



A REDUCED BASIS METHOD FOR MOLECULAR DYNAMICS SIMULATIONS

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Molecular dynamics (MD) simulations are computationally expensive and generally require a large amount of data storage. We propose a method to reduce computational costs and storage requirements using singular value decomposition (SVD) analysis. In particular, we compute the truncated SVD of the MD trajectory in order to obtain a reduced representation of the trajectory. We update the basis defined by the left singular vectors as new information becomes available.

SVD analysis of the computed trajectories will be developed to augment abilities to locate active sites, to identify preferred molecular configurations, and to study periodic behavior. Visualization and manipulation for display purposes can also be vastly improved through the data compression made possible by the truncated SVD - reduced basis approach.

In any trajectory, whether generated by traditional dynamics methods, time-averaged refinements, or a reduced-basis set method, classical principal component analysis may be used to classify and represent the dominant characteristics of the MD trajectory. Here we augment the classical principal component analysis with an SVD updating scheme. We present preliminary results obtained with respect to a harmonic oscillator model and butane.