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SPARSKIT: a basic tool kit for sparse matrix computations

(NASA-CR-185876) SPARSKIT: A BASIC TOOL KIT FOR SPARSE MATRIX COMPUTATIONS (Research Inst. for Advanced Computer Science) 30 p
CSCL 12A
N91-32865
Unclas
G3/64 0043046

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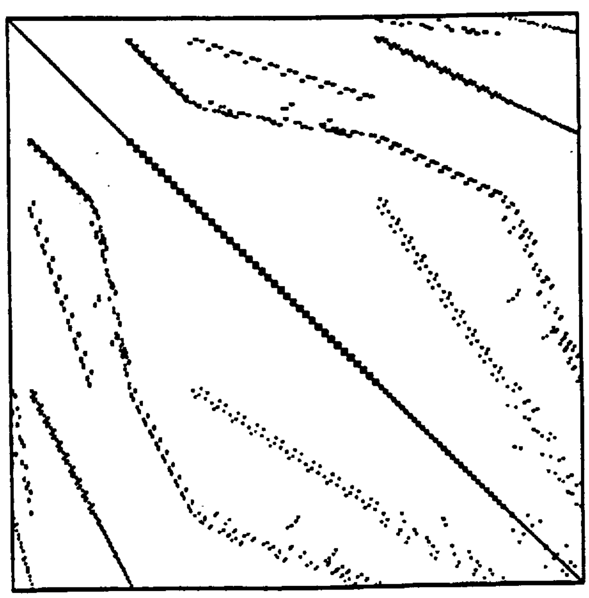

RIACS Technical Report 90.20

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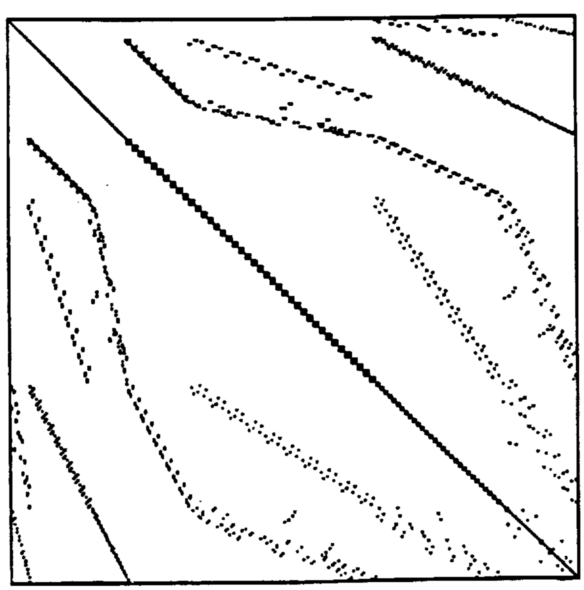

The Research Institute for Advanced Computer Science is operated by Universities Space Research Association (USRA), The American City Building, Suite 311, Columbia, MD 21044, (301)730–2656.

Work reported herein was supported in part by DARPA via Cooperative Agreement NCC 2–387 between NASA and USRA.

SPARSKIT: a basic tool kit for sparse matrix computations

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May 21, 1990

Abstract. This paper presents the main features of a tool package for manipulating and working with sparse matrices. One of the goals of the package is to provide basic tools to facilitate exchange of software and data between researchers in sparse matrix computations. Our starting point is the Harwell/Boeing collection of matrices for which we provide a number of tools. Among other things the package provides programs for converting data structures, printing simple statistics on a matrix, plotting a matrix profile, performing basic linear algebra operations with sparse matrices and so on.

*RIACS, Mail Stop 230-5, NASA Ames Research Center, Moffett Field, CA 94035. This work was supported in part by the NAS Systems Division, via Cooperative Agreement NCC 2-387 between NASA and the University Space Research Association (USRA) and in part by the Department of Energy under grant DE-FG02-85ER25001.

1 Introduction

Research on sparse matrix techniques has become increasingly complex, and this trend is likely to accentuate if only because of the growing need to design efficient sparse matrix algorithms for modern supercomputers. While there are a number of packages and 'user friendly' tools, for performing computations with small dense matrices there is a lack of any similar tool or in fact of any common tools for working with sparse matrices. Yet a collection of a few basic programs to perform some elementary and common tasks may be very useful in reducing the typical time to implement and test sparse matrix algorithms. That a common set of routines shared among researchers does not exist yet for sparse matrix computation is rather surprising. Consider the contrasting situation in dense matrix computations. The Linpack and Eispack packages developed in the 70's have been of tremendous help in various areas of scientific computing. One could speculate that the widespread availability of these packages must have saved millions of hours of coding effort world-wide. In contrast, it is very common that researchers in sparse matrix computation code their own subroutine for such things as converting the storage mode of a matrix or for reordering a matrix according to a certain permutation. One of the reasons for this situation might be the absence of any standard for sparse matrix computations. For instance, the number of different data structures used to store sparse matrices in various applications is staggering. For the same basic data structure there often exist a large number of variations in use. As sparse matrix computation technology is maturing there is a desperate need for some standard for the basic storage schemes and possibly, although this is more controversial, for the basic linear algebra operations.

An important example where a package such as SPARSKIT can be helpful is for exchanging matrices for research or other purposes. In this situation, one must often translate the matrix from some initial data structure in which it is generated, into a different desired data structure. One way around this difficulty is to restrict the number of schemes that can be used and set some standards. However, this is not enough because often the data structures are chosen for their efficiency and convenience, and it is not reasonable to ask practitioners to abandon their favorite storage schemes. What is needed is a large set of programs to translate one data structure into another. In the same vein, subroutines that generate test matrices would be extremely valuable since they would allow users to have access to a large number of matrices without the burden of actually passing large sets of data.

A useful collection of sparse matrices known as the Harwell/Boeing collection, which is publically available [4], has been widely used in recent years for testing and comparison purposes. Because of the importance of this collection many of the tools in SPARSKIT can be considered as companion tools to it. For example, SPARSKIT supplies simple routines to create a Harwell/Boeing (H/B) file from a matrix in any format, tools for creating pic files in order to plot a H/B matrix, a few routines that will deliver statistics for any H/B matrix, etc.. However, SPARSKIT is not limited to being a set of tools to work with H/B matrices. Since one of our main motivations is research on iterative methods, we provide numerous tools that may help researchers in this specific area. SPARSKIT will hopefully be an evolving package that will benefit from contributions from other researchers. This report is a succinct description of the package in its version one release.

