# MULTIGRAPH Users' Guide 2.0

Randolph E. Bank

Department of Mathematics University of California at San Diego La Jolla, California 92093-0112

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### Chapter 1

# Data Structures

#### 1.1 Overview.

The multigraph package can be used to solve large sparse linear systems of equations of the form

$$Ax = b. (1.1)$$

In this chapter, we discuss the main data structures used in the package, and give a brief overview of its overall structure. See [3, 4] for algorithmic details and some numerical results.

We assume that the sparsity pattern of A is symmetric, although the numerical values need not be. We will begin by describing the basic two-level method for solving (1.1) Let B be an  $n \times n$  nonsingular matrix, called the *smoother*, which gives rise to the basic iterative method used in the multigraph preconditioner. In our case, B is an approximate factorization of A, i.e.,

$$B = (L+D)D^{-1}(D+U) \approx P^t A P, \tag{1.2}$$

where L is (strict) lower triangular, U is (strict) upper triangular with the same sparsity pattern as  $L^t$ , D is diagonal, and P is a permutation matrix.

Given an initial guess  $x_0$ , m steps of the smoothing procedure produce iterates  $x_k$ ,  $1 \le k \le m$ , given by

$$r_{k-1} = P^{t}(b - Ax_{k-1})$$

$$B\delta_{k-1} = r_{k-1}$$

$$x_{k} = x_{k-1} + P^{t}\delta_{k-1}$$
(1.3)

The second component of the two-level preconditioner is the *coarse grid correction*. Here we assume that the matrix A can be partitioned as

$$\hat{P}A\hat{P}^t = \begin{pmatrix} A_{ff} & A_{fc} \\ A_{cf} & A_{cc} \end{pmatrix} \tag{1.4}$$

where the subscripts f and c denote fine and coarse, respectively. Similar to the smoother, the partition of A in fine and coarse blocks involves a permutation matrix  $\hat{P}$ . The  $\hat{n} \times \hat{n}$  coarse grid matrix  $\hat{A}$  is given by

$$\hat{A} = \begin{pmatrix} V_{cf} & I_{cc} \end{pmatrix} \begin{pmatrix} A_{ff} & A_{fc} \\ A_{cf} & A_{cc} \end{pmatrix} \begin{pmatrix} W_{fc} \\ I_{cc} \end{pmatrix} 
= V_{cf} A_{ff} W_{fc} + V_{cf} A_{fc} + A_{cf} W_{fc} + A_{cc}.$$
(1.5)

The matrices  $V_{cf}$  and  $W_{fc}^t$  are  $\hat{n} \times (n-\hat{n})$  matrices, with identical sparsity patterns; thus  $\hat{A}$  has a symmetric sparsity pattern. If  $A^t = A$ , we require  $V_{cf} = W_{fc}^t$ , so  $\hat{A}^t = \hat{A}$ .

Let

$$\hat{V} = \begin{pmatrix} V_{cf} & I_{cc} \end{pmatrix} \hat{P}, \qquad \hat{W} = \hat{P}^t \begin{pmatrix} W_{fc} \\ I_{cc} \end{pmatrix}. \tag{1.6}$$

In standard multigrid terminology, the matrices  $\hat{V}$  and  $\hat{W}$  are called *restriction* and *prolongation*, respectively. Given an approximate solution  $x_m$  to (1.1), the coarse grid correction produces an iterate  $x_{m+1}$  as follows.

$$\hat{r} = \hat{V}(b - Ax_m)$$

$$\hat{A}\hat{\delta} = \hat{r}$$

$$x_{m+1} = x_m + \hat{W}\hat{\delta}$$
(1.7)

As is typical of multilevel methods, we define the *Two-Level Preconditioner* M implicitly in terms of the smoother and coarse grid correction. A single cycle takes an initial guess  $x_0$  to a final guess  $x_{2m+1}$  as follows:

#### Two-Level Preconditioner

- i.  $x_k$  for  $1 \le k \le m$  are defined using (1.3).
- ii.  $x_{m+1}$  is defined using (1.7).
- iii.  $x_k$  for  $m+2 \le k \le 2m+1$  are defined using (1.3).

The generalization from two-level to multilevel consists of applying recursion to the solution of the equation  $\hat{A}\hat{\delta}=\hat{r}$  in (1.7). Let  $\ell$  denote the number of levels in the recursion. Let  $\hat{M}\equiv\hat{M}(\ell)$  denote the preconditioner for  $\hat{A}$ ; if  $\ell=2$  then  $\hat{M}=\hat{A}$ . Then (1.7) is generalized to:

$$\hat{r} = \hat{V}(b - Ax_m)$$

$$\hat{M}\hat{\delta} = \hat{r}$$

$$x_{m+1} = x_m + \hat{W}\hat{\delta}$$
(1.8)

The general  $\ell$  level preconditioner M is then defined as follows:

#### $\ell$ -Level Preconditioner

- i. if  $\ell = 1$ , M = A; i.e., solve (1.1) directly.
- ii. if  $\ell > 1$ , then, starting from initial guess  $x_0$ , compute  $x_{2m+1}$  using (iii)-(v):
- iii.  $x_k$  for  $1 \le k \le m$  are defined using (1.3).
- iv.  $x_{m+1}$  is defined by (1.8), using p=1 or p=2 iterations of the  $\ell-1$  level scheme for  $\hat{A}\hat{\delta}=\hat{r}$  to define  $\hat{M}$ , and with initial guess  $\hat{\delta}_0=0$ .
- v.  $x_k$  for  $m+2 \le k \le 2m+1$  are defined using (1.3).

The case p=1 corresponds to the symmetric V-cycle, while the case p=2 corresponds to the symmetric W-cycle. We note that there are other variants of both the V-cycle and the W-cycle, as well as other types of multilevel cycling strategies [6]. However, in our code we restrict attention to just the symmetric V-cycle, with m=1 presmoothing and postsmoothing iterations.

For the coarse mesh solution ( $\ell = 1$ ), our procedure is somewhat non-traditional. Instead of direct solution of (1.1), we compute an approximate solution using one smoothing iteration.

If A is symmetric then so is M, and the  $\ell$ -Level Preconditioner is used as a preconditioner for the composite step conjugate gradient method (CSCG). In the nonsymmetric case, the  $\ell$ -level Preconditioner is used in conjunction with the composite step biconjugate gradient method (CSBCG). See [1] for details of these Krylov space methods.

