

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 ${ }^{\dagger}$

## bin packing

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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 <br> max-degree-4 graphs 

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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: weakly NP-hard [Joss \& Toussaint 2000]

- reduction from Partition: divide $n$ integers into 2egual sums
- horizontal bars for integers
- vertical bars in between, length $<\frac{1}{n}$
$\Rightarrow$ can flip horizontal bars left \& right
- build lock that folds in essentially one way: I

$\Rightarrow$ key must align with lock
OPEN: pseudopolynomial-time algorithm?


# Flattening Fixed-Angle Chains Is Strongly NP-Hard 

Erik D. Demaine* and Sarah Eisenstat*

MIT Computer Science and Artificial Intelligence Laboratory, 32 Vassar St., Cambridge, MA 02139, USA

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





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

rigid edge (unspinnable)

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



Courtesy of Erik D. Demaine and Sarah Eisenstat. Used with permission.
[Demaine \& Eisenstat 2011]

## 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 $P^{\prime}$ which contains $P$. This convex polygon $P^{\prime}$ will contain the area $P$ and 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.

Fig. 1a and 1 b 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.

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.

Table 1 removed due to copyright restrictions.
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Доказательство этой теоремы, данное Б. Секефальви-Надем [см. B. Sz.-N ady, Amer. Math. Monthly 46, 1939, стp. 176-177], неверно. "The proof of this theorem, given by B. Sz. Nagy, is incorrect"

Table 1 removed due to copyright restrictions.
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## "Bing and Kazarinoff remark that Nagy's proof is invalid, but there is no basis for this claim."

Demaine, Gassend, O'Rourke, Toussaint $2008_{24}$

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 $P^{\prime}$ which contains $P$. This convex polygon $P^{\prime}$ will contain the area $P$ and 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 Bêla 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 $A_{1}{ }^{0}, A_{2}{ }^{\circ}, \cdots, A_{\sigma}{ }^{\circ}$ be the vertices of the given simple polygon $P^{0}$. Applying the process $n$ times leads to a polygon $P^{n}$, the points $A_{\%}^{0}(\nu=1,2, \cdots, \sigma)$ being carried thereby into the points $A_{v^{n}}^{n}$. Let us denote by $C^{n}$ the least convex polygon containing $P^{n}$ in its interior. Each polygon in the sequence $P^{0}, C^{0}, P^{1}$, $C^{1}, P^{2}, C^{2}, \cdots$ 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 $A_{\nu^{n}}^{n}(n=0,1,2, \cdots)$ 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 $\left(B, A_{v}^{n}\right) \leqq \operatorname{dist}\left(B, A_{v}^{n+1}\right)$ for $n \geqq m$. Especially we have: dist $\left(A_{v}^{m}, A_{v}^{n}\right) \leqq \operatorname{dist}\left(A_{v}^{m}, A_{v}^{n+1}\right)$ for $n \geqq m$. From this it follows that the sequence of the points $A_{\nu^{n}}(n=0,1,2, \cdots)$ may have only a single point of accumulation. It is thus convergent: $A_{\nu}^{n} \rightarrow A$, for $n \rightarrow \infty$

The polygon $P=\left(\overline{A_{1} A_{2}}, \overline{A_{2} A_{3}}, \cdots, \overline{A_{\sigma-1} A_{\sigma}}, \overline{A_{\sigma} A_{1}}\right)$, being the limit of the sequence $P^{n}$, is also the limit of the sequence $C^{n}$ and is therefore convex.

Denote by $c_{p}(r)$ the interior of the circle of radius $r$ drawn around $A_{\nu}$ 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; $A_{\sigma}$ being denoted also as $A_{0}, A_{1}$ as $A_{\sigma+1}$ ). 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 $n \geqq n_{0}(\mu)$ we shall certainly have: $A_{\nu^{n}} \epsilon c_{\nu}(\rho)$ 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 $n \geqq n_{0}(\mu): A_{\mu} n_{0}(\mu)=A_{\mu}{ }^{n}$. So is $A_{\mu}{ }^{n}=A_{\mu}$ for $n \geqq n_{0}(\mu)$.

Let now $A_{\mu_{1}}, A_{\mu_{2}}, \cdots, A_{\mu_{1}}$, be all the convexity-points of $P$. We have then $A_{\mu_{r}}^{N}=A_{\mu_{r}}(r=1,2, \cdots, s)$ for $N=\max \left(n_{0}\left(\mu_{1}\right), n_{0}\left(\mu_{2}\right), \cdots, n_{0}\left(\mu_{s}\right)\right)$.

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

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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 $A_{1}{ }^{0}, A_{2}{ }^{0}, \cdots, A_{\dot{\circ}}{ }^{0}$ be the vertices of the given simple polygon $P^{0}$. Applying the process $n$ times leads to a polygon $P^{n}$, the points $A_{>}(\nu=1,2$, being carried thereby into the points $A n^{n}$. Let us denote by $C^{n}$ the least convex ${ }^{\bullet}$ 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 of all polygons $P^{n}$ being plainly the same, there is a circle containing all $P^{n}$ s in
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Fevens, Hernandez, Mesa, Morin, Soss, Toussaint 2001


Thurston 2001


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[Dumitrescu \&
Hilscher 2009]

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### 6.849 Geometric Folding Algorithms: Linkages, Origami, Polyhedra

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