2 Data structures for sparse matrices and the conversion routines

One of the difficulties in sparse matrix computations is the variety of types of matrices that are encountered in practical applications. The purpose of each of these schemes is to gain efficiency both in terms of memory utilization and arithmetic operations. As a result many different ways of storing sparse matrices have been devised to take advantage of the structure of the matrices or the specificity of the problem from which they arise. For example if it is known that a matrix consists of a few diagonals one may simply store these diagonals as vectors and the offsets of each diagonal with respect to the main diagonal. If the matrix is not regularly structured, then one of the most common storage schemes in use today is what we refer to in SARSKIT as the Compressed Sparse Row (CSR) scheme. In this scheme all the nonzero entries are stored one row after the other in a one-dimensional real array A together with an array JA containing their column indices and a pointer array which contains the addresses in A and JA of the beginning of each row. Also of importance because of its simplicity is the coordinate storage scheme in which the nonzero entries of A are stored in any order together with their row and column indices. Many of the other existing schemes are specialized to some extent. The reader is referred to the book by Duff et al. [3] for more details.

2.1 Storage Formats

Currently, the conversion routines of SPARSKIT can handle twelve different storage formats. These include some of the most commonly used schemes but they are by no means exhaustive. We found it particularly useful to have all these storage modes when trying to extract a matrix from someone else's application code in order, for example, to analyze it with the tools described in the next sections or, more commonly, to try a given solution method which requires a different data structure than the one originally used in the application. Often the matrix is stored in one of these modes or a variant that is very close to it. We hope to add many more conversion routines as SPARSKIT evolves.

In this section we describe in detail the storage schemes that are handled in the FORMATS module. For convenience we have decided to label by a three character name each format used. We start by listing the formats and then describe them in detail in separate subsections (except for the dense format which needs no detailed description).

DNS Dense format

BND Linpack Banded format

CSR Compressed Sparse Row format

CSC Compressed Sparse Column format

COO Coordinate format

ELL Ellpack-Itpack generalized diagonal format

DIA Diagonal format

BSR Block Sparse Row format

MSR Modified Compressed Sparse Row format

SSK Symmetric Skyline format

NSK Nonsymmetric Skyline format

JAD The Jagged Diagonal scheme

In the following sections we denote by A the matrix under consideration and by N its row dimension and NNZ the number of its nonzero elements.

2.1.1 The Compressed Sparse Row and related formats (CSR, CSC and MSR)

The Compressed Sparse Row format is the basic format used in SPARSKIT. The data structure for Compressed Sparse Row consists of three arrays.

- A real array A containing the real values a_{ij} stored row by row, from row 1 to N. The length of A is NNZ.
- An integer array JA containing the column indices of the elements a_{ij} as stored in the array A. The length of JA is NNZ.
- An integer array IA containing the pointers to the beginning of each row in the arrays A and JA. Thus the content of $IA(i)$ is the position in arrays A and JA where the i-th row starts. The length of IA is $N+1$ with $IA(N+1)$ containing the number $IA(1)+NNZ$, i.e., the address in A and JA of the beginning of a fictitious row $N+1$.

The Compressed Sparse Column format is identical with the Compressed Sparse Row format except that the columns of A are stored instead of the rows. In other words the Compressed Sparse Column format is simply the Compressed Sparse Row format for the matrix A^T.

The Modified Sparse Row (MSR) format is a rather common variation of the Compressed Sparse Row format which consists of keeping the main diagonal of A separately. The corresponding data structure consists of a real array A and an integer array JA. The first N positions in A contain the diagonal elements of the matrix, in order. The position $N+1$ of the array A is not used. Starting from position $N+2$, the nonzero elements of A, excluding its diagonal elements, are stored row-wise. Corresponding to each element $A(k)$ the integer $JA(k)$ is the column index of the element $A(k)$ in the matrix A. The $N+1$ first positions of JA contain the pointer to the beginning of each row in A and JA. The advantage of this storage mode is that many matrices have a full main diagonal, i.e., $a_{ii} \neq 0, i = 1, \ldots, N$, and this diagonal is best represented by an array of length N. This storage mode is particularly useful for triangular matrices with non-unit diagonals. Often the diagonal is then stored in inverted form (i.e. $1/a_{ii}$ is stored in place of a_{ii}) because triangular systems are often solved repeatedly with the same matrix many times, as is the case for example in preconditioned Conjugate Gradient methods. The column oriented analogue of the MSR format, called MSC format, is also used in some of the other modules, but no transformation to/from it to the CSC format is necessary: for example to pass from CSC to MSC one can use the routine to pass from the CSR to the MSR formats, since the data structures are identical. The above three storage modes are used in many well-known packages.

2.1.2 The banded Linpack format (BND)

Banded matrices represent the simplest form of sparse matrices and they often convey the easiest way of exploiting sparsity. There are many ways of storing a banded matrix. The one we adopted here follows the data structure used in the Linpack banded solution routines. The motivation here is that one can often make use of this well-known package if the matrices are banded. For fairly small matrices (say, $N < 2000$ on supercomputers, $N < 200$ on fast workstations, and with a bandwidth of $O(N^{\frac{1}{2}})$), this may represent a viable and simple way of solving linear systems. One must first transform the initial data structure into the banded linpack format and then call the appropriate band solver. For large problems it is clear that a better alternative would be to use a sparse solver such as MA28, which requires the input matrix to be in the coordinate format.

In the BND format the nonzero elements of A are stored in a rectangular array ABD with the nonzero elements of the j-th column being stored in the $j-th$ column of ABD. We also need to know the number ML of diagonals below the main diagonals and the number MU of diagonals above the main diagonals. Thus the bandwidth of A is $ML+MU+1$ which is the minimum number of rows required in the array ABD. An additional integer parameter is needed to indicate which row of ABD contains the lowest diagonal.

2.1.3 The coordinate format (COO)

The coordinate format is certainly the simplest storage scheme for sparse matrices. It consists of three arrays: a real array of size NNZ containing the real values of nonzero elements of A in any order, an integer array containing their row indices and a second integer array containing their column indices. Note that this scheme is as general as the CSR format, but from the point of view of memory requirement it is not as efficient. On the other hand it is attractive because of its simplicity and the fact that it is very commonly used. Incidentally, we should mention a variation to this mode which is perhaps the most economical in terms of memory usage. The modified version requires only a real array A containing the real values a_{ij} along with only one integer array that contains the integer values $(i-1)N+j$ for each corresponding nonzero element a_{ij}. It is clear that this is an unambiguous representation of all the nonzero elements of A. There are two drawbacks to this scheme. First, it requires some integer arithmetic to extract the column and row indices of each element when they are needed. Second, for large matrices it may lead to integer overflow because of the need to deal with integers which may be very large (of the order of N^2). Because of these two drawbacks this scheme has seldom been used in practice.

