

# Sparse Matrix Multiplication Package (SMMP)\*

Randolph E. Bank<sup>†</sup>

Craig C. Douglas<sup>‡</sup>

April 23, 2001

**Abstract:** Routines callable from FORTRAN and C are described which implement matrix–matrix multiplication and transposition for a variety of sparse matrix formats. Conversion routines between various formats are provided.

**Keywords:** sparse matrices, matrix multiplication, transposition, numerical linear algebra

**AMS MOS Classification:** Numerical Analysis (Numerical Linear Algebra)

## 1 Introduction

The routines described here perform matrix-matrix multiplies, transposes, and format conversions for sparse matrices. There are three formats supported. These include the old and new Yale sparse matrix package formats [5, 6, 7] and the more efficient one for square matrices advocated by Bank and Smith [1]. In each case, only the nonzeros are stored, not the zeros (or as few as possible).

The principal use of these routines will probably be in implementing parallel computation algorithms. For example, in one variant of parallel multigrid [2, 3], as the number of coarse grid problems per level grows, it becomes increasingly difficult to generate the coefficient matrices based on grids, as a serial multigrid solver does.

In §2, we describe the sparse matrix formats we support. In §3, we describe the structure of the package and the calling sequences of each routine. In §4, we describe the algorithms implemented by the package. Finally, in §5 are instructions for getting a copy of the code.

The routines described here differ from those in either SPARSKIT (see [9]) or the proposed sparse BLAS (see [4] and [8]). There is some overlap with SPARSKIT, but we are more interested in a data format not supported in SPARSKIT. The sparse BLAS have interfaces for multiplying a sparse matrix by a dense one, but not for multiplying two sparse matrices. Also, our routines are in the public domain with absolutely no restrictions on their use while the others are not.

## 2 Sparse matrix formats

In this section, we define three methods for storing a sparse matrix  $M$ . Let  $M = D + L + U$ , where  $D$  is the main diagonal part of  $M$ ,  $L$  is the strictly lower triangular part of  $M$ , and  $U$  is the strictly upper triangular part of  $M$ . We define the number of nonzeros of  $M$  as  $NZ(M)$ .

---

\*To appear in *Advances in Computational Mathematics*, 1 (1993), first issue. The algorithms and routines described here were developed while both authors were visiting the Center for Applied Mathematics, Department of Mathematics, Purdue University.

<sup>†</sup>University of California at San Diego, Department of Mathematics C012, P. O. Box 109, LaJolla, CA 92093. E-mail: [rbanke@ucsd.edu](mailto:rbanke@ucsd.edu)

<sup>‡</sup>Department of Computer Science, Yale University, P. O. Box 2158 Yale Station, New Haven, CT 06520-2158 and Mathematical Sciences Department, IBM Research Division, Thomas J. Watson Research Center, P. O. Box 218, Yorktown Heights, NY 10598-0218, USA. E-mail: [na.cdouglas@na-net-ornl.gov](mailto:na.cdouglas@na-net-ornl.gov).

The old Yale sparse matrix format [6, 7] requires three vectors:

$$\begin{array}{ll}
 IA : \boxed{IA} & \text{length } N + 1 \\
 JA : \boxed{JA} & \begin{array}{l} \text{length } NZ(M) \\ \text{or } NZ(D + U) \end{array} \\
 A : \boxed{M} & \begin{array}{l} \text{length } NZ(M) \\ \text{or } NZ(D + U) \end{array}
 \end{array}$$

$M$  is stored in row form. If  $M$  is symmetric, the elements of  $L$  do not have to be stored in  $A$ . The first element of row  $I$  is  $A(IA(I))$ . The length of row  $I$  is determined by  $IA(I + 1) - IA(I)$ , which is why  $IA$  requires  $N + 1$  elements instead of the obvious  $N$  elements. The column indices of  $M$  are stored in the  $JA$  vector. For element  $A(J)$ , its column index is  $JA(J)$ . The elements in a row may be stored in any order.

