Local Topology and Perestroikas in Protein Folding Dynamics

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Protein folding is usually analyzed through geometric observables, while the role of local topology remains less explored. We introduce a local-topological framework for protein structure and folding dynamics by extending Arnold's perestroikas to discrete piecewise-linear Cα backbones using the discrete Frenet formalism. In this setting, inflection, flattening, and branch points become local markers of conformational rearrangements, and a folding index together with a correlation function quantify their thermal evolution. Folded globular proteins are shown to possess a modular organization that can be represented by multisoliton solutions of a discretized nonlinear Schrödinger equation. Using myoglobin as a representative example, and combining a DNLS-based free-energy model with Glauber dynamics, we identify three thermally distinct regimes: a folded phase, a molten-globule phase, and a self-avoiding random-walk phase. The transitions between them are driven by temperature-induced perestroikas: unfolding starts when flattening and branch points that define soliton centers are rearranged, while higher temperatures lead to cascading topological reorganizations and progressive loss of modular structure. These results show that topological order parameters complement standard geometric observables and provide a compact statistical-physics framework for understanding protein folding and unfolding transitions.