#### 1.2 Matrix Data Structures.

Let A be an  $n \times n$  matrix with elements  $A_{ij}$ , and a symmetric sparsity structure; that is, both  $A_{ij}$  and  $A_{ji}$  are treated as nonzero elements (i.e. stored and processed) if  $|A_{ij}| + |A_{ji}| > 0$ . All diagonal entries  $A_{ii}$  are treated as nonzero regardless of their numerical values.

Our data structure is a modified and generalized version of the data structure introduced in the (symmetric) Yale Sparse Matrix Package [5]. It is a row-wise version of the data structure described in [2]. In our scheme, the nonzero entries of A are stored in a linear array a, and accessed through an integer array ja. Let  $\eta_i$  be the number of nonzeros in the strict upper triangular part of row i, and set  $\eta = \sum_{i=1}^n \eta_i$ . The array ja is of length  $n+1+\eta$  and the array a is of length  $n+1+\eta$  if  $A^t = A$ . If  $A^t \neq A$ , then the array a is of length  $n+1+2\eta$ . The entries of ja(i)  $1 \leq i \leq n+1$  are pointers defined as follows:

$$ja(1) = n + 2$$
  
 $ja(i+1) = ja(i) + \eta_i, \quad 1 \le i \le n$ 

The locations ja(i) to ja(i+1)-1 contain the  $\eta_i$  column indices corresponding to the row i in the strictly upper triangular matrix.

In a similar manner, the array a is defined as follows:

$$a(i) = A_{ii}, \quad 1 \le i \le n$$
 
$$a(n+1) \quad \text{is arbitrary}$$
 
$$a(k) = A_{ij}, \quad 1 \le i \le n, \quad j = ja(k), \quad ja(i) \le k \le ja(i+1) - 1$$

If  $A^t \neq A$ , then

$$a(k+\eta) = A_{ji}, \quad 1 \le i \le n, \quad j = ja(k), \quad ja(i) \le k \le ja(i+1) - 1$$

In words, the diagonal is stored first, followed by the strict upper triangle stored rowwise. If  $A^t \neq A$ , then this is followed by the strict lower triangle stored column-wise. Since A is structurally symmetric, the column indexes for the upper triangle are identical to the row indexes for the lower triangle, and hence need not be duplicated in storage.

As an example, let

$$A = \begin{pmatrix} A_{11} & A_{12} & A_{13} & 0 & 0 \\ A_{21} & A_{22} & 0 & A_{24} & 0 \\ A_{31} & 0 & A_{33} & A_{34} & A_{35} \\ 0 & A_{42} & A_{43} & A_{44} & 0 \\ 0 & 0 & A_{53} & 0 & A_{55} \end{pmatrix}$$

Then

	1	2	3	4	5	6	7	8	9	10	11
ja	7	9	10	12	12	12	2	3	4	4	5
a	$A_{11}$	$A_{22}$	$A_{33}$	$A_{44}$	$A_{55}$		$A_{12}$	$A_{13}$	$A_{24}$	$A_{34}$	$A_{35}$
	Diagonal					Upper Triangle					

	12	13	14	15	16
$\int ja$					
a	$A_{21}$	$A_{31}$	$A_{42}$	$A_{43}$	$A_{53}$
	Lower Triangle				

If desired, the user can specify a block structure for the matrix A. This block structure is used only in the coarsening phase of the algorithm (i.e. in creating  $\hat{V}$  and  $\hat{W}$ ). If the matrix has nblock blocks, the user provides and integer array ib of length nblock + 1, defined as follows: Let  $\xi_i$  be the order of block i, for  $1 \le i \le nblock$ . Then

$$ib(1) = 1$$
  
 $ib(i+1) = ib(i) + \xi_i, \quad 1 \le i \le nblock.$ 

For the case of just one block, one should set

$$ib(1) = 1$$
$$ib(2) = n + 1$$

The data structure for storing  $B = (L+D)D^{-1}(D+U)$  is quite analogous to that for A. It consists of two arrays, ju and u, corresponding to ja and a, respectively. The first n+1 entries of ju are pointers as in ja, while entries ju(i) to ju(i+1)-1 contain column indices of the nonzeros of row i in of U. In the u array, the diagonal entries of D are stored in the first n entries. Entry n+1 is arbitrary. Next, the nonzero entries of U are stored, in correspondence to the column indices in ju. If  $L^t \neq U$ , the nonzero entries of L follow, stored column-wise.

The data structure we use for the  $n \times \hat{n}$  matrix  $\hat{W}$  and the  $\hat{n} \times n$  matrix  $\hat{V}$  are similar. It consists of an integer array jv and a real array v. The nonzero entries of  $\hat{W}$  are stored row-wise, including the rows of the block  $I_{cc}$ . As usual, the first n+1 entries of jv are pointers; entries jv(i) to jv(i+1)-1 contain column indices for row i of  $\hat{W}$ . In the v array, the nonzero entries of  $\hat{W}$  are stored row-wise in correspondence with jv but shifted by n+1 since there is no diagonal part. If  $\hat{V}^t \neq \hat{W}$ , this is followed by the nonzeros of  $\hat{V}$  stored column-wise.

#### 1.3 The ka Data Structure.

To avoid excessive clutter in the calling sequences, all of the relevant matrices for all of the levels are stored in just two arrays, an integer array ja and a real array a. In order to keep track of the internal structure of these arrays, a matrix of pointers, ka, is created in subroutine mginit and used in subroutine mg. A casual user need not be concerned with this array (other than allocating storage for it), but it is available to the user should access to the various matrices generated by the multigraph method be desired. ka is a  $10 \times (lvl + 1)$  integer array, where  $lvl \leq maxlvl$  is the number levels employed by the method. Column i corresponds to variables associated mainly with level lvl + 1 - i; that is, the first column is associated with the finest level, the second column with the next finest level, and so on.

i	ka(i,*)
1	n, the order of the matrix
2	nptr, pointer for multilevel vector arrays
3	japtr pointer for the integer data structure $ja$
4	iaptr pointer for the real data structure $a$
5	juptr pointer for the integer data structure $ju$
6	iuptr pointer for the real data structure $u$
7	jvptr pointer for the integer data structure $jv$
8	ivptr pointer for the real data structure $v$
9	iqptr pointer for the inverse permutation for $P$
10	ibptr block labels, computed from the $ib$ array

Table 1.1. The ka array.