The new Yale sparse matrix format [5] requires two vectors:

$$\begin{array}{ll}
 IJA : \boxed{IA \quad | \quad JA} & \begin{array}{l} \text{length } N + 1 + NZ(M - D) \\ \text{or } N + 1 + NZ(U) \end{array} \\
 A : \boxed{D \quad | \quad 0 \quad | \quad L \text{ and } U} & \begin{array}{l} \text{length } N + 1 + NZ(M - D) \\ \text{or } N + 1 + NZ(U) \end{array}
 \end{array}$$

$M$  is still stored in row form. The  $IA$ - $JA$  vectors of the old format are combined into a single vector, sometimes referred as an  $IJA$  vector. As before, the first element of row  $I$  is  $A(IJA(I))$ . In this case, the main diagonal of  $M$  is separated out from the nonzeros of  $L$  and  $U$ . The diagonal for row  $I$  is in  $A(I)$ . There is a zero after  $D$  so that the  $JA$  and  $L/U$  parts of the  $IJA$  and  $A$  vectors are aligned properly. Technically, the rows of  $A$  should be stored in ascending column order. However, this is not enforced.

The Bank-Smith sparse matrix format [1] requires  $M$  to be a square matrix with a symmetric (or nearly so) zero structure. It requires two vectors:

$$\begin{array}{ll}
 IJA : \boxed{IA \quad | \quad JA} & \text{length } N + 1 + NZ(U) \\
 A : \boxed{D \quad | \quad 0 \quad | \quad U^T \quad | \quad L} & \begin{array}{l} \text{length } N + 1 + NZ(M - D) \\ \text{or } N + 1 + NZ(U) \end{array}
 \end{array}$$

While  $M$  is stored strictly in row form, in a real sense it is stored in both column and row form. Since we assume that  $M$  has a symmetric zero structure (or  $L$  and  $U$  are padded by a small number of zeros), we need only store the row indices for  $U$  (when  $U$  is stored in column form). These are also the column indices for  $L$  (when  $L$  is stored in row form). However, we store the transpose of  $U$  in row form instead of  $U$ . If  $M$  is symmetric, the elements of  $L$  do not have to be stored in  $A$ . The first element of column  $I$  of  $U$  is  $A(IA(I))$ . The length of column  $I$  is determined by  $IA(I + 1) - IA(I)$ , which is why  $IA$  requires  $N + 1$  elements instead of the obvious  $N$  elements. The row indices of  $U$  are stored in the  $JA$  vector. For element  $A(J)$ , its row index is  $JA(J)$ . The elements in a column must be stored in ascending row order. We define  $LSHIFT$  to be 0 if  $M$  is symmetric and  $IA(N + 1) - IA(1)$  if  $M$  is nonsymmetric. The first element of  $L$  is  $A(IA(1) + LSHIFT)$ .  $L$  is stored in row format. The column index of an element  $A(IA(I) + J + LSHIFT)$  is  $JA(IA(I) + J)$ .

For all three sparse matrix formats, we can assume there are three vectors  $IA$ ,  $JA$ , and  $A$  which describe  $M$ . Except for the old Yale sparse matrix format, the vectors  $IA$  and  $JA$  are really the same vector  $IJA$ . We also need a variable  $DIAGA$  which is one if the diagonal is separated from the rest of the nonzeros and zero otherwise. Last, we need a variable  $SYMA$  which is one if  $M$  is stored in a symmetric manner and zero otherwise.

### 3 Calling sequences

In this section, we describe the five routines which comprise the package. These include two routines to multiply matrices, a routine for the transpose of a matrix, and two routines to convert between various sparse matrix formats.

For each routine in this section, the calling sequence assumes distinct  $IA$  and  $JA$  vectors for each matrix. Suppose a matrix is actually stored using an  $IJA$  vector. Then the routine should be called with  $IJA$  as an argument twice, once for each  $IA$  and  $JA$ . The  $IJA$  vector should not be subscripted to point to either of the  $IA$  or  $JA$  parts; the routines will do this automatically.

