

Implementation of protein folding algorithms in the HP model on a grid lattice with diagonals



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Abstract

In this Thesis project we want to analyze different protein folding algorithm. We start in understanding what we mean with protein folding, how we deal with this problem, what are the solution that we can adopt. Then, we want to look at the history of this operation and how we develop techniques and programs. We will discover that HP model in lattice is the most common and used solution. We understand the reason behind this choice and then we use this to simplify and obtain folded protein in a given dimensional space. We use algorithms to manage the folding technique and we analyze the results and the actual implementations of simple algorithms in two dimensions.

When we have our results we can compare and add different point of view in the consideration of the lattice space. We can consider that our bonds (we will see later what we mean with bonds) can be not only horizontal and vertical but also in diagonals and this consideration open a new door and start a new way of approaching these algorithms. We implement and analyze three new more algorithms in two and we extend the algorithm idea in three dimensions, using the diagonals as principal idea. We analyze the overall results. In this way, we have a lot of methods to fold protein following the HP model.

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