## Chapter 2

# Multigraph Routines

#### 2.1 Overview.

The multigraph implementation consists of four main routines, mginit, mgilu, mg, and cycle. Subroutine mginit is the initialization routine that creates the levels and their associated data structures. Subroutine mgilu performs a subset of the operations of mginit, and can be used when one solves a sequence of linear systems with a family of related matrices (e.g. in a Newton iteration). Subroutine mgilu computes new values for all of the real variables (a, u and v), while retaining the integer data structures produced by mginit; this significantly reduces the initialization time. Subroutine mg solves (1.1) using either the composite set conjugate gradient or composite step biconjugate gradient method. Subroutine cycle is the V-cycle preconditioner called by mg. It is documented separately, as it can be called directly as the preconditioner in other iterative solvers. For such a situation, we also provide subroutines mtxmlt and perm for matrix multiplication and reordering, respectively. Two other routines, gphplt and mtxplt, are visualization tools that are discussed in Chapter 3.

This version of the multigraph package is written in FORTRAN90. There is only one version of the source code. The precision of the arithmetic is governed through the module mthdef where the precision of integer and floating point numbers can be specified through the parameters iknd and rknd, respectively. Module mthdef is included in every subroutine and function in the package, and thus represents a global specification of precision.

# 2.2 Subroutine mginit.

mginit is called using the statement:

call mginit( n, ispd, nblock, ib, maxja, ja, maxa, a, ncfact, maxlvl, maxfil, ka, lvl, dtol, method, iflaq )

A discussion of these parameters follows.

- n is an integer specifying the order of the system of equations.
- ispd is an integer specifying the symmetry of the matrix. ispd = 1 indicates that symmetric storage is used; ispd = 0 indicates that nonsymmetric storage is used.
- nblock is an integer specifying the number of blocks in the matrix (see Section 1.2).
- ib is an integer array of size nblock + 1 containing the block structure, as defined in Section 1.2.
- maxja is an integer specifying the size of the array ja.
- ja is an array of integers, containing all the integer data structures for all levels defined in Chapter 1. On input, the head of ja should contain the integer data structure corresponding the the linear system (1.1) to be solved.
- maxa is an integer specifying the size of the array a. A good (but inexact) guide is to choose  $maxa \sim maxja$  when ispd = 1 and  $maxa \sim 2 maxja$  when ispd = 0.
- a is an array of reals, containing all the real data structures for all levels defined in Chapter 1. On input, the head of a should contain the real data structure corresponding the the linear system (1.1) to be solved.
- ncfact is an integer specifying the coarsening factor. If the matrix at a given level is of order n, then the matrix for the next coarser level will be of order  $\hat{n} \approx n/ncfact$ . We require  $ncfact \geq 2$ .
- maxlvl is an integer specifying the maximum number of levels to be used.
- maxfil is an integer specifying the maximum storage allowed for certain matrices. In particular, the ja and ju arrays for a system of order  $n_i$  will have maximum size  $n_i + 1 + n_i \max fil$ . Note that  $\max fil$  controls the average number of nonzeros per row, but NOT necessarily the fill-in in any particular row.
- ka is a 10×(lvl+1) integer array, which on output contains pointers as defined in Section 1.3.
- lvl is an integer, which on output contains the number of levels actually generated by mginit. In particular  $lvl \leq maxlvl$ .
- dtol is a nonnegative real, specifying the drop tolerance for the ILU factorizations.

- method is an integer specifying the smoother for the multigraph algorithm. method = 0 is the default ILU with drop tolerance; method = 1 is ILU(0) ( $ja \equiv ju$  at all levels); method = 2 is symmetric Gauss-Seidel ( $ja \equiv ju$  and  $a \equiv u$  at all levels). method = 1 and method = 2 are provided mainly as a baseline to compare with method = 0; however, for certain problems they can provide comparable performance using less time and space for the initialization, and therefore are independently useful.
- iflag is an integer that on output contains the error flag. iflag = 0 signifies no error; iflag = 20 signifies insufficient storage. Although this could refer to maxja, maxa, or lenz, the typical failure is for lenz.

## 2.3 Subroutine mgilu.

Subroutine mgilu performs a subset of the computations of mginit. In particular, for a related family of matrices, one can save the level and fill-in structures (essentially the contents of the ja array) and simply compute new numerical values for matrix elements (the a array). One calls mginit for the first member of the family of matrices and then mgilu for the remainder. For example, in a Newton iteration, one might expect the changes in the Jacobian matrices to be sufficiently small that the level and fill-in structures could be used for all (or perhaps just several) Newton steps. Thus one would call mginit once to initialize the arrays and compute the first set of matrices, and then call mgilu for all other matrices, which would then reuse the level and fill-in structure from the call to mginit.

mgilu is called using the statement:

```
call mgilu( ja, a, lvl, ka )
```

A discussion of these parameters follows.

- ja is an array of integers, containing all the integer data structures for all levels defined in Chapter 1. This should be the output from the original call to mginit.
- a is an array of reals, containing all the real data structures for all levels defined in Chapter 1. On input, the head of a should contain the real data structure corresponding the the linear system (1.1) to be solved.
- *lvl* is an integer, which contains the number of levels. This should be the output from the original call to *mginit*.
- ka is a 10×(lvl+1) integer array, which contains pointers as defined in Section
  1.3. This should be the output from the original call to mginit.

It is important to note that mginit reorders the original matrix stored in the ja and a data structures. mgilu assumes that the new matrix provided in a corresponds to this reordering. The inverse permutation array for the ordering can

be found using the pointer iqptr = ka(9,1). If p(i) is the permutation, and q(i) the inverse permutation, then  $p(q(i)) = i, 1 \le i \le n$ .

As a convenience, we provide subroutine jamap0, which takes a pair (i, j) in the original ordering and provides pointers to the locations of  $A_{ij}$  and  $A_{ji}$  in the reordered data structures. jamap0 is called using the statement:

```
call jamap0( i, j, n, ispd, ij, ji, ja )
```

A discussion of these parameters follows.