2.1.4 The diagonal format (DIA)

The matrices that arise in many applications often consist of a few diagonals. This structure has probably been the first one to be exploited for the purpose of improving performance of matrix by vector products on supercomputers, see references in [8]. To store these matrices we may store the diagonals in a rectangular array $DIAG(1:N, 1:NDIAG)$ where $NDIAG$ is the number of diagonals. We also need to know the offsets of each of the diagonals with respect to the main diagonal. These will be stored in an array $IOFF(1:NDIAG)$. Thus, in position (i,k) of the array $DIAG$ is located the element $a_{i,i+ioff(k)}$ of the original matrix. The order in which the diagonals are stored in the columns of $DIAG$ is unimportant. Note also that all the diagonals except the main diagonal have fewer than N elements, so there are positions in $DIAG$ that will not be used.

In many applications there is a small number of non-empty diagonals and this scheme is enough. In general however, it may be desirable to complement this data structure, e.g., by a compressed sparse row format. A general matrix is therefore represented as the sum of a diagonal-structured matrix and a general sparse matrix. The conversion routine CSRDIA which converts from the compressed sparse row format to the diagonal format has an option to this effect. If the user wants to convert a general sparse matrix to one with, say, 5 diagonals, and if the input matrix has more than 5 diagonals, the rest of the matrix (after extraction of the 5 desired diagonals) will be put, if desired, into a matrix in the CSR format. In addition, the code may also compute the most important 5 diagonals if wanted, or it can get those indicated by the user through the array $IOFF$.

2.1.5 The Ellpack-Itpack format (ELL)

The Ellpack-Itpack format [6, 9, 5] is a generalization of the diagonal storage scheme which is intended for general sparse matrices with a limited maximum number of nonzeros per row. Two rectangular arrays of the same size are required, one real and one integer. The first, $COEF$, is similar to $DIAG$ and contains the nonzero elements of A. Assuming that there are at most $NDIAG$ nonzero elements in each row of A, we can store the nonzero elements of each row of the matrix in a row of the array $COEF(1:N, 1:NDIAG)$ completing the row by zeros if necessary. Together with $COEF$ we need to store an integer array $JCOEF(1:N, 1:NDIAG)$ which contains the column positions of each entry in $COEF$.

2.1.6 The Block Sparse Row format (BSR)

Block matrices are common in all areas of scientific computing. The best way to describe a block matrix is by saying that it is a sparse matrix whose nonzero entries are square dense blocks. Block matrices arise from the discretization of partial differential equations when there are several degrees of freedom per grid point. There are restrictions to this scheme. Each of the blocks is treated as a dense block. If there are zero elements within each block they must be treated as nonzero elements with the value zero.

There are several variations to the method used for storing sparse matrices with block structure. The one considered here, the Block Sparse Row format, is a simple generalization of the Compressed Sparse Row format.

We denote here by $NBLK$ the dimension of each block, by $NNZR$ the number of nonzero blocks in A (i.e., $NNZR = NNZ/(NBLK^2)$) and by NR the block dimension of A, (i.e., $NR = N/NBLK$), the letter R standing for 'reduced'. Like the Compressed Sparse Row format we need three arrays. A rectangular real array $A(1:NNZR, 1:NBLK, 1:NBLK)$ contains the nonzero blocks listed (block)-row-wise. Associated with this real array is an integer array $JA(1:NNZR)$ which holds the actual column positions in the original matrix of the $(1,1)$ elements of the nonzero blocks. Finally, the pointer array $IA(1:NR+1)$ points to the beginning of each block row in A and JA.

The savings in memory and in the use of indirect addressing with this scheme over Compressed Sparse Row can be substantial for large values of $NBLK$.

2.1.7 The Symmetric Skyline format (SSK)

A Skyline matrix is often referred to as a variable band matrix or a profile matrix [3]. The main attraction of skyline matrices is that when pivoting is not necessary then the skyline structure of the matrix is preserved during Gaussian elimination. If the matrix is symmetric we need only to store its lower triangular part. This is a collection of rows whose length varies. A simple method used to store a Symmetric Skyline matrix is to place all the rows in order from 1 to N, [2] in a real array A and then keep an integer array which holds the pointers to the beginning of each row. The column positions of the nonzero elements stored in A can be easily derived and are therefore not kept.

2.1.8 The Non Symmetric Skyline format (NSK)

Conceptually, the data structure of a nonsymmetric skyline matrix consists of two substructures. The first consists of its lower part of A stored in skyline format and the second of its upper triangular part stored in a column oriented skyline format (i.e., the transpose is stored in standard row skyline mode). Several ways of putting these substructures together may be used and there are no compelling reasons for preferring one strategy over another one. We chose to store contiguously each row of the lower part and column of the upper part of the matrix. The real array A will contain the 1-st row followed by the first column (empty), followed by the second row followed by the second column, etc.. An additional pointer is needed to indicate where the diagonal elements, which separate the lower from the upper part, are located in this array.

2.1.9 The Jagged Diagonal Format (JAD)

This storage mode is very useful for the efficient implementation of iterative methods on parallel and vector processors [8]. Starting from the CSR format, the idea is to first reorder the rows of the matrix decreasingly according to their number of nonzeros entries. Then, a new data structure is built by constructing what we call "jagged diagonals" (j-diagonals). We store as a dense vector, the vector consisting of all the first elements in A, JA from each row, together with an integer vector containing the column positions of the corresponding elements. This is followed by the second jagged diagonal consisting of the elements in the second positions from the left. As we build more and more of these diagonals, their length decreases. The number of j-diagonals is equal to the number of nonzero elements of the first row, i.e., to the largest number of nonzero elements per row. The data structure to represent a general matrix in this form consists, before anything, of the permutation array which reorders the rows. Then the real array A containing the jagged diagonals in succession and the array JA of the corresponding column positions are stored, together with a pointer array IA which points to the beginning of each jagged diagonal in the arrays A, JA. The advantage of this scheme for matrix multiplications has been illustrated in [8] and in [1] in the context of triangular system solutions.

2.2 The FORMATS conversion module

It is important to note that there is no need to have a subroutine for each pair of data structures, since all we need is to be able to convert any format to the standard row-compressed format and then back to any other format. There are currently 23 different conversion routines in this module all of which are devoted to converting from one date structure to another.

