Protein Folding in 2D and 3D

15-48 EC masters' thesis project

For: Master Students that know how to program - and are interested.
                 If you've ever done a course in heuristics, it is a pre.
Load: 15 - 48 EC, depending on blocks (see below)
Period (approx.): From September 2021 onward
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Introduction video: https://bit.ly/3DWGFrG

About the project

Proteins are long strands of amino acids that control many important processes in the human body. It is known that proteins are stored 'folded' inside the cells of the body, and that the specific folding significantly influences their functioning. 'Misfolded' proteins can play a role in cancer, Alzheimer's disease and cystic fibrosis.

In a protein, hydrophobic amino acids (H) like to lie 'adjecntly', polar amino acids (P) do not have that preference. When two hydrophobic amino acids lie next to each other, an 'H-bond' is formed due to the attractive forces between the two. And the more bonds, the more stable the protein. The HP-model, containing of just two types of amino acids, arranges these in a grid or a lattice.
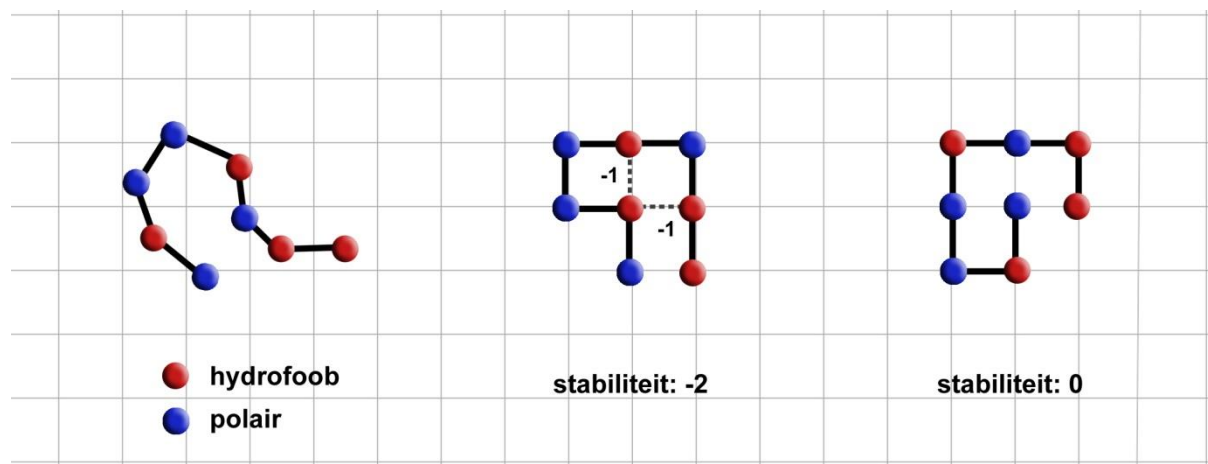

Figure 1 What's the most stable fold for this 8-piece protein?

Each block is about 15-18 EC's worth. You can choose blocks to your liking, though there is a strong emphasis on doing Block #1 first. Generally, we can adapt blocks as we go along, but once a block is finished, we're not going back, only forward.

Block #1

Delve up some basic literature, program an exact algorithm, and make 100 random protein strands of 20,25,30,35 and 40 amino acids and optimally fold the proteins in 2D. Are there differences in runtime?

Block #2

Fold the same proteins in 3D and compare the hardness to the 2D folds.

Block #3

Use a beam search algorithm, and experiment with the beam width for both the 2D and the 3D folds.

Block #4

Use two more amino acids than just H and P. Does it make sense from a biological point of view? How is the hardness affected?

References

No references as yet