Non-Linear Dynamics of Protein Folding: The Anti-Chaos of Life

Bernard S. Gerstman and Prem Chapagain

Department of Physics
Florida International University
University Park
Miami, FL 33199
305-348-3115
gerstman@biophys.fiu.edu

We have used a well known computer lattice model to generate a time series of protein unfolding data. Analysis of the data using heat capacity algorithms shows that the model gives physically realistic results and adds to the confidence in the biophysical relevance of the model. We show how the output data from the model can be used with analytical techniques of non-linear dynamics to obtain important information about the complex underlying protein dynamics. We calculate Lyapunov exponents for protein behavior under different biochemical conditions. Highly organized proteins in their native state can be followed under conditions in which the protein remains folded but executes small scale thermal fluctuations. For these computer runs that do not unfold, the Lyapunov exponents are close to zero. However, when conditions are changed such that the protein unfolds, we find positive Lyapunov exponents implying chaotic dynamics.