The naming mechanism adopted is to use a 6-character name for each of the subroutines the first 3 for the input format and the last 3 for the output format. Thus COOCSR does the conversion from the coordinate format to the Compressed Sparse Row format. However it was necessary to break the naming rule in one exception. We needed a version of COOCSR that is in-place, i.e., which can take the input matrix, and convert it directly into a CSR format by using very little additional work space. This routine is called COICSR. Each of the formats has a routine to translate it to the CSR format and a routine to convert back to it from the CSR format. The only exception is that a CSCCSR routine is not necessary since the conversion from Column Sparse format to Sparse Row format can be performed with the same routine CSRCSC. This is essentially a transposition operation.

Considerable effort has been put in attempting to make the conversion routines in-place, i.e., in allowing some or all of the output arrays to be the same as the input arrays. The purpose is to save storage whenever possible without sacrificing performance. The added flexibility can be very convenient in some situations. When the additional coding complexity to permit the routine to be in place was not too high this was always done. If the subroutine is in-place this is clearly indicated in the documentation. There is one case where we found it necessary to provide the in-place version as well as the regular version: COICSR is an in-place version of the COOCSR routine. We would also like to add that other routines that avoid the CSR format for some of the more important data structures may eventually be included. For now, there is only one such routine [1] namely, COOELL.

2.3 Internal format used in SPARSKIT

Most of the routines in SPARSKIT use internally the Compressed Sparse Row format. The selection of the CSR mode has been motivated by several factors. Simplicity, generality, and widespread use are certainly the most important ones. However, it has often been argued that the column scheme may have been a better choice. One argument in this favor is that vector machines usually give a better performance for such operations as matrix vector by multiplications for matrices stored in CSC format. In fact for parallel machines which have a low overhead in loop synchronization (e.g., the Alliants), the situation is reversed, see [8] for details. For almost any argument in favor of one scheme there seems to be an argument in favor of the other. Fortunately, the difference provided in functionality is rather minor. For example the subroutine APLB to add two matrices in CSR format, described in Section 5.1, can actually be also used to add two matrices in CSC format, since the data structures are identical. Several such subroutines can be used for both schemes, by pretending that the input matrices are stored in CSR mode whereas in fact they are stored in CSC mode.

3 Manipulation routines

The module UNARY of SPARSKIT consists of a number of utilities to manipulate and perform basic operations with sparse matrices. The following sections give an overview of this part of the package.

3.1 Miscellaneous operations with sparse matrices

There are a large number of non-algebraic operations that are commonly used when working with sparse matrices. A typical example is to transform A into $B = PAQ$

[1] Contributed by E. Rothman from Cornell University.

where P and Q are two permutation matrices. Another example is to extract the lower triangular part of A or a given diagonal from A. Several other such 'extraction' operations are supplied in SPARSKIT. Also provided is the transposition function. This may seem as an unnecessary addition since the routine CSRCSC already does perform this function economically. However, the new transposition provided is in place, in that it may transpose the matrix and overwrite the result on the original matrix, thus saving memory usage. Since many of these manipulation routines involve one matrix (as opposed to two in the basic linear algebra routines) we created a module called UNARY to include these subroutines.

Another set of subroutines that are sometimes useful are those involving a 'mask'. A mask defines a given nonzero pattern and for all practical purposes a mask matrix is a sparse matrix whose nonzero entries are all ones (therefore there is no need to store its real values). Sometimes it is useful to extract from a given matrix A the 'masked' matrix according to a mask M, i.e., to compute the matrix $A \odot M$, where $\odot$ denotes the element-wise matrix product, and M is some mask matrix.

3.2 The module UNARY

This module of SPARSKIT consists of a number of routines to perform some basic non-algebraic operations on a matrix. The following is a list of the routines currently supported with a brief explanation.

SUBMAT Extracts a square or rectangular submatrix from a sparse matrix. The input is a matrix in CSR format the output is a matrix in CSR format. The output matrix can, if desired, be overwritten on the input matrix (Algorithm is "in place").

FILTER Filters out elements from a matrix according to their magnitude. The input is a matrix in CSR format, the output is a matrix in CSR format, obtained from the input matrix by removing all its elements that are smaller than a certain threshold. The threshold is computed for each row according to one of three provided options. The algorithm is in place.

TRANSP This is an in-place transposition routine, i.e., it is an in place version of the CSRCSC routine in FORMATS.

COPMAT Copy of a matrix into another matrix (both stored CSR).

GETDIA Extracts a specified diagonal from a matrix. An option is provided to transform the input matrix so that the diagonal is removed from its entries. Otherwise the diagonal is extracted and the input matrix remains untouched.

GETL This subroutine extracts the lower triangular part of a matrix, including the main diagonal. The algorithm is in-place.

GETU Extracts the upper triangular part of a matrix. Similar to GETL.

LEVELS Computes the level scheduling data structure for lower triangular matrices, see [1].

AMASK Extracts $C = A \odot M$, i.e., performs the mask operation. This routine computes a sparse matrix from an input matrix A by extracting only the elements in A, where the corresponding elements of M are nonzero. The mask matrix M, is a sparse matrix in CSR format without the real values, i.e., only the integer arrays JM and IM are of the CSR format are passed.

CPERM Permutes the columns of a matrix, i.e., computes the matrix $B = AQ$ where Q is a permutation matrix.

RPERM Permutes the rows of a matrix, i.e., computes the matrix $B = PA$ where P is a permutation matrix.

DPERM Permutes the rows and columns of a matrix, i.e., computes $B = PAQ$ given two permutation matrices P and Q. This routine gives a special treatment to the common case where $Q = P^T$.

VPERM Performs an in-place permutation of a vector, i.e., performs $x := Px$, where P is a permutation matrix.

RETMX Returns the maximum absolute value in each row of an input matrix.

DIAPOS Returns the positions in the arrays A and JA of the diagonal elements, for a matrix stored in CSR format.

EXTBDG Extracts the main diagonal blocks of a matrix.

GETBWD Returns bandwidth information on a matrix. This subroutine returns the bandwidth of the lower part and the upper part of a given matrix. May be used to determine these two parameters for converting a matrix into the BND format.

BLKFND Attempts to find the block-size of a matrix.

BLKCHK Checks whether a given integer is the block size of A. This routine is called by BLKFND.

INFDIA Computes the number of nonzero elements of each of the $2n-1$ diagonals of a matrix. (The first diagonal is the diagonal with offset $-n$ which consists of the entry $a_{n,1}$ and the last is the diagonal with offset n).

AATDGR Computes the number of nonzero elements in each row of the matrix AA^T.

