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A Model Comparison for Characterizing Protein Motions from Structure[1] CHARLES DAVID, Department of Bioinformatics and Genomics, University of North Carolina at Charlotte, Charlotte, NC, 28223 USA, DONALD JACOBS, Department of Physics and Optical Science, University of North Carolina at Charlotte, Charlotte, NC, 28223 USA — A comparative study is made using three computational models that characterize native state dynamics starting from known protein structures taken from four distinct SCOP classifications. A geometrical simulation is performed, and the results are compared to the elastic network model and molecular dynamics. The essential dynamics is quantified by a direct analysis of a mode subspace constructed from ANM and a principal component analysis on both the FRODA and MD trajectories using root mean square inner product and principal angles. Relative subspace sizes and overlaps are visualized using the projection of displacement vectors on the model modes. Additionally, a mode subspace is constructed from PCA on an exemplar set of X-ray crystal structures in order to determine similarly with respect to the generated ensembles. Quantitative analysis reveals there is significant overlap across the three model subspaces and the model independent subspace. These results indicate that structure is the key determinant for native state dynamics.

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Charles David
Department of Bioinformatics and Genomics,
University of North Carolina at Charlotte, Charlotte, NC, 28223 USA

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