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Multiscale modeling of macromolecular dynamics

CECILIA CLEMENTI, Rice University, Department of Chemistry

The understanding of emerging collective behaviors in biomolecular complexes represents a major challenge in modern biophysics. As a first step toward the study of such processes we have applied multi-resolution nonlinear dimensionality reduction and diffusion analysis to obtain reliable low-dimensional representations and models for the dynamics of apparently high-dimensional complex systems such as proteins in a biological environment. The results clearly show that the proposed methods can efficiently find low dimensional representations of complex processes such as protein folding, and suggest strategies to simplify significantly the study of such processes.