ATADGR Computes the number of nonzero elements in each row of the matrix A^TA.

APBDGR Computes the number of nonzero elements in each row of the matrix $A+B$, given two matrices A and B.

RNRMS Computes the norms of the rows of a matrix. The usual three norms $\|.\|_1, \|.\|_2$, and $\|.\|_\infty$ are supported.

CNRMS Computes the norms of the columns of a matrix. Similar to RNRMS.

RSCAL Scales the rows of a matrix by their norms. The same three norms as in RNRMS are available.

CSCAL Scales the columns of a matrix by their norms. The same three norms as in RNRMS are available.

4 Input/Output routines

The INOUT module of SPARSKIT comprises a few routines for reading, writing, and for plotting and visualizing the structure of sparse matrices. These routines are essentially geared towards the utilization of the Harwell/Boeing collection of matrices. There are currently only three subroutines in this module.

READMT Reads a matrix in the Harwell/Boeing format.

PRTMT Creates a Harwell Boeing file from an arbitrary matrix in CSC or CSC format.

PLTG Creates a pic file for plotting the pattern of a matrix.

The routines readmt and prtmt allow to read and create files containing matrices stored in the H/B format. For details concerning this format the reader is referred to

[4]. While the purpose of readmt is clear, it is not obvious that one single subroutine can write a matrix in H/B format and still satisfy the needs of all users. For example for some matrices all nonzero entries are actually integers and a format using say a 10 digit mantissa may entail an enormous waste of storage if the matrix is large. The solution provided is to compute internally the best formats for the integer arrays IA and JA. A little help is required from the user for the real values in the arrays A and RHS. Specifically, the desired format is obtained from a parameter of the subroutine by using a simple notation, see documentation for details.

We found it extremely useful to be able to visualize a sparse matrix, notably for debugging purposes. A simple look at the plot can sometimes reveal whether the matrix obtained from some reordering technique does indeed have the expected structure. For now two simple plotting mechanisms are provided. First, a preprocessor to the Unix utility 'Pic' allows one to generate a pic file from a matrix that is in the Harwell/Boeing format or any other format. For example for a Harwell/Boeing matrix file, the command is of the form

$$PltMat < HBfilename$$

The output file is then printed by the usual troff or TeX commands. A translation of this routine into one that generates a post-script file is also available in the module UNSUPP (see Section 8). We should point out that the plotting routines are very simple in nature and should not be used to plot large matrices. For example the pltmt routine outputs one pic command line for every nonzero element. This constitutes a convenient tool for document preparation for example. Matrices of size just up to a few thousands can be printed this way. Several options concerning size of the plot and caption generation are available.

Another set of utilities for viewing profiles of sparse matrices on Sun screens is also available, see Section 8.

5 Basic algebraic operations

The usual algebraic operations involving two matrices, such as $C = A + B$, $C = A + \beta B$, $C = AB$, etc.., are fairly common in sparse matrix computations. These basic matrix operations are included in the module called BLASSM. In addition there are a large number of basic operations, involving a sparse matrix and a vector, such as matrix-vector products and triangular system solutions that are very commonly used. Some of these are included in the module MATVEC. Sometimes it is desirable to compute the patterns of the matrices $A + B$ and AB, or in fact of any result of the basic algebraic operations. This can be implemented by way of job options which will determine whether to fill-in the real values or not during the computation. We now briefly describe the contents of each of the two modules BLASSM and MATVEC.

5.1 The BLASSM module

Currently, the module BLASSM (Basic Linear Algebra Subroutines for Sparse Matrices) contains the following nine subroutines:

AMUB Performs the product of two matrices, i.e., computes $C = AB$, where A and B are both in CSR format.

APLB Performs the addition of two matrices, i.e., computes $C = A + B$, where A and B are both in CSR format.

APLSB Performs the operation $C = A + \sigma B$, where σ is a scalar, and A, B are two matrices in CSR format.

APMBT Performs either the addition $C = A + B^T$ or the subtraction $C = A - B^T$.

APLSBT Performs the operation $C = A + sB^T$.

DIAMUA Computes the product of diagonal matrix (from the left) by a sparse matrix, i.e., computes $C = DA$, where D is a diagonal matrix and A is a general sparse matrix stored in CSR format.

AMUDIA Computes the product of a sparse matrix by a diagonal matrix from the right, i.e., computes $C = AD$, where D is a diagonal matrix and A is a general sparse matrix stored in CSR format.

APLDIA Computes the sum of a sparse matrix and a diagonal matrix, $C = A + D$.

APLSCA Performs an in place addition of a scalar to the diagonal entries of a sparse matrix, i.e., performs the operation $A := A + \sigma I$.

Still missing from this list, and to be added in the near future are the routines

AMUBT to multiply A by the transpose of B, $C = AB^T$, and

ATMUB to multiply the transpose of A by B, $C = A^T B$.

Operations of the form $tA + sB$ have been avoided as their occurrence does not warrant additional subroutines. Several other operations similar to those defined for vectors have not been included. For example the scaling of a matrix in sparse format is simply a scaling of its real array A, which can be done with the usual BLAS1 scaling routine, on the array A.

5.2 The MATVEC MODULE

In its current status, this module contains matrix by vector products and various sparse triangular solution methods. The contents are as follows.

AMUX	Performs the product of a matrix by a vector. Matrix stored in Compressed Sparse Row (CSR) format.
ATMUX	Performs the product of the transpose of a matrix by a vector. Matrix A stored in Compressed Sparse Row format. Can also be viewed as the product of a matrix in the Compressed Sparse Column format by a vector.
AMUXE	Performs the product of a matrix by a vector. Matrix stored in Ellpack/Itpack (ELL) format.
AMUXD	Performs the product of a matrix by a vector. Matrix stored in Diagonal (DIA) format.
AMUXJ	Performs the product of a matrix by a vector. Matrix stored in Jagged Diagonal (JAD) format.
LSOL	Unit lower triangular system solution. Matrix stored in Compressed Sparse Row (CSR) format.
LDSOL	Lower triangular system solution. Matrix stored in Modified Sparse Row (MSR) format. Diagonal elements inverted.
LSOLC	Unit lower triangular system solution. Matrix stored in Compressed Sparse Column (CSC) format.
LDSOLC	Lower triangular system solution. Matrix stored in Modified Sparse Column (MSC) format with diagonal elements inverted.
LDSOLL	Unit lower triangular system solution with the level scheduling approach. Matrix stored in Modified Sparse Row format, with diagonal elements inverted.

