

Abstract Submitted
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Chaos Theory and Protein Dynamics¹ JAMES BUI, JAMES CLARAGE, University of St. Thomas — Chaos theory, commonly known as the butterfly effect, states that a small change in a complex system may cause large changes in the system as time moves forward. This phenomenon was first discovered by Henri Poincare in the 1880's. The computer programs NAMD, VMD (Visual Molecular Dynamics) and Mathematica were used to calculate the movements and graphically analyze the trajectories of the protein ubiquitin. A small change was applied to a single atom's initial position in the x-coordinate to see how it would affect the future dynamics and trajectory of the protein. Our findings indicate an exponential divergence from the controlled trajectory with a Lyapunov exponent = 10.5 [1/ps]. In other words after less than a picosecond (trillionth of a second) the dynamics of a small biophysical system is no longer predictable, even though the underlying Newtonian physical laws are completely deterministic.

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