Abstract Submitted
for the NWS18 Meeting of
The American Physical Society

The Influence of Free-Energy Surfaces on Mode-Dependent Protein Dynamics[1] ERIC BEYERLE, MARINA GUENZA, Univ of Oregon — The analysis and description of protein motions is greatly facilitated by reducing the effective dimensionality of the system through coarse-graining and transforming to decoupled normal-mode coordinates. Principal-component analysis (PCA) is a popular method used to quantify and visualize the motions of proteins through a normal mode decomposition of an appropriate covariance matrix. However, its description of mode-dependent dynamics does not account for barriers on free-energy surfaces. We have found that the inclusion of free-energy barriers can influence the dynamics predicted by each mode. Here we compare the dynamics predicted by our method (the Langevin Equation for Protein Dynamics, LE4PD) and PCA. The comparison is facilitated by analytically mapping the bond-bond connectivity matrix used in the LE4PD onto the covariance matrix used in PCA. We find that the motions of PCA are restricted to specific regions of the free-energy surface and that they are not, in general, 'aware' of the most-probable energetic pathways present along each normal mode. A more detailed description of the dynamics represented by each mode is found by using the finite-temperature string method to find the most probable pathway along the free-energy surface.

[1]NSF Grant CHE-1362500, XSEDE ACI-1053575

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Date submitted: 20 Apr 2018 Electronic form version 1.4