USOL	Unit upper triangular system solution. Matrix stored in Compressed Sparse Row (CSR) format.
UDSOL	Upper triangular system solution. Matrix stored in Modified Sparse Row (MSR) format. Diagonal elements inverted.
USOLC	Unit upper triangular system solution. Matrix stored in Compressed Sparse Column (CSC) format.
UDSOLC	Upper triangular system solution. Matrix stored in Modified Sparse Column (MSC) format with diagonal elements inverted.

Most of the above routines are very short and rather straightforward. A long test program is provided to run all of the subroutines on a large number of matrices that are dynamically generated using the MATGEN module.

6 The basic statistics and information routines

It is sometimes very informative when analyzing solution methods, to be able in a short amount of time to obtain some statistical information about a sparse matrix. The purpose of the subroutine infol, is to print out such information. The question we had to address at first was to determine what type of information was the most useful without being too expensive to obtain. The simplest and most common statistics are: total number of nonzero elements, average number of nonzero elements per row (with standard deviation), band size. Our preliminary package Infol contains the above and a number of other features. For example it answers the following questions: Is the matrix lower triangular, upper triangular? does it have a symmetric structure? If not how close is it from having this property? Is it weakly row-diagonally dominant? What percentage of the rows are weakly diagonally dominant? Same questions for column diagonal dominance. A sample output from infol is listed in Figure1. This print-out was generated by typing

infol < pores_2

where pores_2 is a file containing a matrix in H/B format.

If the Harwell-Boeing matrix is symmetric then Infol takes this information into account to obtain the correct information instead of the information on the lower triangular part only. Moreover, in cases where only the pattern is provided (no real values), then infol will print a message to this effect and will then give information related only to the structure of the matrix. The output for an example of this type is shown in Figure 2. We should point out that the runs for these two tests were basically instantaneous on a Sun-4 workstation.

```
* * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * *
* unsymmetric matrix from pores                                              *
*                    Key = pores_2  , Type = rua                              *
* * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * *
  *  Dimension N                                        =       1224  *
  *  Number of nonzero elements                         =       9613  *
  *  Average number of nonzero elements/Column          =     7.8538  *
  *  Standard deviation for above average               =     5.4337  *
  *  Nonzero elements in strict upper part              =       4384  *
  *  Nonzero elements in strict lower part              =       4005  *
  *  Nonzero elements in main diagonal                  =       1224  *
  *  Weight of longest column                           =         30  *
  *  Weight of shortest column                          =          2  *
  *  Weight of longest row                              =         30  *
  *  Weight of shortest row                             =          2  *
  *  Matching elements in symmetry                      =       6358  *
  *  Relative Symmetry Match (symmetry=1)               =     0.6614  *
  *  Average distance of a(i,j)  from diag.             =  0.615E+02  *
  *  Standard deviation for above average               =  0.103E+03  *
  *-----------------------------------------------------------------*
  *  Frobenius norm of A                                =  0.150E+09  *
  *  Frobenius norm of symmetric part                   =  0.100E+09  *
  *  Frobenius norm of nonsymmetric part                =  0.951E+08  *
  *  Maximum element in A                               =  0.378E+08  *
  *  Percentage of weakly diagonally dominant rows      =  0.481E+00  *
  *  Percentage of weakly diagonally dominant columns   =  0.490E-02  *
  *-----------------------------------------------------------------*
  *  Lower bandwidth  (max: i-j, a(i,j) .ne. 0)         =        470  *
  *  Upper bandwidth  (max: j-i, a(i,j) .ne. 0)         =        471  *
  *  Maximum Bandwidth                                  =        736  *
  *  Average Bandwidth                                  =  0.190E+03  *
  *  Number of nonzeros in skyline storage              =     340385  *
  *  90% of matrix is in the band of width              =        527  *
  *  80% of matrix is in the band of width              =        145  *
  *  The total number of nonvoid diagonals is           =        367  *
  *  The 10 most important diagonals are (offsets)      :             *
  *     0     1    -1    -2     2    -3   -32  -264   264    32      *
  *  The accumulated percentages they represent are     :             *
  *  12.7  24.6  31.7  37.9  43.6  49.0  52.4  55.7  58.6  61.4      *
  *-----------------------------------------------------------------*
  *  The matrix does not have a block structure                      *
  *-----------------------------------------------------------------*
```

Figure 1: Sample output from Info1

```
* * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * *
* SYMMETRIC PATTERN FROM CANNES,LUCIEN MARRO,JUNE 1981.                        *
*                    Key = CAN 1072 , Type = PSA                              *
* No values provided - Information on pattern only                            *
* * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * *
    *  Dimension N                                    =        1072  *
    *  Number of nonzero elements                     =        6758  *
    *  Average number of nonzero elements/Column      =     11.6082  *
    *  Standard deviation for above average           =      5.6474  *
    *  Nonzero elements in strict upper part          =        5686  *
    *  Nonzero elements in strict lower part          =        5686  *
    *  Nonzero elements in main diagonal              =        1072  *
    *  Weight of longest column                       =          35  *
    *  Weight of shortest column                      =           6  *
    *  Matching elements in symmetry                  =        6758  *
    *  Relative Symmetry Match (symmetry=1)           =      1.0000  *
    *  Average distance of a(i,j)  from diag.         =   0.110E+03  *
    *  Standard deviation for above average           =   0.174E+03  *
    *-----------------------------------------------------------------*
    *  Lower bandwidth  (max: i-j, a(i,j) .ne. 0)     =        1048  *
    *  Upper bandwidth  (max: j-i, a(i,j) .ne. 0)     =        1048  *
    *  Maximum Bandwidth                              =        1055  *
    *  Average Bandwidth                              =   0.376E+03  *
    *  Number of nonzeros in skyline storage          =      277248  *
    *  90% of matrix is in the band of width          =         639  *
    *  80% of matrix is in the band of width          =         343  *
    *  The total number of nonvoid diagonals is       =         627  *
    *  The  5 most important diagonals are (offsets)  :              *
    *     0    -1    -2    -3    -4                                  *
    *  The accumulated percentages they represent are  :             *
    *  15.9  24.7  29.7  33.9  36.3                                  *
    *-----------------------------------------------------------------*
    *  The matrix does not have a block structure                    *
    *-----------------------------------------------------------------*
```

Figure 2: Sample output from Info1 for matrix with pattern only

7 Matrix generation routines

One of the difficulties encountered when testing and comparing numerical methods, is that it is sometimes difficult to guarantee that the matrices compared are indeed identical. Even though a paper may give full details on the test problems considered, programming errors or differences in coding may lead to the incorrect matrices and the incorrect conclusions. This has often happened in the past and is likely to be avoided if the matrices were generated with exactly the same code. The module MATGEN of SPARSKIT includes several matrix generation routines. Currently, the matrices generated by SPARSKIT are of the following type.

