, Morin, Soss, Toussaint 2001



### Thurston 2001

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[Dumitrescu & Hilscher 2009]

6.849 Geometric Folding Algorithms: Linkages, Origami, Polyhedra Fall 2012

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