Computational Studies of Protein Folding

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Abstract
Proteins are known to fold into tertiary structures that determine their functionality in living organisms. The goal of our research is to better understand the protein folding process. Using MATLAB, we created an algorithm that models the folding process via a Monte Carlo time step approach. Specifically, amino acids in the chain at each time step are allowed to fold to certain locations according to a set of rules. These rules are based on two main criteria: folds must maintain bond length and should be thermally and energetically favorable. One central goal of our research is to examine whether the folding process can be viewed through the lens of self-organized criticality. In particular we are interested in whether there are features of the folding process that are independent of the size of the protein.

What is Protein Folding?
Protein folding is the process in which a string of amino acids under goes folding to find an equilibrium state where system energy is minimized. The particular sequence of amino acid types in the protein determine the unique tertiary structure formed at the end of the folding process. To aid in the successful folding of the protein an annealing function has been inserted into the code. Annealing is the process of lowering the temperature as the protein folds. This is useful to our simulation because it provides a logical method to make a manual shut off practical. The annealing function follows a Boltzmann distribution, \( T = T_0 \exp \left( -\frac{E}{kT} \right) \), where \( T \) is temperature, \( T_0 \) is the initial temperature, \( C \) is a constant, and \( E \) is the energy of the protein, not \( E < 0 \) in the simulation. It is these structures that determine the protein’s biological function. A number of diseases are believed to be caused when proteins fails to fold to the proper structure. So a better understanding of the folding process may help shed light on how these diseases could be prevented or treated.

What is Self Organized Criticality?
Self-organized criticality (SOC) is a theory of complex dynamic processes that deals in complex systems evolve on their own into critical states where a small disturbance, by a domino effect, can result in larger events called avalanches. Avalanches come in all sizes, ranging from insignificant to catastrophic. The first and simplest example used to illustrate self-organized criticality is the sand pile model. Imagine dropping grains of sand, one at a time, on a flat surface. The grains will form small piles. Eventually the slope of one of more of these piles will become steep enough that a grain slips and tumbles down the hill. This causes other grains to tumble as well, thus creating an avalanche.

Our Algorithm
Our model works by a simple algorithm illustrated in (Figure 2) above.

1. The algorithm starts by finding the current energy level of the system and temporarily stores it for comparison later.
2. The annealing function finds the temperature of the protein based on its current energy. This is useful to our simulation because it provides a logical method to make a manual shut off practical. The annealing function follows a Boltzmann distribution, \( T = T_0 \exp \left( -\frac{E}{kT} \right) \), where \( T \) is temperature, \( T_0 \) is the initial temperature, \( C \) is a constant, and \( E \) is the energy of the protein, not \( E < 0 \) in the simulation. It is these structures that determine the protein’s biological function. A number of diseases are believed to be caused when proteins fails to fold to the proper structure. So a better understanding of the folding process may help shed light on how these diseases could be prevented or treated.

The Annealing function

Power Law Behavior

What’s Next?

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