- *i* and *j* are the indices for the desired matrix element, given in the original ordering.
- n is an integer specifying the order of the system of equations.
- ispd is an integer specifying the symmetry of the matrix. ispd = 1 indicates that symmetric storage is used; ispd = 0 indicates that nonsymmetric storage is used.
- On output, ij and ji are pointers to the a array where matrix entries  $A_{ij}$  and  $A_{ji}$ , respectively, are stored. ij = ji if i = j or ispd = 1, and ij = ji = 0 if entry (i, j) is not present in the data structure.
- ja is an array of integers, containing all the integer data structures for all levels defined in Chapter 1. This should be the output from the original call to mginit.

# 2.4 Subroutine mg.

Subroutine mg solves the linear system (1.1) using the output from mginit (or mgilu). In the nonsymmetric case, subroutine mg can also solve problems of the form

$$A^t x = b. (2.1)$$

mg is called using the statement:

call mg( ispd, lvl, mxcg, eps1, ja, a, dr, br, ka, relerr, iflag, hist )

A discussion of these parameters follows.

- ispd is an integer specifying the symmetry of the matrix. ispd = 1 indicates that symmetric storage is used; ispd = 0 indicates that nonsymmetric storage is used. ispd = -1 indicates that nonsymmetric storage is used and one should solve (2.1).
- lvl is an integer specifying the number of levels. This should be the output from the call to mginit.
- mxcg is an integer specifying the maximum number of CSCG iterations (ispd = 1) or CSBCG iterations ( $ispd \neq 1$ ).

- eps1 it the convergence tolerance. The iteration terminates when the residual norm is reduced by a factor of eps1 or when mxcg iterations is achieved, whichever occurs first.
- ja is an array of integers, containing all the integer data structures for all levels defined in Chapter 1. This should be the output from the call to mginit.
- a is an array of reals, containing all the real data structures for all levels
  defined in Chapter 1. This should be the output from a call to mginit or
  mgilu.
- dr is a real array of size n, which on output contains the solution of the linear system.
- br is a real array of size n, which on input contains the right hand side of the linear system.
- ka is a 10×(lvl+1) integer array, which contains pointers as defined in Section
   1.3. This should be the output from the call to mginit.
- relerr is a real number which on output specifies the ratio of the norms of initial and final residuals.
- iflag is an integer that on output contains the error flag. iflag = 0 signifies no error; iflag = 12 indicates that the error tolerance eps1 was not reached in mxcg iterations, but the iteration appeared to be converging. iflag = -12 indicates that the iteration appeared to diverge. hist is a real array of size 22, which collects data used by the graphics routine gphplt.

# 2.5 Subroutines cycle, mtxmlt and perm.

Subroutine cycle implements the V-cycle preconditioner, and is called as needed by mg. It is documented separately here, as it can be used as a preconditioner in other preconditioned iterative methods. cycle is called using the statement:

```
call cycle( ispd, lvl, ja, a, x, b, ka )
```

A discussion of these parameters follows.

- ispd is an integer specifying the symmetry of the matrix. ispd = 1 indicates that symmetric storage is used; ispd = 0 indicates that nonsymmetric storage is used. ispd = -1 indicates that nonsymmetric storage is used and one should solve (2.1).
- *lvl* is an integer specifying the number of levels. This should be the output from the call to *mginit*.
- ja is an array of integers, containing all the integer data structures for all levels defined in Chapter 1. This should be the output from the call to mqinit.

- a is an array of reals, containing all the real data structures for all levels defined in Chapter 1. This should be the output from a call to mginit or mgilu.
- x is a real array of size n, which on output contains the approximate solution of the linear system.
- b is a real array of size n, which on input contains the right hand side of the linear system.
- ka is a 10×(lvl+1) integer array, which contains pointers as defined in Section
   1.3. This should be the output from the call to mginit.

Subroutine mtxmlt computes b = Ax or  $b = A^tx$ . It is a companion routine to cycle for use in a preconditioned iterative method. mtxmlt is called using the statement:

```
call\ mtxmlt(\ n,\ ja,\ a,\ x,\ b,\ ispd\ )
```

A discussion of these parameters follows.

- *n* is an integer specifying the order of the system of equations.
- ja is an array of integers, containing all the integer data structures for all levels defined in Chapter 1. This should be the output from the call to mginit.
- a is an array of reals, containing all the real data structures for all levels defined in Chapter 1. This should be the output from a call to mginit or mgilu.
- x is a real array of size n, which on contains the input vector.
- b is a real array of size n, which on output contains Ax or  $A^{t}x$ .
- ispd is an integer specifying the symmetry of the matrix. ispd = 1 indicates that symmetric storage is used; ispd = 0 indicates that nonsymmetric storage is used. In both cases b = Ax is computed. ispd = -1 indicates that nonsymmetric storage is used and  $b = A^t x$  is computed.

Both cycle and mtxmlt assume that all vectors are ordered according the minimum degree ordering computed in mginit. If the input and output are provided in the original ordering, then subroutine perm should be called as necessary to reorder the data.

perm is called using the statement:

```
call\ perm(\ n,\ x,\ ja,\ isw\ )
```

A discussion of these parameters follows.

• *n* is an integer specifying the order of the system of equations.

- x is a real array of size n, which contains the vector to be reordered.
- ja is an array of integers, containing all the integer data structures for all levels defined in Chapter 1. This should be the output from the call to mginit.
- isw is an integer switch. If isw = 1, the input is assumed to be in the original order, and the output is reordered using the order generated in mginit. If isw = -1, the input is assumed to be ordered using the order provided by mginit and the output is restored to the original order.

## Chapter 3

# **Graphics**

#### 3.1 Overview.

The graphics tools associated with the multigraph package consist of subroutines *gphplt* and *mtxplt*. These routines are written in self-contained, portable FORTRAN, addressing the graphics output device through subroutines *pline*, *pfill*, *pframe* and *pltutl*. The specifications for these routines are given in Section 3.4.

Subroutine gphplt displays various graphs and charts containing timings, convergence histories, and other items of interest. Subroutine mtxplt displays sparse matrices associated with the multigraph solver.

# 3.2 Subroutine gphplt.

gphplt is called using the statement

```
call gphplt( ip, rp, sp, hist, ka, time )
```

Subroutine gphplt uses three parameters specified in the ip array and one parameter specified in the sp array.

- *igrsw* is an integer switch specifying the graphs to be drawn. The possibilities are given in Table 3.1,
- gdevce is an integer switch specifying the graphics output device.
- mxcolr is an integer specifying the number of colors available; we assume mxcolr > 2.
- *gtitle* is an string specifying the title for the graph.