1. Scalar 5-point and 7-point matrices arising from discretization of the elliptic type equation:

$$Lu = \frac{\partial}{\partial x}(a\frac{\partial}{\partial x}u) + \frac{\partial}{\partial y}(b\frac{\partial}{\partial y}u) + \frac{\partial}{\partial z}(c\frac{\partial}{\partial z}u) + \frac{\partial}{\partial x}(du) + \frac{\partial}{\partial y}(eu) + \frac{\partial}{\partial z}(fu) + gu \quad (1)$$

   on rectangular regions with Dirichlet boundary conditions. The user provides the functions $a, b, c, ..., g$ and the result is a matrix in general sparse format, possibly printed in a file in the H/B format.

   For now only centered differences are considered. However, an option will be added in the future to allow upwinded schemes for the first order derivatives.

2. Block 5-point and 7-point matrices arising from discretization of the elliptic type equation (1) in which u is now a vector of $nfree$ components, and $a, b, c, ..., g$ are $nfree \times nfree$ matrices provided by the user.

3. Finite element matrices created from the heat conduction problem

$$-\nabla.K\nabla u = f \quad (2)$$

   on a domain D with Dirichlet boundary conditions. A coarse initial domain is described by the user and the code does an arbitrary user-specified number of refinements of the grid and assembles the matrix, in CSR format. Linear triangular elements are used. If only the matrix is desired the heat source f can be zero. Arbitrary grids can be used, but the user may also take advantage of six initial grids supplied by the package for simple test problems.

4. Test matrices [2] from Zlatev et. al. [10] and Osterby and Zlatev [7]. The first two matrix generators described in the above references are referred to as $D(n, c)$ and $E(n, c)$ respectively. A more elaborate class where more than two parameters can be varied, is referred to as the class $F(m, n, c, r, \alpha)$ in [7, 10]. The three subroutines to generate these matrices are called MATRF2 (for the class $F(m, n, c, r, \alpha)$), DCN (for the class $D(c, n)$) and ECN (for the class $E(c, n)$). These codes can generate rectangular as well as square matrices and allow a good flexibility in making the matrices more or less dense and more or less well conditioned.

[2]These subroutines have been contributed to the author by E. Rothman from Cornell University.

8 The UNSUPP directory

In addition to the basic tools described in the previous sections, SPARSKIT includes a directory called UNSUPP includes software that is not necessarily portable or that does not fit in all previous modules. For example software for viewing matrix patterns on some particular workstation may be found here. Another example is all the different reordering schemes, such as minimum degree ordering, or nested dissection etc.. Many of these are available from NETLIB but others may be contributed by researchers for comparison purposes.

In version 1 the following items are available in UNSUPP.

MATVIEW A FORTRAN/suncore program to plot a Harwell/Boeing matrix on a sun screen. This must be used with suntools. Also provided is a makefile to produce the executable 'viewmat'. Then the usage is *viewmat* $< HB_{file}$ where HB_{file} is a file containing a matrix in Harwell-Boeing format.

MATVIEWP Similar to MATVIEW but allows to zoom on a rectangular part of the matrix. A makefile is also provided to produce the executable viewmatp. To execute one just types 'matviewp' and there will be a prompt asking for the name of the matrix and for the row and column indices $i1, i2, j1, j2$ that limit the submatrix to be viewed.

PLTMTPS a translation of the pltmt subroutine in INOUT/inout.f to produce a post-script file rather than a pic file. Does not yet offer the same functionality as pltmt.

ILUT Preconditioned GMRES algorithm with three preconditioners. The main item here is a robust preconditioner called ILUT (unpublished) which uses a dual thresholding strategy for dropping elements. Arbitrary accuracy is allowed in ILUT. The standard ILU(0) and MILU(0) are also provided. All can be used with the same PGMRES routine which supports only right preconditioning.

The two basic programs for viewing matrix patterns on a sun screen will eventually be replaced by programs for the X-windows environment which is fast becoming a standard. The ILUT code is provided mainly for facilitating comparisons between iterative algorithms.

9 Distribution

The first release of the package follows the Linpack-Eispack approach in that it aims at providing efficient and well tested subroutines written in portable FORTRAN. Similarly to the Linpack and Eispack packages, the goal is to make available a common base of useful codes for a specific area of computation, in this case sparse linear algebra. The package is in the public domain and will be made accessible through the internet.

Currently, the package is organized in six distinct subdirectories, each containing one or more modules. The six directories and the modules they contain are the following: INOUT (inout.f), FORMATS (formats.f, unary.f), BLASSM (blassm.f, matvec.f), MATGEN (genmat.f, zlatev.f), INFO (dinfo1.f), UNSUPP (various routines). Test programs with unix makefiles are provided in each subdirectory to test a large number of the subroutines. Each directory contains a README file listing contents, and giving additional information.

For information concerning distribution contact the author at na.saad@na-net.stanford.edu.

10 Conclusion and Future Plans

It is hoped that SPARSKIT will be useful in many ways to researchers in different areas of scientific computing. In the first version of SPARSKIT, there are few sparse problem solvers, such as direct solution methods, or eigenvalue solvers. Some of these are available from different sources and we felt that it was not appropriate to provide additional ones. The original motivation for SPARSKIT is that there is a gap to fill in the manipulation and basic computations with sparse matrices. Once this gap is filled with some satisfaction, then additional functionality may be added.

We briefly mentioned in the introduction the possibility of using SPARSKIT to develop an interactive package. Large matrices of dimension tens of of thousands can easily be manipulated with the current supercomputers, in real time. One of the difficulties with such an interactive package is that we do not yet have reliable routines for computing eigenvalues/eigenvectors of large sparse matrices. The state of the art in solving linear systems is in a much better situation. However, one must not contemplate to perform the same type of computations as with small dense matrices. As an example, getting all the eigenvalues of a sparse matrix is not likely to be too useful when the matrix is very large.

Beyond interactive software for sparse linear algebra, one can envision the integration of SPARSKIT in a larger package devoted to solving certain types of Partial Differential Equations, possibly interactively.

