Introduction

There are many unanswered questions when it comes to protein folding. These questions are interesting because the tertiary structure of proteins determines its functionality in living organisms. How do proteins consistently reach their final tertiary structure from the primary sequence of amino acids? What explains the complexity of tertiary structures? Our research uses a simple hydrophobic-polar lattice-bound computational model to investigate self-organized criticality as a possible mechanism for generating complexity in protein folding and protein tertiary structures.

Self-Organized Criticality (SOC)

- a dynamical system at a critical state
- characterized by power law behavior
- both time and scale invariant

Sand Pile Model

Critical Trait: steepness of slope
Critical State: critical slope is reached
Avalanches: grains of sand falling of steep slopes
Avalanche Size: number of grains falling the distribution of avalanches follows a power law

Protein Folding Model

Critical Trait: minimizing energy
Critical State: non-native structure
Avalanches: rapid changes in structure (due to overcoming energy barriers)
Avalanche Size: number of consecutive folds

The Boltzmann factor, a probability function, allows some folds to occur that don’t decrease the energy of the protein.

Model and Algorithm

Algorithm:
- The model starts with linear chain made up of a specific sequence of hydrophobic or polar amino acids on a 3D lattice.
- Randomly, an amino acid is chosen for the first move.
- Is there a possible move? No, then a new amino acid is chosen. Yes, move one.
- Current energy of the protein. If $E < 0$, fold.
- If $E > 0$, then using the Boltzmann factor, the thermal energy is tested. If satisfied a fold occurs.

Avalanche Distributions

- Some evidence that specific primary structures exhibit SOC behavior (power law and scaling)
- further analysis needed to establish SOC behavior
- larger proteins, different primary structures, improved sampling statistics, KS test

Discussion of Results

- Is SOC connected to tertiary structure?
- How does the ratio of H-P amino acids in the protein affect SOC behavior?
- Do more sophisticated models exhibit SOC?
- variable bond length
- alternate avalanche definition
- molecular dynamics
- Explore contact maps of tertiary structure

Future Research

- Is SOC connected to tertiary structure?
- How does the ratio of H-P amino acids in the protein affect SOC behavior?
- Do more sophisticated models exhibit SOC?
- variable bond length
- alternate avalanche definition
- molecular dynamics
- Explore contact maps of tertiary structure

Figure 1 Representation of sand pile model

Figure 2 Avalanche size distribution for the sand pile model

Figure 3 Flow chart for simulation

Figure 4 Sample folded protein

Figure 5 Avalanche distributions for 2 different primary structure types

Figure 6 Scaled avalanche distributions for one sequence type (left) and both sequence types (right)