The case igrsw = 0 is probably the most useful. In the large frame, a convergence history of the multigraph iteration is displayed; iteration number appears on the x-axis, and  $\log(relerr)$  appears on the y-axis. In one of the smaller frames,

igrsw	displayed graph
0	convergence history
1	storage profile
-1	timings
2	ip array
-2	$rp  ext{ array}$
3	ka array
-3	sp array

Table 3.1. The values of igrsw.

times for mginit and mg are displayed in a pie chart. In the other, storage statistics for various matrices are displayed;  $\log(n)$  for each level appears on the x-axis, and the average number of nonzeros in ja, ju and jv for each level are displayed in different colors on the y-axis. The cases  $igrsw = \pm 1$  are permutations of the three frames.

The case igrsw=2 displays the ip array, an integer array of size 100 containing global parameters used by the test driver program. The case igrsw=-2 displays the rp array, a real array of size 100 containing global parameters used by the test driver program. The case igrsw=-3 displays the sp array, a character\*80 array of size 100 containing global parameters used by the test driver program. Finally, igrsw=3 displays the sizes of all major arrays on all levels.

The remaining arguments are summarized by:

- hist is a real array of size 22, which contains the convergence history. It is the output from subroutine mg.
- ka is a 10×(lvl+1) integer array, which contains pointers as defined in Section
  1.3. This should be the output from the call to mginit.
- time is a real array of size 2, containing the execution times of mginit and mg.

# 3.3 Subroutine mtxplt.

Subroutine mtxplt displays the sparsity structure of the stiffness matrix A, the LDU factors from the ILU, or the error matrix E associated with an approximate factorization. mtxplt is called using the statement

```
call mtxplt( ip, rp, sp, ja, a, ka )
```

Subroutine mtxplt uses several parameters specified in the ip and rp arrays and one parameter specified in the sp array.

• imtxsw specifies the matrix to be displayed, as summarized in Table 3.2. If

imtxsw > 0, the magnitude of matrix elements is displayed; if imtxsw < 0, the (signed) value is displayed.

- mdevce is an integer switch specifying the graphics output device.
- mxcolr is an integer specifying the number of colors available; we assume  $mxcolr \geq 2$ .
- iscale in an integer that specifies the scaling to be used for the cases  $imtxsw = \pm 2, \pm 4, \pm 6$  as summarized in Table 3.2.
- lines is an integer that specifies the line drawing option, as summarized in Table 3.2.
- numbers in an integer that specifies numbering options, as summarized in Table 3.2.
- (mx, my, mz) are three integers specifying the viewing perspective.
- ncon is an integer specifying the number of colors in the cases cases  $imtxsw = \pm 2, \pm 4, \pm 6$ .
- level is an integer,  $1 \leq level \leq lvl$ , specifying the level of the matrix to be displayed. If level > lvl or level < 1, then lvl is used.
- (smin, smax) are real numbers that optionally specify lower and upper bounds for the color range for the cases  $imtxsw = \pm 2, \pm 4, \pm 6$ . Matrix elements with values falling outside the given range are colored white.
- rmag is a real number specifying the magnification factor.
- (cenx, ceny) are real numbers that specify the center of the picture when rmag > 1.
- *mtitle* is an string specifying the title for the graph.

The remaining arguments are summarized by:

- ja is an array of integers, containing all the integer data structures for all levels defined in Chapter 1. This should be the output from the call to mginit.
- a is an array of reals, containing all the real data structures for all levels
  defined in Chapter 1. This should be the output from a call to mginit or
  mgilu.
- ka is a  $10 \times (lvl+1)$  integer array, which contains pointers as defined in Section 1.3. This should be the output from the call to mqinit.

imtxsw	displayed matrix		
±1	LDU colored by element type		
$\pm 2$ LDU colored by element			
$\pm 3$	A colored by element type		
±4	A colored by element size		
±5	E colored by element type		
±6	E colored by element size		
iscale	scale		
0	linear		
1	logarithmic		
2	$\sinh^{-1}$		
lines	line drawing option		
0 no lines			
-2	matrix element boundaries		
numbrs	labeling option		
0	no labels		
-1	matrix element values		
-2	matrix element locations		

Table 3.2. The values of switches.

# 3.4 Graphics Interface.

The four device dependent routines in the graphics package are

```
subroutine pltutl( ncolor, red, green, blue) subroutine pframe( list ) subroutine pline( x, y, z, n, icolor ) subroutine pfill( x, y, z, n, icolor )
```

Subroutine pltutl takes various actions depending on the value of the integer ncolor. ncolor > 0 specifies initialization; ncolor denotes the number of colors to be used and satisfies  $2 \le ncolor \le mxcolr$ . red, green and blue are vectors of length ncolor. The entries red(i), green(i), and blue(i),  $1 \le i \le ncolor$ , are floating point numbers on the interval [0,1], corresponding to rgb values for the ith color. Color number 1 is always white (red(1) = green(1) = blue(1) = 1.0), and color number 2 is always black (red(2) = green(2) = blue(2) = 0.0). The rgb values of the remaining entries depend on the picture to be drawn and the value of mxcolr. pltutl should create a color map with the required colors, as these will be referenced in future calls to pline and pfill. If pltutl is called with ncolor < 0, the drawing is complete and any necessary postprocessing should be carried out (e.g., close the plot file).

The drawing space used by the graphics routines is always assumed to be either

the unit square  $(0,1) \times (0,1)$  or the rectangle  $(0,1.5) \times (0,1)$ . For devices that have a so-called z-buffer, the drawing space is either the unit cube  $(0,1) \times (0,1) \times (0,1)$  or the brick  $(0,1.5) \times (0,1) \times (0,1)$ . The graphics display itself is always viewed as rectangular with aspect ratio 3/2, which is either a single rectangular frame or three square frames. These frames are numbered 1 to 4 as illustrated in Figure 3.1. The graphics routines write their output to various *lists*. A list consists of a frame, and certain attributes (rotating/non-rotating, lighted/non-lighted). Some attributes may not have realizations for certain graphics devices. The nine available lists are summarized in Table 3.3.

