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Performance of Parallel Symmetric Eigensolvers in Quantum Chemistry Codes on CRAY T3E

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Nearly one-third of the projects on the Cray supercomputer complex in Jülich pertain to the area of computational chemistry. For projects in quantum chemistry ZAM offers several extensive software packages running on CRAY T3E [1]. The solution of the symmetric eigenvalue problem is a compute-intensive task in many quantum-chemical calculations. We studied the performance of symmetric eigensolvers from different parallel libraries on CRAY T3E: GA_DIAG_STD from Global Arrays used in NWChem [2] (calling PDSPEV from PeIGS), PSSYEVX from ScaLAPACK contained in the Cray scientific library and used in DGauss [3], and PSSYEV from the public domain version 1.6 of ScaLAPACK. All eigensolvers use the following three-step-algorithm:
1. reduction of the full symmetric matrix to tridiagonal form;
2. solution of the tridiagonal eigenproblem;
3. back transformation of the eigenvectors.

PSSYEVX and PDSPEV use bisection and inverse iteration for the solution of the symmetric tridiagonal eigenproblem, in PSSYEV a modified QR-algorithm is applied. PDSPEV uses a parallel version for the reorthogonalization of eigenvectors whereas PSSYEVX does reorthogonalization of all eigenvectors belonging to one cluster of eigenvalues on a single node. This means that for large clusters of eigenvalues reorthogonalization with PSSYEVX is not possible because of memory exhaustion.

If there are no large clusters of eigenvalues or if reorthogonalization is not needed then PSSYEVX is significantly faster than PDSPEV as it is written in a blocked version using BLAS 3 and BLAS 2 operations whereas PDSPEV is based on BLAS 1 routines. On machines with small level 1 caches only the use of BLAS 3 routines can deliver good performance. If eigenvectors for large clusters of eigenvalues are needed orthogonal to a high precision then PSSYEV from ScaLAPACK is the best performing routine. The eigenvalues of the tridiagonal matrix are computed simultaneously on all processors and the eigenvectors are computed in parallel.

References

[1] http://www.fz-juelich.de/zam/mathe/chem_soft

[2] http://www.emsl.pnl.gov:2080/docs/nwchem

[3] http://www.oxmol.co.uk/software/unichem