We multiply two sparse matrices, resulting in a third:

$$C = AB.$$

Matrix-matrix multiplication is performed in two steps. These routines only support the Yale sparse matrix formats. First, the nonzero structure of the resulting matrix is determined symbolically in *SYMBMM*:

```
subroutine SYMBMM (N,M,L, IA,JA,DIAGA, IB,JB,DIAGB,
                  IC,JC,DIAGC, INDEX)

integer         N,M,L, IA(*),JA(*),DIAGA,
                IB(*),JB(*),DIAGB, IC(*),JC(*),DIAGC,
                INDEX(*)
```

The number of rows and columns of the matrices are

matrix	rows	columns
$A$	$N$	$M$
$B$	$M$	$L$
$C$	$N$	$L$

*INDEX* is a scratch vector of length  $\max\{L, M, N\}$ . It is used to store linked lists. The output of *SYMBMM* is *IC* and *JC*. They are dependent on the value of *DIAGC*.

Once the nonzero structure for  $C$  is known, the numerical matrix-matrix multiply is computed in *NUMBMM*:

```
subroutine NUMBMM (N,M,L, IA,JA,DIAGA, A, IB,JB,DIAGB, B,
                  IC,JC,DIAGC, C, TEMP)

integer         N,M,L, IA(*),JA(*),DIAGA,
                IB(*),JB(*),DIAGB, IC(*),JC(*),DIAGC
real           A(*), B(*), C(*)
```

*TEMP* is a scratch vector of length  $\max\{L, M, N\}$ . It is used to store partial sums.

We may also compute the transpose of a matrix, resulting in a second:

$$B = A^T.$$

We do this operation in *TRANSP*:

```
subroutine TRANSP (N,M, IA,JA,DIAGA, A, IB,JB, B, MOVE)

integer         N,M, IA(*),JA(*),DIAGA,
                IB(*),JB(*), MOVE
real           A(*), B(*)
```

The number of rows and columns of the matrices are

matrix	rows	columns
$A$	$N$	$M$
$B$	$M$	$N$

We assume that  $B$  will use the same diagonal storage method that is used for  $A$ . We do not actually move the elements of  $A$  into  $B$  unless  $MOVE$  is one.

Finally, we have two routines for converting between one of the Yale formats and the Bank-Smith format. This only makes sense when the matrices are square. The routine  $YTOBS$  will convert a Yale format sparse matrix into the Bank-Smith format:

```
subroutine YTOBS (N, IA, JA, DIAGA, SYMA, A, IB, JB, B, MOVE)
```

```
integer N, IA(*), JA(*), DIAGA, SYMA,
        IB(*), JB(*), MOVE
real A(*), B(*)
```

By definition,  $DIAGB$  must be one. Hence, we do not need it as an argument. We determine whether or not  $B$  should be stored in a symmetric or nonsymmetric manner from  $SYMA$ . We do not actually move the elements of  $A$  into  $B$  unless  $MOVE$  is one.

The routine  $BSTOY$  will convert a Bank-Smith format sparse matrix into one of the Yale formats:

```
subroutine BSTOY (N, IA, JA, SYMA, A, IB, JB, DIAGB, B, MOVE)
```

```
integer N, IA(*), JA(*), SYMA,
        IB(*), JB(*), DIAGB, MOVE
real A(*), B(*)
```

We determine which of the two formats by the value of  $DIAGB$ . We determine whether or not  $B$  should be stored in a symmetric or nonsymmetric manner from  $SYMA$ . We do not actually move the elements of  $A$  into  $B$  unless  $MOVE$  is one.

## 4 Algorithms

In this section, we describe the algorithms for  $SYMBMM$ ,  $NUMBMM$ , and  $TRANSP$ . We use a metalanguage rather than real code. One of the facets of these algorithms is their ability to work well with matrices in a variety of formats.

### 4.1 SYMBMM

Initialization consists of setting up the first row pointer and clearing all of the links (contained in  $INDEX$ ):

```
1      do i ∈ {1, ⋯, max{l, m, n}} {
2          indexi = 0
3      }
4      if (diagc == 0) {
5          ic1 = 1
6      }
7      else {
8          ic1 = n + 2
9      }
```

$INDEX$  is used to store links. If an entry in  $INDEX$  is nonzero, it is a pointer to the next column with a nonzero. The links are determined as they are found, and are unordered.

