Parallelizing Large-scale Vibronic Calculations

Scott Rabidoux[1], John Stanton[2], Victor Eijkhout[3]
[1] Institute for Computational Engineering and Sciences, UT
[2] Department of Chemistry, University of Texas - Austin
[3] Texas Advanced Computing Center

An efficiently parallelized matrix-vector product routine to be used in iterative methods for computing extremal spectral values of the vibronic Hamiltonian has been developed. A key insight into parallelization is provided by viewing the Hamiltonian matrix as a derivation of a stencil in a multi-dimensional domain. By block distributing this domain, rather than the matrix, we can achieve near linear speedup of the matrix-vector product operation. The new code is demonstrated by applications to the simulation of the $\tilde{A}^2E' \leftarrow \tilde{X}^2A'_2$ dark state spectrum of NO_3 and to other cases with up to nine active modes and 100 billion (!!!) basis functions.