
TUCKER CARRINGTON, Queen's University

Using sparse grids to solve the vibrational Schroedinger equation

In principle, it is straightforward to compute the vibrational spectrum of a molecule without neglecting coupling and anharmonicity: one must calculate eigenvalues and eigenvectors of a matrix representing the Hamiltonian in an appropriate basis. In practice, this is difficult because the matrix is very large. To obviate the N^2 memory and N^3 CPU costs of standard diagonalisation methods, it is now common to use iterative algorithms (e.g. Lanczos, Davidson, Filter Diagonalisation) for computing eigenvalues and eigenvectors. It is easy to efficiently implement iterative algorithms when a direct product basis is used. However, for a molecule with more than four atoms, a direct product basis set is large and (although iterative algorithms eliminate the need to store the matrix) minimising the number of basis functions required to obtain converged eigenvalues would be advantageous. Can this be done without jeopardizing the efficiency of the matrix-vector products required by all iterative algorithms? One way to reduce the number of basis functions is to discard unimportant functions from a direct product basis. In this talk I shall present new basis-size reduction ideas of this type that are compatible with efficient matrix-vector products.