Acknowledgements. The idea of creating a tool package for sparse matrices germinated while the author was at the Center for Supercomputing Research and Development of the University of Illinois (1986-1987) and part of this work was performed there. Initially the author has benefited from helpful comments from Iain Duff (then visiting CSRD) and a number of colleagues at CSRD. Billy Stewart and his students at NCSU used a preliminary version of SPARSKIT in a class project and made some valuable comments. Ernie Rothman contributed some software. The author has also benefited from helpful discussions from a number of other colleagues, including Mike Heroux, Giuseppe Radicatti, Ahmed Sameh, Horst Simon, Phuong Vu, and Harry Wijshoff.

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APPENDIX: QUICK REFERENCE

For convenience we list in this appendix the most important subroutines in the various modules of SPARSKIT. More detailed information can be found either in the body of the paper or in the documentation of the package.

FORMATS Module

- CSRDNS : converts a row-stored sparse matrix into the dense format.
- DNSCSR : converts a dense matrix to a sparse storage format.
- COOCSR : converts coordinate to to csr format
- COICSR : in-place conversion of coordinate to csr format
- CSRCOO : converts compressed sparse row to coordinate format.
- CSRSSR : converts compressed sparse row to symmetric sparse row format.
- SSRCSR : converts symmetric sparse row to compressed sparse row format.
- CSRELL : converts compressed sparse row to ellpack format
- ELLCSR : converts ellpack format to compressed sparse row format.
- CSRMSR : converts compressed sparse row format to modified sparse row format.
- MSRCSR : converts modified sparse row format to compressed sparse row format.
- CSRCSC : converts compressed sparse row format to compressed sparse column format (transposition).
- CSRDIA : converts the compressed sparse row format into the diagonal format.
- DIACSR : converts the diagonal format into the compressed sparse row format.
- BSRCSR : converts the block-row sparse format into the compressed sparse row format.
- CSRBSR : converts the compressed sparse row format into the block-row sparse format.
- CSRBND : converts the compressed sparse row format into the banded format (linpack style).

- BNDCSR : converts the banded format (linpack style) into the compressed sparse row storage.
- CSRSSK : converts the compressed sparse row format to the symmetric skyline format
- SSKSSR : converts symmetric skyline format to symmetric sparse row format.
- CSRJAD : converts the csr format into the jagged diagonal format
- JADCSR : converts the jagged-diagonal format into the csr format
- COOELL : converts the coordinate format into the Ellpack/Itpack format.

UNARY Module

- SUBMAT : extracts a submatrix from a sparse matrix.
- FILTER : filters elements from a matrix according to their magnitude.
- TRANSP : in-place transposition routine (see also csrcsc in formats)
- COPMAT : copies a matrix into another matrix (both stored csr).
- GETDIA : extracts a specified diagonal from a matrix.
- GETL : extracts lower triangular part.
- GETU : extracts upper triangular part.
- LEVELS : gets the level scheduling structure for lower triangular matrices.
- AMASK : extracts $C = A \odot M$
- DPERM : permutes a matrix ($B = PAQ$) given two permutations P, Q
- CPERM : permutes the columns of a matrix ($B = AQ$)
- RPERM : permutes the rows of a matrix ($B = PA$)
- VPERM : permutes a vector (in-place)
- RETMX : returns the max absolute value in each row of the matrix.
- DIAPOS : returns the positions of the diagonal elements in A.
- EXTBDG : extracts the main diagonal blocks of a matrix.
- GETBWD : returns the bandwidth information on a matrix.

- BLKFND : finds the block-size of a matrix.
- BLKCHK : checks whether a given integer is the block size of A.
- INFDIA : obtains information on the diagonals of A.
- AMUBDG : obtains the number of nonzeros in each row of AB.
- APBDGR : obtains the number of nonzero elements in each row of $A + B$.
- RNRMS : computes the norms of the rows of A.
- CNRMS : computes the norms of the columns of A.
- RSCAL : scales the rows of a matrix by their norms.
- CSCAL : scales the columns of a matrix by their norms.

INOUT Module

- READMT : reads matrices in the boeing/Harwell format.
- PRTMT : prints matrices in the boeing/Harwell format.
- PLTMT : produces a 'pic' file for plotting a sparse matrix.

INFO Module

- DINFO1 : obtains a number of statistics on a sparse matrix.

MATGEN Module

- GEN57PT : generates 5-point and 7-point matrices.
- GEN57BL : generates block 5-point and 7-point matrices.
- GENFEA : generates finite element matrices in assembled form.
- GENFEU : generates finite element matrices in unassembled form.
- ASSMB1 : assembles an unassembled matrix (as produced by genfeu).
- MATRF2 : Routines for generating sparse matrices by Zlatev et al.
- DCN: Routines for generating sparse matrices by Zlatev et al.

- ECN: Routines for generating sparse matrices by Zlatev et al.

BLASSM Module

- AMUB : computes $C = A * B$.
- BPLB : computes $C = A + B$.
- APLSB : computes $C = A + sB$.
- APMBT : Computes $C = A \pm B^T$.
- APLSBT : Computes $C = A + s * B^T$.
- DIAMUA : Computes $C = Diag * A$.
- AMUDIA : Computes $C = A * Diag$.
- APLDIA : Computes $C = A + Diag$.
- APLSCA : Computes $A := A + sI$ (s = scalar).

MATVEC Module

- AMUX : A times a vector. Compressed Sparse Row (CSR) format.
- ATMUX : A^T times a vector. CSR format.
- AMUXE : A times a vector. Ellpack/Itpack (ELL) format.
- AMUXD : A times a vector. Diagonal (DIA) format.
- AMUXJ : A times a vector. Jagged Diagonal (JAD) format.
- LSOL : Unit lower triangular system solution. Compressed Sparse Row (CSR) format.
- LDSOL : Lower triangular system solution. Modified Sparse Row (MSR) format.
- LSOL : Unit lower triangular system solution. Compressed Sparse Column (CSC) format.
- LDSOLC: Lower triangular system solution. Modified Sparse Column (MSC) format.
- LDSOLL: Lower triangular system solution with level scheduling. MSR format.

- USOL : Unit upper triangular system solution. Compressed Sparse Row (CSR) format.
- UDSOL : Upper triangular system solution. Modified Sparse Row (MSR) format.
- USOLC : Unit upper triangular system solution. Compressed Sparse Column (CSC) format.
- UDSOLC: Upper triangular system solution. Modified Sparse Column (MSC) format.

UNSUPP Module

- ILUT: ILUT(k) preconditioned GMRES mini package.
- MATVIEW : suncore code for viewing a matrix on a sun station.
- MATVIEWP: suncore code for viewing a submatrix on a sun station.
- PLTMTPS : creates a post Script file to plot a sparse matrix.