

Abstract Submitted
for the MAR07 Meeting of
The American Physical Society

Model for the simultaneous evolution of protein sequences and conformations LONGHUA HU, ALEXANDER GROSBERG, Department of Physics, University of Minnesota — Protein molecule folds because its sequence is quenched while its conformation dynamically evolves governed by the quenched sequence. Sequence design procedures known in the literature usually operate by computationally annealing the sequence on the background of properly quenched conformation. There are suggestions in the literature to invigorate both the sequence design and the computational folding algorithms by considering the simultaneous evolution of both sequence and conformation, assuming that these two sets of degrees of freedom interact with thermostats of two different temperatures. To examine this procedure, we study the model of random walks on the graph in which each vertex represents the state of a protein, including both sequence and conformation. The graph has bonds of two sorts, some represent change of conformation (physical motion), while others represent change of sequence ('mutation'). We show that when sequence and conformation dynamics are governed by different temperatures, there cannot be any equilibrium, and we analyze the stationary currents in the system which are realized by never stopping cascade of sequence rearrangements followed by conformational moves followed by sequence moves and so on, ad infinitum.

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Date submitted: 25 Nov 2006

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