When graphics is initiated for a certain list, say list k, subroutine pframe(k) is called to indicate that subsequent calls of pline and pfill contain data to be written to list k. pframe(-k) indicates that the output to the given list should be terminated. By convention, graphics routines are allowed only one open list at a time. Therefore, when pframe is invoked with a positive argument, the given list should be opened and the mapping from the unit cube or brick to the actual device coordinates for the given list should be computed. If rotation or lighting attributes are available, these should be set as specified in Table 3.3. When pframe is invoked with a negative argument, the given list should be closed.

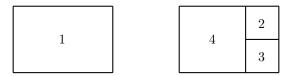


Figure 3.1. Frame definitions.

list	frame	rotating	lighted
1	1	no	no
2	2	no	no
3	3	no	no
4	4	no	no
5	4	yes	no
6	4	yes	no
7	4	yes	yes
8	4	yes	yes
9	4	no	yes

**Table 3.3.** list specifications for pframe.

Subroutine pline has arguments x, y, z, n, and icolor. x, y, and z are vectors of length  $n \geq 2$ . The points (x(i), y(i), z(i)) will lie in the unit cube or the brick

 $(0,1.5) \times (0,1) \times (0,1)$ . The z coordinate is useful only for devices that have a z-buffer, and can be ignored in other cases. *icolor* is an integer between 1 and ncolor, where ncolor was the argument that initialized pltutl, indicating the color to be used. pline should draw the given polyline (x(i), y(i), z(i)) to (x(i+1), y(i+1), z(i+1)),  $1 \le i \le n-1$ , with the specified color in the proper frame.

Subroutine pfill has arguments x, y, z, n, and icolor. x, y, and z are vectors of length  $n \geq 3$ . The points (x(i), y(i), z(i)) will lie in the unit cube or the brick  $(0,1.5)\times(0,1)\times(0,1)$ , and define an n-sided (planar) polygonal region with sides (x(i), y(i), z(i)) to (x(i+1), y(i+1), z(i+1)) for  $1 \leq i \leq n-1$ , and (x(n), y(n), z(n)) to (x(1), y(1), z(1)). icolor is an integer between 1 and ncolor, where ncolor was the argument that initialized pltutl, indicating the color to be used. pfill should color the specified polygon with the specified color in the proper frame.

# Chapter 4

# **Test Driver**

#### 4.1 Overview.

Program atest is the test driver used in the development and testing of the multigraph solver. atest is a flexible program in that it accepts simple command strings directing it to call subroutines or perform other tasks. It is not limited to a fixed sequence of tasks on a particular run; any routine can be called as often as desired, with certain parameters reset for each call at the discretion of the user.

The program atest can operate in three modes, governed by the switch mode. If mode = -1, atest runs as an interactive program, accepting commands from the user via a terminal window. If mode = 0, atest runs interactively, accepting commands from the user via an X-WINDOWS interface. This interface is based on the MOTIF widget set and can be used only in environments supporting X-WINDOWS. Finally, if mode = 1, atest runs as a batch program, reading commands from a journal file and sending all output to appropriate output files.

A common command syntax is used for all three modes. This is described first for the case mode = -1 in Section 4.2. The extensions used in the X-WINDOWS interface are described in Section 4.3.

Several files are written by atest. The file bfile contains a complete record of all commands and printed output produced during the session. The file jwfile contains a record of all commands read and processed during the session, formatted as a journal file. See Section 4.8 for a discussion of journal files. atest sets the default values bfile = output.out and jwfile = journl.jnl. atest also creates a temporary file jtfile = jnltmp.jnl which it uses in connection with journal files.

#### 4.2 Terminal Mode.

In terminal mode, commands are entered from a terminal window in character strings of 80 characters, counting blanks. The syntax of a command can take several forms, but the root command is always a single letter. The commands that are currently recognized by *atest* are summarized in Table 4.1.

command:

Command	Action
f	call mginit
s	call $mg$
g	call gphplt
m	call $mtxplt$
l	create a linear system
r	read data set from a file
j	read journal file
q	quit

Table 4.1. Available commands for atest.

The terminal window prompt is the string command:. At this prompt, one can enter a command string (e.g., s), reset parameters as described below, or enter a blank line to see a list of the available commands. In this latter case the terminal window will appear as follows.

```
command:
factor f    solve s    gphplt g    mtxplt m
linsys l    read r    journl j    quit q
command:
```

A syntax error in a given command string causes the entire string to be ignored. atest will display the string command error and present the command prompt for a new input string.

The most simple commands are just single lower case letters as shown in Table 4.1. However, associated with most commands are various parameters which can be reset before calling the given routine. To see a listing of the parameters associated with a given command and their current values, without executing the command itself, enter the command in upper case at the command prompt. For example, the command M will display the parameters which can be interactively reset in connection with mtxplt.

```
command: M
imtxsw i 2
                  iscale s 0
                                    lines 1 0
                                                      numbrs n 0
mdevce d 3
                        mx 1
                                          my 1
                                                      mz.
                                                            mz. 1
                  mx
                                    my
                  level 1 0
                                    mxcolr mc 100
                                                            sn 0.0
ncon c 11
                                                      smin
smax
     sx 0.0
                  rmag
                        m 1.0
                                    cenx cx 0.5
                                                      ceny
                                                            cy 0.5
mtitle t "mtxplt"
```

These are eleven integer, five real, and one string parameters affecting subroutine mtxplt which can be interactively reset by the user. To the right of each parameter is a one- or two-letter alias (to avoid typing long names), followed by the current value. To reset some parameters associated with a command c (c = s, f, g, etc.), without invoking the command itself, one can type a string of the form

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```
command:C name1=value1, name2=value2, ..., namek=valuek
```

Note that the root command appears in upper case. The *namek* refer to variable names or their aliases, and valuek refer to integer, real, or string values. Several parameters can be reset, with different entries separated by commas. Values for integer parameters should be integers, while values for real parameters can be specified using integer, fixed point, or exponential notation. There are three types of string parameters: short, file, and long. Short and file strings contain no blank characters, or special characters used by atest ("=,) and hence can be entered directly. Long strings, such a titles for graphics output, could have blanks and other reserved characters and must appear within double quotes. Long string parameters can contain any printable ASCII characters (other than double quotes). Blank spaces are ignored everywhere but within the value field of a long string parameter. A syntax error in the input line (e.g., a misspelled variable name) causes the entire command to be ignored and no variables to be reset. atest will respond command error and then ask for the next command. For example, here we reset iscale = 1, ncon = 20, cenx = .3, rmaq = 10, and mtitle = A new title for mtxplt. Subroutine mtxplt is not called, but the parameters are updated and redisplayed as

