A brief review of the ITPACK project *

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Abstract: Over the past several years a number of research-oriented software packages for solving large sparse systems of linear algebraic equations have been developed within the Center for Numerical Analysis as part of the ITPACK Project. This report includes a brief discussion of each of the packages. References are given to other reports and papers which describe the individual packages in more detail.

1. Introduction

The ITPACK Project was established in the mid-1970s by the Center for Numerical Analysis at The University of Texas at Austin. The objective was the development and evaluation of iterative algorithms for solving large systems of linear algebraic equations with sparse coefficient matrices using theoretical analysis and experimental studies. The emphasis was on linear systems arising in the solution of partial differential equations by discretizations involving finite difference methods or finite element methods. Several software packages have been developed in connection with this research, to provide software tools for carrying out experimental studies for a variety of algorithms over a range of test problems. The ITPACK packages have been modified, improved, enhanced, and changed through various versions over a period of years. The following packages have been developed:

ITPACK 1: a prototype package which is no longer available.

ITPACK 2C: contains seven iterative algorithms designed primarily for symmetric positive definite (SPD) systems.

ITPACKV 2C: a vectorized package based on ITPACK 2C but with a modified data storage scheme and coding techniques for improved performance on vector computers.

ITPACK 3A: allows a combination of a number of preconditioners and acceleration procedures; designed to handle systems which are not necessarily SPD.

ITPACK 3B: similar to ITPACK 3A but is activated by a high-level language.

NSPCG: contains a large number of preconditioners/accelerator combinations with several different data storage schemes; designed for SPD or non-SPD systems and with vectorization in mind.

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The object of this report is to give a very brief description of each of these packages. More detailed summaries and more complete information can be found in the references.

2. ITPACK 1

The development of the ITPACK software began when Professor Garrett Birkhoff suggested that there was a need for general purpose software for solving linear systems of algebraic equations based on iterative methods similar to that based on direct methods which was being developed under the LINPACK project. Before that time, many iterative computer programs had been written in the Center for Numerical Analysis but primarily to support research studies. These programs were designed for solving self-adjoint elliptic partial differential equations with iterative methods embedded in the code. One of the reasons for the lack of general purpose software was the absence of accurate procedures for choosing iteration parameters and for deciding when to stop the iteration process. A number of iteration algorithms were developed, based on adaptive selection of acceleration parameters and automatic stopping procedures. Many are described in the book by Hageman and Young (1981) [5]. An earlier book by Young (1971) [41] presented many of the basic theoretical principles associated with iterative methods.

Initially, prototype software for ITPACK was written based on preliminary iterative algorithms with the emphasis on designing algorithms with these key features (adaptive parameter determination and automatic stopping). In ITPACK 1.0 the focus shifted from partial differential equations to large sparse linear systems. Which storage scheme to use was a major issue from the beginning. As with some of the latter version of the package, ITPACK 1.0 allowed the user to select from several different sparse storage formats. (Selecting the appropriate storage scheme to use is still an unresolved problem today since the structure of the matrices in the applications and the computer architectures keep changing. The current trend seems to be toward matrix-free packages which require the user to provide routines for matrix-vector operations). Some of the early work on ITPACK is described by the following authors: Kincaid and Young (1975) [25]; Kincaid and Grimes (1977) [24]; Hayes and Young (1977) [6]; Kincaid, Grimes and Young (1979) [21,22]; Grimes, Kincaid, MacGregor and Young (1979) [4].

3. ITPACK 2C and ITPACKV 2C

The ITPACK 2C package described by Kincaid, Respess, Young and Grimes (1982) [17] includes seven iterative algorithms including the Successive Overrelaxation (SOR) method as well as the Jacobi, Symmetric Successive Overrelaxation (SSOR) and Reduced System (RS) methods, each with Chebyshev or conjugate gradient acceleration. Adaptive procedures are used to determine the iteration parameters. The package is designed primarily for linear systems where the coefficient matrix is symmetric and positive definite (SPD). It can handle mildly nonsymmetric systems in a formal manner. The nonzeros from the coefficient matrix of the system are stored in three linear arrays A-IA-JA. A double precision version of this package is available for use on short-word-length computers.

The basic iterative algorithms used in ITPACK 2C are found in the book by Hageman and Young (1981) [5] and in the following reports and papers: Grimes, Kincaid and Young (1979) [3],
Kincaid and Young (1979, 1980) [20,23]; Young and Kincaid (1980, 1983) [39,40]; Kincaid (1981) [18]; Young, Jea and Kincaid (1984) [36]. Various versions of the user’s guide for this package were written before the final refereed paper on ITPACK 2C was published by Kincaid, Respess, Young and Grimes (1982) [17].

A vectorized package, called ITPACKV 2C, was constructed by modifying ITPACK 2C to improve overall performance on vector computers. The algorithms used are exactly the same as those in ITPACK 2C. The primary modification involved changing the sparse data structure used to store the matrix in such a way as to obtain longer vectors and less indirect addressing. This storage format uses two two-dimensional arrays COEF-JCOEF and is the same one used in the ELLPACK package for solving elliptic partial differential equations (Rice and Boisvert, 1985 [31]). Most of the routines from ITPACKV 2C are included in ELLPACK as iterative modules in the solution phase of this package (Kincaid, Oppe, Respess, and Young, 1985 [11]). The user who does not need ELLPACK to generate the linear system is encouraged to obtain the ITPACK software and to use it as a stand-alone package.

