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Towards an Automatic and Application-based Eigensolver Selection

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The computation of eigenvalues and eigenvectors is an important and often time-consuming phase in computer simulations. Recent efforts in the development of eigensolver libraries have given users good algorithm implementations without the need for users to spend much time in programming. Yet, given the variety of algorithms that are available to domain scientists, choosing the "optimal" algorithm for a particular application is a daunting task. In addition, as simulations become increasingly sophisticated and larger, it becomes infeasible for a user to try out every reasonable algorithm configuration in a timely fashion. Therefore, there is a need for an automated tool that is able to guide the user through the maze of various solvers with different configurations.

In this talk, we will describe a high-end, intelligent sparse eigensolver toolbox, EigAdept, which comprises the following components:

- A uniform and extensible interface for a collection of parallel sparse eigensolvers. The collection focuses on a class of solvers based on projection methods which are amenable to scalable implementations, which include ARPACK (implicitly restarted Arnoldi method), BLZPACK (block Lanczos method), TRLan (thick-restart Lanczos method), the Jacobi-Davidson method and the multi-level sub-structuring (AMLS) method. The Arnoldi/Lanczos-based solvers are enhanced with shift-and-invert capabilities using the scalable sparse direct linear solvers such as SuperLU and MUMPS.
- An intelligent engine to guide the user through the maze of various solvers and to automate the process of algorithm selection. To achieve that, a "history" knowledge base (algorithm selection criteria, or decision tree) incorporates initial information from our prior experience as well as from the literature (e.g., from "Templates for the Solution of Algebraic Eigenvalue Problems: a Practical Guide", edited by Bai et al.) The contents of

the knowledge base are gradually improved as more problems are solved, and can be ”adapted” at runtime through the repeated solutions of similar eigensystems from a specific application domain. An efficient data analyzer takes a user’s problem specification at runtime, queries the knowledge base, and finds the best match of an algorithm configuration with the target problem.

- Highly-tuned performance-critical kernels for high-end architectures. We identify and isolate the performance-critical kernels (e.g., parallel sparse matrix-vector multiplication), and provide highly-tuned versions for them. The methodolody of automatic performance tuning consists of both off-line optimization guided by detailed performance model, and on-line optimization by running the kernels in the pruned space of possible implementations. Furthermore, these tuned kernels will be made as standard-alone components, so that they can be used directly in any new eigensolver technology, or even in other areas of matrix computations.

EigAdept is implemented in C++ with Fortran interface. We have implemented distinct class structures for eigensolvers, linear equation solvers, and matrix types, so that for each eigensolver algorithm, we can easily support different sparse matrix formats, or use different linear solvers internally (e.g., for performing shift-and-invert). We use MySQL relational database to facilitate the implementation of the intelligent engine. MySQL is a free open source database software with a reliable C API. We will illustrate, with some case studies, that EigAdept can be a valuable tool for users from application domains, as well as for experts doing algorithm research.