Sparse Interpolatory Models for Molecular Dynamics Computations

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The objective of this project is to design a simulator which will be a test bed for quantum chemistry experiments. The tool will allow one to excite a molecule to one of several excited states, allow it to relax at that state, change the excited state, and continue the process until finally allowing the molecule to return to the ground state. The goals of the experiment are to obtain a different molecular configuration at the end and to have enough data to construct the energy landscape near the relaxation path.

The relaxation of the molecule, once the state of excitation is fixed, is determined a gradient flow equation for the bond and torsion angles. The problems are that the energy computation is expensive, there can be hundreds of angles, and therefore computing gradients one needs to integrate the differential equation is not practical.

In this talk we will discuss several stages of model reduction for this problem, the most important of which is an application of sparse interpolation. We will present recent results showing that the tool works and performs well in parallel.