ARPACK

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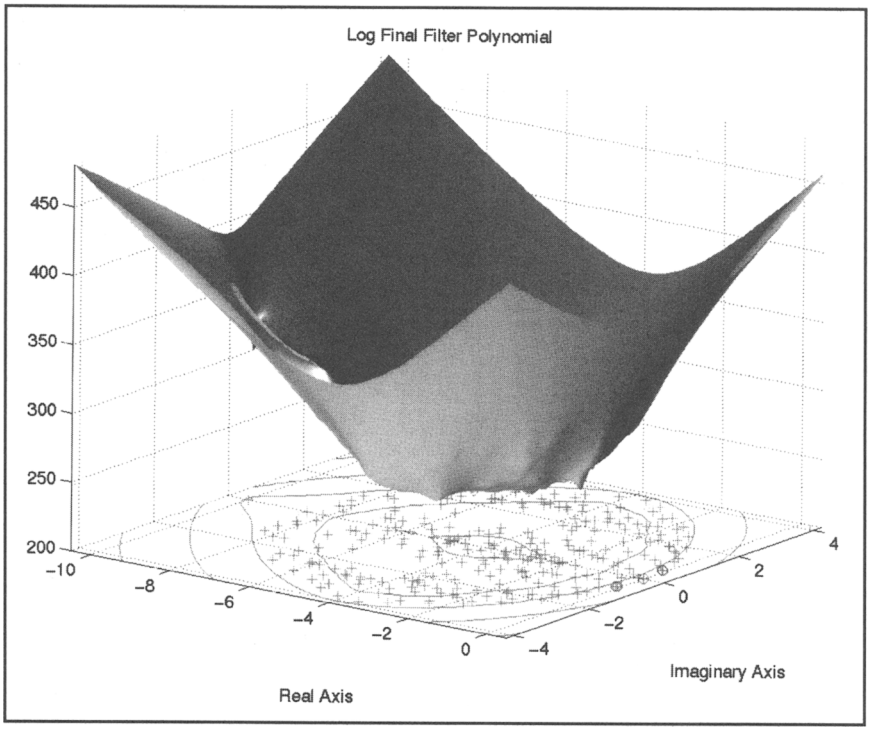

Users' Guide

Solution of Large-Scale Eigenvalue Problems with Implicitly Restarted Arnoldi Methods

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Preface

The development of ARPACK began as a research code written in Matlab [1] and then in Fortran 77 in 1990. Initially, the code was developed to study and verify the properties of the implicitly restarted Arnoldi method described in [44]. Preliminary experience with that code showed considerable promise in performance and also seemed to provide a solid foundation for the development of serious mathematical software for large structured eigenvalue problems.

During the academic year 1991–92, Dr. Phuong Vu (at that time with Cray Research) was granted permission to work in a half-time appointment to the NSF Center for Research on Parallel Computation at Rice University on the development of ARPACK. At the outset, we attempted to design the software to be efficient and portable on conventional high performance computing architectures. Of course, our design was also intended to be easily modified to effectively utilize a variety of parallel architectures (resulting in P_ARPACK). Phuong's experience with users at Cray Research suggested that a reverse communication interface was essential. We are deeply indebted to Phuong for the design and implementation of this interface. He set the coding and documentation style and developed the initial implementation of all of the basic computational routines for real (single- and double-precision) matrices. His fundamental design has served us well as we have improved and expanded upon the package over the past few years.

We wish to thank the numerous users with applications and also our fellow numerical analysts who worked with initial "alpha" and then "beta" versions of the code. Their feedback and patience throughout this development has been invaluable. This interaction has often given us a wonderful sense of community and the words "it solved my problem!" always managed to brighten up the drudgery of developing and maintaining the software. In particular, we would like to mention Jean-Philippe Brunet, Daniela Calvetti, Lawrence Cowsar, Olivier Daube, David Day, Stewart Edwards, Ralph T. Goodwin III, Ed Hayes, Lennart Johnsson, Michiel Kooper, Karl Meerbergen, Frank Milde, Seymour Parter, Phil Pendergast, George Phillips, John Red-Horse, Lothar Reichel, Tod Romo, Will Sawyer, Jennifer Scott, Rajesh Kumar Singh, Allison Smith, Allister Spence, Zdenko Tomasic, Henk Van der Vorst.

[1] Matlab is a registered trademark of The MathWorks, Inc., 24 Prime Park Way, Natick, MA 01760, USA, tel. 508-647-7000, fax 508-647-7001, info@mathworks.com, http://www.mathworks.com.

We wish to give special thanks to Kristi Maschhoff. She implemented the modifications required to produce the portable and parallel package P_ARPACK, redesigned both the makefiles and distribution mechanisms for ARPACK and P_ARPACK, and set up the ARPACK web site.

ARPACK is freely available through the world wide web and by anonymous ftp (see Chapter 1). It relies heavily upon the LAPACK software [1] and upon the BLAS [21, 11, 10]. Portability with performance, accuracy, and robustness is a direct consequence. We are greatly indebted to the authors of that software and more generally to the larger numerical analysis community that has contributed in many ways to its development.

Finally, we would like to thank the National Science Foundation, DARPA, and the Department of Energy for their generous support of this project (see below for full citation).

How to use this Guide

This users' guide is not intended to be read sequentially. There is a great deal of repetition amongst several of the subsections in Chapter 3 and also in Appendix A. We decided that it would be better to discuss each major problem class: real symmetric, real nonsymmetric, and complex as complete individual units even though this inevitably resulted in redundancy. We expect users to turn to the section that discusses the problem class of interest and to find everything related to that class in one complete section. We think this is preferable to searching back and forth to reference a general description in order to understand a special case of interest.

Chapter 1 gives an overview and contains general information. Chapter 2 provides installation instructions and describes how to get started. It is recommended for those who are just beginning with eigenvalue computations and also for those who are unfamiliar with reverse communication. Chapter 3 gives a detailed description of how to use all of the capabilities of ARPACK. Those wishing to learn a little about the underlying numerical methods should turn to Chapter 4. This discussion provides a broad overview of the methods. It gives a reasonably detailed description of the Arnoldi process with implicit restarting and what to expect. It also attempts to provide some understanding of the spectral transformation. Numerous references are provided for those who desire a more detailed level of understanding. Chapter 5 discusses implementation and usage details within the main computational routines. Experienced users of large-scale eigenvalue methods can probably turn directly to Appendix A and find the discussion of the driver routine that is appropriate for their problem. These drivers are intended to be used as templates that are easily modified for a particular application. Trace debugging and check-pointing are discussed in Appendix B. Finally, there are listings of the top-level reverse communication interface routines `XYaupd` for reference. The source code for all of the computational routines is available with the distribution. Each of these is

fully documented in the header and many users have found that documentation sufficient to get started with.

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