The main loop consists of three components: initialization, a long loop that merges row lists, and code to copy the links into the  $JC$  vector. The initialization part is as follows:

```

10      do  $i \in \{1, \dots, n\}$  {
11           $istart = -1$ 
12           $length = 0$ 

```

The start column ( $istart$ ) is reset and the number of column entries for the  $i$ -th row is assumed empty. The loop to merge row lists is as follows:

```

13      do  $jj \in \{ia_i, \dots, ia_{i+1}\}$  {
14          if ( $jj == ia_{i+1}$ ) {
15              if ( $diaga == 0 \mid$ 
16                   $i > \min\{m, n\}$ ) {
17                  next  $jj$ 
18              }
19               $j = i$ 
20          }
21          else {
22               $j = ja_{jj}$ 
23          }
24          if ( $index_j == 0 \ \& \ diagb == 1 \ \&$ 
25               $j \leq \min\{l, m\}$ ) {
26               $index_j = istart$ 
27               $istart = j$ 
28               $length = length + 1$ 
29          }
30          do  $k \in \{ib_j, \dots, ib_{j+1} - 1\}$  {
31              if ( $index_{jb_k} == 0$ ) {
32                   $index_{jb_k} = istart$ 
33                   $istart = jb_k$ 
34                   $length = length + 1$ 
35              }
36          } (end of k loop)
37      } (end of jj loop)

```

Lines 14-22 determine if the  $jj$  loop has to execute an “extra” iteration when  $A$  is stored in the new Yale sparse matrix format. Lines 23-27 add column  $j$  to the linked list. Lines 28-34 determine the intersection of this row  $i$  with the nonzeros in column  $j$  of  $B$ . Finally, we copy the links into the  $JC$  vector as the column indices:

```

36      if ( $diagc == 1 \ \& \ index_i \neq 0$ ) {
37           $length = length - 1$ 
38      }
39       $ic_{i+1} = ic_i + length$ 
40      do  $j \in \{ic_i, \dots, ic_{i+1} - 1\}$  {
41          if ( $diagc == 1 \ \& \ istart == i$ ) {
42               $istart = index_{istart}$ 
43               $index_i = 0$ 
44          }
45           $jc_j = istart$ 
46           $istart = index_{istart}$ 

```

```

47              $index_{jc_j} = 0$ 
48             } (end of j loop)
49      $index_i = 0$ 
50     } (end of i loop)

```

Lines 36-38 remove the diagonal element from the row if  $C$  is stored in the new Yale sparse matrix format. Note that in lines 43 and 47 the nonzero links are cleared. Due to the small number of links (with respect to  $N$ ), it would be extremely inefficient to clear the entire vector. The resulting vectors  $IC$  and  $JC$  contain the nonzero structure of  $C = AB$ .

## 4.2 NUMBMM

Initialization consists of clearing all of the partial sums:

```

1     do  $i \in \{1, \dots, \max\{l, m, n\}\}$  {
2          $temp_i = 0$ 
3     }

```

The main loop forms the partial sums and then copies the completed sums into the correct locations in the sparse matrix structure:

```

4      do i ∈ {1, …, n} {
5          do jj ∈ {iai, …, iai+1} {
6              if (jj == iai+1) {
7                  if (diaga == 0 |
8                      i > min{m, n}) {
9                      next jj
10                     }
11                     j = i
12                     ajj = ai
13                 }
14                 else {
15                     j = jajj
16                     ajj = ajj
17                 }
18                 if (diagb == 1 & j ≤ min{l, m}) {
19                     tempj = tempj + ajj * bj
20                 }
21                 do k ∈ {ibj, …, ibj+1 - 1} {
22                     tempjbk = tempjbk + ajj * bk
23                 } (end of k loop)
24             } (end of jj loop)
25         if (diagc == 1 & i ≤ min{l, n}) {
26             ci = tempi
27             tempi = 0
28         }
29         do j ∈ {ici, …, ici+1 - 1} {
30             cj = tempjcj
31             tempjcj = 0.
32         } (end of j loop)
33     } (end of i loop)

```

Lines 6-16 determine if the  $jj$  loop has to execute an “extra” iteration when  $A$  is stored in the new Yale sparse matrix format. Lines 20-22 accumulate the product for row  $j$ , and store it in lines 28-31. Lines 17-19 and 24-27 deal with special cases when a matrix is stored in the new Yale sparse matrix format. The resulting vector  $C$  contains the numerical product  $AB$ .