```
command:M s=1, ncon=20, cenx=.3, rmag=1.e1, t="A new title for mtxplt"
imtxsw i 2
                  iscale s 1
                                    lines 1 0
                                                      numbrs n 0
mdevce d 3
                  mx
                        mx 1
                                    my
                                           my 1
                                                      mz
                 level 1 0
    c 20
                                    mxcolr mc 100
     sx 0.0
                 rmag m 10.0
                                    cenx cx 0.3
                                                       ceny
                                                             cy 0.5
mtitle t "A new title for mtxplt"
```

#### command:

One can reset some parameters for a given command c, and then invoke the command itself, using a string of the form

```
command:c name1=value1, name2=value2, ..., namek=valuek
```

Note that the only difference is that the root command now appears in lower case rather than upper case. Thus

```
command:m s=1, ncon=20, cenx=.3, rmag=1.e1, t="A new title for mtxplt"
```

resets the indicated parameters as in the previous example. However, instead of displaying the updated values, subroutine mtxplt is called.

Finally, the graphics commands (g and m) have a short form allowing one crucial parameter (igrsw and imtxsw, respectively) to be reset without typing even the alias. For example,

is the short form for

```
command:g igrsw=0
```

The short and long forms of these commands cannot be mixed. Thus

```
command:g0, gdevce=1
```

is not valid.

#### **4.3** X-WINDOWS **Mode.**

When mode = 0, the driver atest creates an X-WINDOWS interface, The functional capabilities are the same as for the terminal window mode, but the possibilities for data entry are more varied. An example of the X-WINDOWS interface appears in Figure 4.1.

Figure 4.1. The X-WINDOWS interface.

The main display contains three elements. The upper portion of the display contains *command buttons*. Below the command buttons is a one line *command window*. The bottom portion of the display is the *history window*. The interface supports up to 10 graphics popup displays, based on the graphics interface defined in Section 3.4.

The command buttons stand in one to one correspondence with the basic atest command set shown in Table 4.1. In particular, clicking the left mouse button

(button one) with the pointer over a command button is equivalent to the typed lower-case version of that command. For example, clicking mouse button one on the mtxplt command button causes subroutine mtxplt to be called as in the command m. On the other hand, clicking on the right mouse button (button three) with the pointer over a command button is equivalent to the upper case version of the command. Clicking mouse button three on the mtxplt command button causes the parameters for the mtxplt command to be displayed in a popup reset window, as in the typed command M. This is shown is figure 4.2.

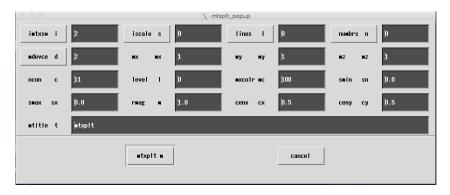


Figure 4.2. mtxplt reset window.

The parameters associated with a given command are displayed in the reset window in a format similar to terminal mode. However, parameter values are displayed in one line text-editing windows, and can be reset by typing in the new value. For some parameter names (e.g., imtxsw in Figure 4.2), the name has a raised button border. Clicking on the name causes a display of radio buttons, listing available options for the given parameter, to popup. Clicking on the appropriate option causes the parameter to be reset to the corresponding value. The radio button popup associated with the parameter imtxsw appears in Figure 4.3.

For file selection commands (*read* and *journl*), the generic reset window is replaced by the Motif file-selection widget. The file-selection popup for the *read* command is shown in Figure 4.4.

The history window displays the contents of the output file, bfile, as it is created. If the file becomes sufficiently large, only the tail of the file is displayed.

The X-WINDOWS driver also supports 10 graphics popup displays (numbered 0-9). The parameter ngraph,  $0 \le ngraph \le 10$ , states the number of windows to create initially. Graphics popups can be dismissed an recreated as necessary. These windows use only X-WINDOWS primitives, and display static images which cannot be manipulated (e.g. rotated) with the mouse. Graphics popups can be resized in the usual way, but maintain a 3/2 aspect ratio. Also, any existing image is erased upon resize, and must be redrawn.

When executing a journal file in X-WINDOWS mode, if a graphics command (g or m) is executed, depending on the graphics device selected, atest can pause after the picture is drawn, and create a small popup continue button. In this case, atest

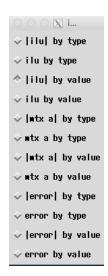


Figure 4.3. *imtxsw popup*.

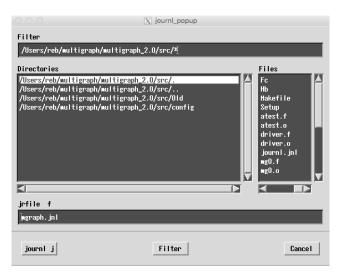


Figure 4.4. read file selection popup.

waits until the user dismisses the *continue* popup before continuing to execute the journal file. This allows time for the user to view the picture before processing the next command in the journal file.

The X-WINDOWS display can be interactively resized in the usual way. However, *atest* will adjust the user-specified resizing such that an overall aspect ratio of 3/2 is maintained. *atest* also imposes a minimum size requirement on the main window.

The string parameters bgclr and btnbg allow the user to specify the background

4.4. Batch Mode. 27

and button background colors for the main display. MOTIF automatically defines the remaining colors used in the display. These parameters can be given any of the named colors supported by X-WINDOWS.

Finally, we remark that the X-WINDOWS interface does not follow the pattern of many X-WINDOWS programs, in that the multigraph solver was not integrated into the X-WINDOWS system with the X-WINDOWS interface serving as the main routine. Indeed, the X-WINDOWS interface is realized as a collection of C language subroutines called by a FORTRAN driver. These routines use the same database of FORTRAN character strings as the terminal window interface to define their displays, and return command strings of the same type described in the terminal windows interface. Both the X-WINDOWS interface and the terminal window interface are quite generic, in that neither contains direct links to any of the main routines in the package. Thus changes in the behavior the routines comprising the package have no impact on the interface routines and at most modest impact on the database of character strings that define the displays.

#### 4.4 Batch Mode.

When mode = 1, the atest driver runs as a batch program. All commands are read from the journal file specified in jrfile. One should choose appropriate graphics output devices (e.g., Postscript or XPM files rather than X-windows displays) to ensure that the program runs correctly.

# 4.5 Array Dimensions and Initialization.

atest has six labeled common blocks:

