Polygonal Chains:
from Pocket Flipping to Protein Folding

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Although *polygonal chains*—open chains of rigid links connected at joints—are the simplest type of bar-and-joint linkage, they nevertheless have both a wide range of applicability and a rich mathematical structure leading to intriguing computational questions. It is characteristic and apt that, in a sense, this area of investigation was initiated by Paul Erdős in 1935, with a problem he posed in the *American Mathematics Monthy* [Erd35]. He asked whether every polygon may be convexified by a finite number of simultaneous "pocket flips." The answer was provided in a later issue by de Sz. Nagy [dSN39], who proved that, restricting to one flip at a time, a finite number of flips suffice to convexify any polygon. Toussaint has shown how this theorem has been rediscovered over the years since [Tou99], but a close examination has revealed that none of the proofs are entirely sound, including Nagy's original. I will present a recent proof developed in collaboration with Erik Demaine, Blaise Gassend, and Godfried Toussaint [DO06].

The question of characterizing the conditions under which a polygonal chain can be *locked*, that is, its configuration space has more than one connected component, has fueled research in this area for more than a decade. Although many of the main questions were resolved by the celebrated proof of Connelly, Demaine, and Rote that chains cannot lock in 2D [CDR03], intriguing related problems remain open. In particular, the interlocking of several chains is not entirely understood, and the reconfigurations of fixed-angle chains constitute a complex choreography even less understood.

It is this latter topic that connects to protein folding, for the backbone of amino acids in a protein acts in many ways like a fixed-angle polygonal chain. Recently the class of "producible" protein chains (producible via a model of the ribosome) has been shown, surprisingly, to be identical to the flattenable chains [DLO03]. This work connects the seemingly abstract investigations into locked chains to the computational pragmatics of protein folding. Finally, I describe a raft of new and apparently difficult questions suggested by this work, concerning "unit" and "nearly unit" chains.

References

[CDR03] Robert Connelly, Erik D. Demaine, and Günter Rote. Straightening polygonal arcs and convexifying polygonal cycles. *Discrete & Computational Geometry*, 30(2):205–239, September 2003.

[dSN39] Béla de Sz. Nagy. Solution to problem 3763. *Amer. Math. Monthly*, 46:176–177, 1939.

[DLO03] Erik D. Demaine, Stefan Langerman, and Joseph O'Rourke. Geometric restrictions on producible polygon protein chains. In *Lecture Notes Comput. Sci.*, volume 2906, pages 395–404. Springer-Verlag, 2003. *Algorithmica*, to appear, 2005.

[DO06] Erik D. Demaine and Joseph O'Rourke. *Geometric Folding Algorithms: Linkages, Origami, and Polyhedra*. Cambridge University Press, 2006. In preparation. `http://www.fucg.org`.

[Erd35] Paul Erdős. Problem 3763. *Amer. Math. Monthly*, 42:627, 1935.

[Tou99] Godfried T. Toussaint. The Erdős-Nagy theorem and its ramifications. In *Proc. 11th Canad. Conf. Comput. Geom.*, pages 9–12, 1999.

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