

Advanced Full CI Implementation for Teraflop Computing

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As supercomputing passes through the era of teraflop computing and approaches the era of petaflop computing, a great challenge for computational chemistry applications is to make good use of the potential enormous computing power. In this poster we presented advanced FULL CI implementation for state-of-art parallel and vector supercomputers.

Single processor performance is fundamental in archiving high performance. In this poster we presented both DAXPY based and DGEMM based implementations. We concluded that using system optimized BLAS3 kernel is still the most effective way to achieve high performance as of today's computing technology.

As the most basic operation in FCI, excitation list computing also presents the major parallel scalability bottleneck because it is duplicated to avoid otherwise enormous communication required. In the poster efficient string mapping algorithm is presented. Furthermore, we show that explicit generation of excitation pairs can be entirely avoided by combining the intermediate string driven approach with a matrix multiplication kernel.

For scalable applications heavy disk I/O activity must be avoided on supercomputers. To perform large benchmark calculations we designed a relaxed single vector iterative diagonalization method which has fast convergence.

Finally, the linear parallel scalability of our implementations is demonstrated by examples. Benchmark calculation was performed on C_2 using triple zeta basis and about 65 billion determinants. Each CI iteration takes only 4 minutes and the sustained performance is about 3.5 Tflops on 432 MSP of the Cray-X1.

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