```
common /atest1/ip(100),rp(100),sp(100)
common /atest2/iu(100),ru(100),su(100)
common /atest3/mode,jnlsw,jnlr,jnlw,ibatch
common /atest4/jcmd,cmdtyp,list
common /atest5/idevce
common /atest6/nproc,myid,mpisw,mpiint,mpiflt
```

The functionality provided by blocks *atest*2, *atest*4 and *atest*6 is not used in the current implementation of the multigraph solver, but is embedded in the generic driver nonetheless.

The ip, rp, and sp and integer, real, and character\*80 arrays of size 100 that contain various global parameters associated with the driver, subroutines mg, mginit,  $gphplt\ mtxplt$ , etc. Their structure and current values can be displayed by appropriate calls to gphplt.

The arrays iu, ru and su are analogous to ip, rp and sp and are provided for user-defined variables used in usrcmd commands (no commands of this class are used in the multigraph package). atest3 contains internal control parameters used by atest; several have corresponding locations in the ip array, allowing the user to specify defaults as necessary. atest4 contains a character\*80 variable list, a

 $character^*6$  variable cmdtyp and an integer jcmd, used for communication between the main user interface routines and subroutine reset, part of the usrcmd.

The block atest5 has a single integer idevce, which specifies the current graphics output device. Finally, atest6 contains five integer parameters relevant for an MPI-based parallel computing environment.

The main program has a parameter statement where values of maxn, maxja, maxa and lenw are defined. In turn, these parameters are used to allocate storage for all the major arrays used by the package. maxn is the maximum order of linear systems to be solved; maxja, maxa and lenw are the sizes of the matrix arrays ja, a, and the work array w, respectively. Their sizes, relative to maxn are problem dependent, and may need to be adjusted by the user in any particular case.

#### 4.6 Matrix Files.

The read command (r) will read a file containing a data defining a matrix and right hand side. Although it increases the file size, matrix files are ASCII (as opposed to binary formats such as XDR) to make them readable by humans. The required format follows:

The first line of the file contains three integers: n, ispd and nblock, (in that order).  $n \geq 1$  is the order of the system; ispd = 0, 1 specifies the symmetry structure, and  $nblock \geq 1$  specifies the number of blocks. The next nblock + 1 lines each contain two integers and are of the form:

$$k = ib(k)$$

defining the ib array. The next n lines each contain one integer and one real, and are of the form:

$$k b_k$$

defining the right hand side. The remaining lines all define matrix elements; each consists of two integers and one real and are of the form:

$$i \quad j \quad A_{ij}$$

The number of nonzeros is not directly specified; EOF (end-of-file) is treated as the end of matrix elements. Diagonal matrix entries should be defined, even if they are zero. If ispd = 1, then either  $a_{ij}$  or  $a_{ji}$  can be used to specify off-diagonal entries (specifying both causes no problems, but increases the file size). Within each major grouping (ib, right hand side, matrix) the entries can be specified in any order. All lines are free format (blank characters are used to separate entries).

#### 4.7 Matrix Generators.

The driver provides a few routines to generate families of matrices of varying orders, for example to study the convergence of various multigraph strategies as a function of n. At the moment, six different classes of matrices are available, each arising from standard discretizations of simple PDE's on uniform meshes. The mesh has

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ngrid mesh points in each space dimension. The parameter mtxtyp specifies the matrix to be generated. A brief summary of each class follows:

- $mtxtyp = 0 \ (star5)$ : This is the usual 5-point star finite difference discretization for  $-\Delta u$  on a uniform  $ngrid \times ngrid$  square mesh.  $n = ngrid^2$ ;  $A_{ii} = 4$  for all diagonal entries, and  $A_{ij} = -1$  for all nonzero off-diagonal entries.
- mtxtyp = 1 (|star5|): This is the same as star5 except  $A_{ij} = 1$  for all nonzero off-diagonal entries. This is not really a PDE discretization, but provides a simple class of symmetric positive definite matrices which are NOT M-matrices.
- $mtxtyp = 2 \ (star7)$ : This is the usual 7-point star finite difference discretization for  $-\Delta u$  on a uniform  $ngrid \times ngrid \times ngrid$  cubic mesh in three space dimensions.  $n = ngrid^3$ ;  $A_{ii} = 6$  for all diagonal entries, and  $A_{ij} = -1$  for all nonzero off-diagonal entries.
- mtxtyp = 3 (stokes): This is the mini-element discretization, with static condensation of cubic bubble functions, for the Stokes equations on a uniform  $ngrid \times ngrid$  square mesh in two space dimensions.  $n = 3 \, ngrid^2$ . These matrices are highly indefinite and correspond to stabilized saddle-point problems. For this class, we choose nblock = 3, with the three blocks corresponding to x-velocity, y-velocity, and pressure.
- $mtxtyp = 4 \ (star9)$ : This is the usual 9-point star finite element discretization for  $-\Delta u$  on a uniform  $ngrid \times ngrid$  square mesh.  $n = ngrid^2$ ;  $A_{ii} = 8$  for all diagonal entries, and  $A_{ij} = -1$  for all nonzero off-diagonal entries.
- mtxtyp = 5 (|star9|): This is the same as star9 except  $A_{ij} = 1$  for all nonzero off-diagonal entries. As with |star5|, this is not really a PDE discretization, but provides a second simple class of symmetric positive definite matrices which are not M-matrices.

#### 4.8 Journal Files.

The j command causes atest to read its command strings from the file jrfile, rather than accepting them interactively from the user. It is the only option available in batch mode. A journal file is an ASCII file containing a sequence of command strings as described in Section 4.2. The symbol # appearing as the first character in a line causes that line to be interpreted as a comment. When the end of the file is reached atest returns to terminal or X-windows mode and again accepts commands interactively. If a q command is encountered in a journal file, atest will exit.

When reading a journal file in X-WINDOWS mode, if a graphics command (g or m) is executed, for some devices atest will pause after the picture is drawn until the continue popup is dismissed. This allows time for the user to view the picture before proceeding to the next command in the journal file.

# 4.9 Timing Routine.

The timing routine  $cpu_time$  is used to compute the execution times for subroutines mginit and mg. If this routine is not available on a particular system, as suitable substitute is generally available.  $cpu_time$  is called only from the main program, and not from any internal subroutines.

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