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Sparse Interpolatory Models for Molecular Dynamics

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We describe a method for using interpolatory models to accurately and efficiently simulate molecular excitation and relaxation. We use sparse interpolation for efficiency and local error estimation and control for robustness and accuracy.

The objective of the project is to design an efficient algorithm for simulation of light-induced molecular transformations. The simulation seeks to follow the relaxation path of a molecule after excitation by light. The simulator is a predictive tool to see if light excitation and subsequent return to the unexcited or ground state will produce a different configuration than the initial one.

We simulate the results of the excitation, rather than the excitation itself. The excitation will change the quantum state of a molecule. Our objective is to design software that will let one explore the possible changes in a molecule after a sequence of excitations.

The goals of the simulation are not only to identify the end point, but to report the entire path in an high-dimensional configuration space so that one can look for nearby paths to interesting configurations and examine the energy landscape near the path to see if low energy barriers make jumping to a different path possible.