### 4.3 TRANSP

We begin by constructing  $ib$ . This requires setting up the first row pointer and counting indices for each column:

```

1      do  $i \in \{1, \dots, m+1\}$  {
2           $ib_i = 0$ 
3      }
4      if ( $move == 1$ ) {
5          do  $i \in \{1, \dots, m+1\}$  {
6               $b_i = 0$ 
7          }
8      }
9      if ( $diaga == 1$ ) {
10          $ib_1 = m+2$ 
11     }
12     else {
13          $ib_1 = 1$ 
14     }
15     do  $i \in \{1, \dots, n\}$  {
16         do  $j \in \{ia_i, \dots, ia_{i+1} - 1\}$ 
17              $ib_{ja_j+1} = ib_{ja_j+1} + 1$ 
18         }
19     }
20     do  $i \in \{1, \dots, m\}$  {
21          $ib_{i+1} = ib_i + ib_{i+1}$ 
22     }

```

Lines 1-3 clear  $IB$ . If we are constructing  $B$  at the same time, then lines 4-8 clear the main diagonal of  $B$ . Lines 9-14 determine where the rows of  $B$  are stored. Lines 15-18 count the number of indices in each column and lines 20-22 converts this information into row pointers.

Next, we construct  $jb$ :

```

23     do  $i \in \{1, \dots, n\}$  {
24         do  $j \in \{ia_i, \dots, ia_{i+1} - 1\}$  {
25              $jj = ja_j$ 
26              $jb_{ib_{jj}} = i$ 
27             if ( $move == 1$ ) }
28                  $b_{ib_{jj}} = a_j$ 
29             }
30              $ib_{jj} = ib_{jj} + 1$ 
31         }
32     }

```

Lines 23-32 put  $i$  as a column index into row  $JA(j)$  in the first possible position (pointed to by  $IB(jj)$ ) and increment the pointer. If we are constructing  $B$  at the same time, then lines 27-29 do the copy.

Finally, we have to restore  $IB$ :



```

33     do i ∈ {m, m - 1, ..., 2} {
34         ibi = ibi-1
35     }
36     if (diaga == 1) {
37         if (move == 1) {
38             j = min(n, m)
39             do i ∈ {1, j} {
40                 bi = ai
41             }
42         }
43         ib1 = m + 2
44     }
45     else {
46         ib1 = 1
47     }

```

Lines 34, 43, and 46 do the real work in restoring  $IB$ . Lines 36-42 finish copying the main diagonal of  $A$  when it is stored in the new Yale sparse matrix format.

## 5 Fortran source code

The Fortran source code for this package is freely available from Netlib as the file `linalg/smmp.shar`.

## References

- [1] R. E. Bank and R. K. Smith, *General sparse elimination requires no permanent integer storage*, SIAM J. Sci. Stat. Comp., 8 (1987), pp. 574–584.
- [2] C. C. Douglas and W. L. Miranker, *Constructive interference in parallel algorithms*, SIAM J. Numer. Anal., 25 (1988), pp. 376–398.
- [3] C. C. Douglas and B. F. Smith, *Using symmetries and antisymmetries to analyze a parallel multigrid algorithm: the elliptic boundary value case* SIAM J. Numer. Anal., 26 (1989), pp. 1439–1461.
- [4] I. Duff, M. Marrone, and G. Radicati, *A proposal for user level sparse BLAS*, in preparation.
- [5] S. C. Eisenstat and H. C. Elman and M. H. Schultz and A. H. Sherman, *The (new) Yale sparse matrix package*, in Elliptic Problem Solvers II, G. Birkhoff and A. Schoenstadt, editors, Academic Press, New York, 1984, pp. 45–52.
- [6] S. C. Eisenstat and M. C. Gursky and M. H. Schultz and A. H. Sherman, *Yale sparse matrix package I: the symmetric codes*, Int. J. Numer. Methods in Engin., 18 (1982), pp. 1145-1151.
- [7] ———, *Yale sparse matrix package II: the nonsymmetric codes*, Research Report 114, Department of Computer Science, Yale University, New Haven, CT, 1977.
- [8] M. A. Heroux, *Proposal for a sparse BLAS toolkit*, in preparation.
- [9] Y. Saad, *SPARSKIT: a basic tool kit for sparse matrix computations*, preliminary version, 1990. Available by anonymous ftp from `riacs.edu`.