A Hybrid Parallel Block Jacobi Davidson Method

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The Jacobi-Davidson method has been very successful in solving large sparse eigenvalue problems from quantum physics (cf. [1]) - as well as many other application areas - on massively parallel computers. In its original single-vector formulation, however, it suffers from a poor ratio of data transfers to computations. In this paper we present a block variant of Jacobi-Davidson that extends the search space by blocks rather than single vectors. A carefully designed strategy for maintaining stability is developed.

The new implementation is based on a programming model of "threads + kernels". The algorithm is organized in a number of parallel tasks that are handled by control threads to minimize the number of synchronization points. Kernel operations provide optimized numerical operations such as sparse matrix-vector products and operations on "tall skinny" matrices, based on an "MPI+X" programming model (X indicating OpenMP, CUDA and other techniques for intra-node parallelization). The blocked algorithm allows for temporal cache locality when accessing the matrix (and possibly a preconditioner), and the use of BLAS3 operations for the projection operations. The kernels provide optimized data structures and implementations, so that the resulting Eigensolver yields near optimal performance on clusters of multi- and many-core or hybrid CPU/GPU nodes.

For asserting that the method can be used in practice on potentially unstable exascale systems, a fault tolerance scheme is under development. As a first step an asynchronous checkpoint/restart mechanism has been implemented that allows writing backup files efficiently and restarting the solver in case of a system failure.

For validating the method we compute a few exterior eigenpairs of large, sparse and non-Hermitian matrices from quantum mechanics simulations.

References

[1] M. Kinateder, G. Wellein, A. Basermann and H. Fehske. In: E. Krause and W. Jäger (eds.), High Performance Computing in Science and Engineering '00 (Springer-Verlag, Berlin, Heidelberg). ISBN 3-540-41213-1, 188-204, (2001). Jacobi-Davidson algorithm with fast matrix vector multiplication on massively parallel and vector super computers.