The Computation of Rotational and Vibrational Spectrum of Van Der Waals Molecules on Cray-T3D

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The bound states of Van Der Waals Molecules are computed using iterative eigenvalue solver Implicitly Restarted Lanczos Method (IRLM). In this application two techniques are used to make the calculation more efficient. First Chebychev preconditioning is used to speedup the convergence. Secondly tensor product technique is used to calculate the sparse matrix - vector multiplication through dense matrix - matrix multiplications. The result program is many times faster than eispack routines. The parallelization of the program on Cray-T3D shows that the program also scales well on multi-processor supercomputers.