ITPACKV 2C was considerably faster than ITPACK 2C when tested on the CDC Cyber 205 and CRI Cray 1 supercomputers. In some cases, ITPACKV 2C was a factor of ten times faster (Kincaid, Oppe, and Young, in 1982, 1983 [12,16]). Recently, additional comparisons were performed on sample oil reservoir simulation problems using the Cyber 205, Cray X-MP, and Amdahl VP1200 (Oppe and Kincaid, 1987 [29]). The main focus of these papers was on the changes made in the package for efficiency when going from a memory-to-memory supercomputer to a register-to-register supercomputer. It is believed that these modifications are typical of changes that must be considered when transporting software of this type between vector computers. It should be noted that these studies were used to evaluate the performance of the particular software package and, hence, may not be representative of the overall performance of the computers involved. Some of the other publications related to ITPACKV 2C are those by: Kincaid, Oppe and Young (1984, 1986) [12,8,9]; Kincaid and Oppe (1983, 1984) [13,12]; Kincaid and Young (1983b) [15]; Young and Kincaid (1984) [34]; Young, Oppe, Kincaid and Hayes (1985) [35]. The ITPACKV 2C user’s guide was written by Kincaid, Oppe, Respess and Young (1984) [11]. Status reports on the development of the ITPACK 2 packages were written by Kincaid and Young (1983a) [14] as well as Young and Kincaid (1983) [39].

4. ITPACK 3A and 3B

The ITPACK 3A and 3B packages were designed to be modular in that any one of several basic iterative methods could be used with any one of several basic acceleration procedures. Moreover, the packages can handle nonsymmetric and indefinite systems as well as SPD systems. The ITPACK 3A package is written in the form of individual subroutines which can be called by the user. The accelerators available for symmetric systems are conjugate gradient acceleration and Chebyshev acceleration. For nonsymmetric and indefinite systems, the accelerations include ORTHOMIN(s), ORTHODIR(s), ORTHORES(s), Lanczos/ORTHOMIN (biconjugate gradient), Lanczos/ORTHODIR, Lanczos/ORTHORES, and nonsymmetric Chebyshev acceleration. The matrix is stored using the A-IA-JA storage scheme.

ITPACK 3B, on the other hand, is activated by means of a high-level language similar to that used with the ELLPACK package. The user describes the matrix problem and the desired
iterative solution techniques using this language. Then a preprocessor constructs a Fortran
program with the appropriate calls to the library of iterative routines. This package contains
basically the same algorithm as in ITPACK 3A with the same storage scheme but a different user
interface designed to make the package easy to use.

More details on ITPACK 3A and 3B are given by Young and Mai (1984, 1987) [33,34] and
Mai and Young (1986) [27], respectively. Related publications on ITPACK 3 and the algorithms
used therein are those by: Jea (1982) [7]; Mai (1986) [26]; Young, Jea and Mai (1987) [33].

5. NSPCG (a.k.a. ITPACK 4)

The newest software package in the ITPACK collection of software is called NSPCG, for
Nonsymmetric Preconditioned Conjugate Gradient. The package is intended to handle both
symmetric and nonsymmetric systems with structured and unstructured coefficient matrices. As
in ITPACK 2C and ITPACK 3A, the user makes a subroutine call to obtain a particular iterative
algorithm. NSPCG allows various acceleration techniques to be used in conjunction with various
preconditioners by selecting unique names for two parameters in the calling sequence. Details on
the user interface can be found in the report by Oppe, Joubert, and Kincaid (1988) [28]. For
symmetric systems, a number of methods, such as those used in ITPACK 2C, are included. For
nonsymmetric systems, a number of accelerators are included such as generalized conjugate
gradient acceleration, Lanczos acceleration, a least-squares version of conjugate gradient acceler-
ation applied to the normal equations, and many others. Many basic preconditioners are
available, such as Jacobi, modified incomplete Cholesky, line SOR, line least-squares polynomial,
and various others. Furthermore, some of these preconditioners are available with either
left-preconditioners, right-preconditioners, or two-sided preconditioners. Many of the precondi-
tioners have been vectorized to work efficiently on supercomputers such as the Cray X-MP,
Cyber 205, etc. In the interest of portability, the entire package is written in 1977 ANSI Standard
Fortran with no special vector-Fortran syntax. However, some minor installation changes can be
made for different vector computers to enhance vectorization. For example, the Fortran
implementation of gather and scatter instructions can be replaced by calls to machine routines
for these operations when available.

A novel feature of this package is that several different matrix storage schemes are allowable.
The user may represent the matrix of the linear system in one of the following five basic sparse
matrix storage formats: primary storage (ELLPACK format), symmetric diagonal storage,
nonsymmetric diagonal storage, symmetric coordinate storage, and nonsymmetric coordinate. In
addition, the package can be used in a matrix-free mode where the user supplies customized
routines for performing all matrix operations. The package is modular in nature so that almost
any preconditioner may be used with almost any accelerator. Also, any preconditioner may be
used with nearly all of the allowable data storage schemes.

A preliminary version of the NSPCG User's Guide has been written by Oppe, Joubert and
Kincaid (1988) [28], and a companion report outlining the algorithms used is being written.
Testing of the package on applications is in progress using the sample reservoir simulation
problems that were used in the evaluation of ITPACKV 2C (Oppe and Kincaid, 1986, 1987
[30,29]). Additional testing using other large application problems and linear systems from
finite-element solution techniques is planned.
6. Distribution of software

A limited number of copies of these packages are available for distribution with the understanding that they are intended as research tools and may undergo further development. The interested reader should write to the address below for additional information on obtaining the distribution tape(s) of the software and documentation.

Center for Numerical Analysis
RLM Bldg. 13.150
University of Texas at Austin
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A nominal fee is involved to cover handling, mailing charges, etc. Also, reports of difficulties encountered in using these packages plus comments and suggestions for improving them are welcome.

As usual with research software, The University of Texas at Austin and the Center for Numerical Analysis disclaim all warranties with regard to these software packages and documentation. It should be emphasized that they are preliminary, incomplete, and subject to change.

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