Session 20 *(In preparation for Class 20, students are asked to view Lecture 20 and are given the option to view Lecture 21.)*

Topics for Class 20

3D linkage folding: ribosomes, HP protein folding NP-hardness, flattening is strongly NP-hard, flips, flipturns, deflations, pops, popturns.

Detailed Description of Class 20

This class opens with a discussion about the class as a whole, and how the experimental split into video lectures + live classes worked out.

Second, we address a few questions concerning:

- Equilateral vs. equiangular vs. obtuse locked 3D chains
- The shape of the ribosome
- HP protein folding NP-hardness proofs

Third, we cover a new result: Flattening fixed angle chains (and min/max flat span) are **strongly** NP-hard [Demaine & Eisenstat 2011].

Fourth, we cover a fun series of results on polygon (closed chain) reconfiguration via flips, flipturns, deflations, pops, and popturns.

Topics for Lecture 20

Protein folding: Fixed-angle linkages, tree, and chains; span; flattening; flat-state connectivity, disconnectivity of orthogonal partially rigid trees, connectivity of orthogonal open chains; locked fixed-angle chains; producible protein (fixed-angle) chains, ribosome, β-producible chains, helix-like canonical configuration, flat states are producible, producible states are connected.

Detailed Description of Lecture 20

This lecture is about fixed-angle linkages in 3D, which have the constraint that the angles (in addition to the lengths) must remain fixed at all times. Fixed-angle linkages model the mechanics of chemical bonds between atoms in a molecule. In particular, the backbone of a biological protein is a fixed-angle tree in this model, and can be approximated by a fixed-angle chain. We'll cover several results about fixed-angle linkages, all motivated by questions about protein folding:

- Span: What's the farthest or nearest you can fold the endpoints of a fixed-angle chain?
- Flattening: When does a fixed-angle chain have a non-self-intersecting flat state?
- Flat-state connectivity: When can a fixed-angle chain be folded without self-intersection between every pair of flat states?
- Locked: When is a fixed-angle linkage locked? In particular, we'll show that all states of a fixed-angle chain producible by a simple model of the ribosome (which includes all flat states) can reach each other.

A lot is known about each question, though many problems remain open.

Topics for Lecture 21 (optional)

Protein folding: HP model of protein folding, NP-hardness and approximation, unique optimal foldings, protein design.
Interlocked 3D chains: Lubiw's problem, unlocking 2-chains, unlocking two 3-chains and 2-chains, interlocking 3-chains, interlocking 3-chain with 4-chain, interlocking 4-chain with triangle, interlocking 3-chain with quadrangle, topological vs. geometric arguments, rigid and fixed-angle variations.

Detailed Description of Lecture 21 (optional)

This lecture continues our discussion on protein folding, this time focusing on simple theoretical models of the forces, rather than the mechanics, behind protein folding. In particular, we'll see the HP model, a lattice model capturing the hydrophobia of certain amino, which try to hide from the surrounding water. Finding the optimal folding a given protein is NP-complete, but there are some decent constant-factor approximations, and it's also not known whether protein design is similarly hard. We'll see one step in the direction of design: guaranteeing a unique optimal folding.

Then we'll turn to a fun problem of interlocked linkages. It's known that you need five bars to lock an open chain, but can you interlock multiple chains each with less than five bars? The answer is yes, with a nearly complete characterization of the possibilities. One consequence we'll see is how to cut a chain of n bars into around $n/2$ pieces that are not interlocked, while $n/4$ pieces are necessary.

6.849 Geometric Folding Algorithms: Linkages, Origami, Polyhedra
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