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MA62 - A Frontal Code for Sparse Positive-Definite Symmetric Systems from Finite-Element Applications

I S Duff and J A Scott

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MA62 - A frontal code for sparse positive-definite symmetric systems from finite-element applications.*

by

Iain S. Duff and Jennifer A. Scott

Abstract

We describe the design, implementation, and performance of a frontal code for the solution of large sparse symmetric systems of linear finite-element equations. The code is intended primarily for positive-definite systems since numerical pivoting is not performed. The resulting software package, MA62, will be included in Release 13 of the Harwell Subroutine Library (HSL). We illustrate the performance of our new code on a range of problems arising from real engineering and industrial applications. The performance of the code is compared with that of the HSL general frontal solver MA42 and with other positive-definite codes from the Harwell Subroutine Library.

Keywords: sparse symmetric linear equations, symmetric frontal method, Gaussian elimination, finite-element equations, Level 3 BLAS.

AMS(MSC 1991) subject classifications: 65F05, 65F50.

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Department for Computation and Information,
Atlas Centre, Rutherford Appleton Laboratory,
Oxon OX11 0QX, England.

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Contents

1 Introduction

In this report, we discuss the design and use of a code for the solution of the linear systems of equations

$$\mathbf{AX} = \mathbf{B} \tag{1.1}$$

where the n×n matrix **A** is large, sparse, and symmetric. **B** is an n×nrhs (nrhs ≥ 1) matrix of right-hand sides and **X** is the n × nrhs solution matrix. It is assumed that the matrix **A** is an elemental matrix, that is, it is a sum of finite-element matrices

$$\mathbf{A} = \sum_{l=1}^{m} \mathbf{A}^{(l)}, \tag{1.2}$$

where each element matrix $\mathbf{A}^{(l)}$ has nonzeros only in a few rows and columns and corresponds to the matrix from element l. The frontal method was originally developed by Irons (1970) for the solution of symmetric positive-definite systems which come from finite-element discretizations in structural analysis. However, it was later realised that the method could be extended and modified to be applicable to a far wider class of problems, including those for which **A** is any general unsymmetric matrix (see, for example, Hood, 1976, Duff, 1981). A frontal code for unsymmetric systems, MA32, was developed for the Harwell Subroutine Library (1996) by Duff (1981, 1983, 1984). This code was very widely used before being substantially restructured and improved by Duff and Scott (1993, 1996). The upgraded code, MA42, which has superseded MA32 in the Harwell Subroutine Library (HSL), is efficient on a wide range of modern computers and has been used to solve problems from many different application areas.

From the feedback we have received from users, it is apparent that MA42 is frequently used to solve finite-element problems for which the system matrix **A** is symmetric and positive definite. However, apart from offering an option of restricting pivoting to the diagonal, MA42 does not exploit symmetry or positive definiteness and, as a result, the code is more expensive in terms of both storage requirements and operation counts than it need be for this class of problems. MA42 is also complicated by an option allowing the input of the assembled matrix **A** by rows. Our goal is to design and develop an efficient frontal code specifically for symmetric positive-definite elemental matrices. Our new code, MA62, is now available and will be included in the next release of the Harwell Subroutine Library. Details of how to obtain the code are given in Section 6.

The outline of this report is as follows. In Section 2, we briefly review frontal schemes for symmetric positive-definite elemental matrices. The design of MA62, including the user interface, the internal data structures, and the use of high level BLAS, is discussed in Section 3. In Section 4, we illustrate the performance of the new code, and compare it with our general frontal code MA42 and with other Harwell Subroutine Library codes for the solution of symmetric positive-definite systems. Concluding comments are made in Section 5. Specification Sheets for MA62 are given in the Appendix.

2 Frontal schemes

The frontal method is a variant of Gaussian elimination and, for the symmetric system (1.1), involves the matrix factorization

$$\mathbf{A} = (\mathbf{PL})\mathbf{D}(\mathbf{PL})^T, \tag{2.1}$$

where $\mathbf{P}$ is permutation matrix, $\mathbf{D}$ is a diagonal matrix, and $\mathbf{L}$ is a unit lower triangular matrix. If $\mathbf{A}$ is a positive-definite matrix, the entries of $\mathbf{D}$ are positive. The solution process is completed by performing the forward elimination

$$(\mathbf{PL})\mathbf{Z} = \mathbf{B}, \tag{2.2}$$

then the diagonal solution

$$\mathbf{DY} = \mathbf{Z}, \tag{2.3}$$

followed by the back substitution

$$(\mathbf{PL})^T\mathbf{X} = \mathbf{Y}. \tag{2.4}$$

The main feature of the method is that the contributions $\mathbf{A}^{(l)}$ from the finite-elements (see (1.2)) are assembled one at a time and the construction of the assembled coefficient matrix $\mathbf{A}$ is avoided by interleaving assembly and elimination operations. An assembly operation is of the form

$$a_{ij} \Leftarrow a_{ij} + a_{ij}^{(l)}, \tag{2.5}$$

where $a_{ij}^{(l)}$ is the (i,j)th nonzero entry of the element matrix $\mathbf{A}^{(l)}$. A variable is *fully summed* if it is involved in no further sums of the form (2.5) and is *partially summed* if it has appeared in at least one of the elements assembled so far but is not yet fully summed. The Gaussian elimination operation

$$a_{ij} \Leftarrow a_{ij} - a_{il}[a_{ll}]^{-1}a_{lj} \tag{2.6}$$

may be performed as soon as all the terms in the triple product in (2.6) are fully summed. At any stage during the assembly and elimination processes, the fully and partially summed variables are held in a dense matrix, termed the *frontal* matrix. The power of frontal schemes comes from the following observations:

- since the frontal matrix is held as a dense matrix, dense linear algebra kernels, in particular, the Level 3 Basic Linear Algebra Subprograms (BLAS) (Dongarra, DuCroz, Duff and Hammarling, 1990), can be used during the numerical factorization.

- the matrix factors need not be held in-core, which allows large problems to be solved using only modest amounts of high-speed memory,

The number of floating-point operations and the storage requirements for the frontal method are dependent on the size of the frontal matrix at each stage of the computation. Since the size of the frontal matrix increases when a variable appears

for the first time and decreases whenever a variable is eliminated, the order in which the element matrices are input is critical for the efficiency of the method. There has been considerable attention paid to the problem of automatically choosing a good ordering. Many of the proposed algorithms are similar to those for bandwidth reduction of assembled matrices (see, for example, Duff, Reid and Scott, 1989, and the references therein). To give the user the greatest flexibility in deciding how to order the elements, we have chosen not to incorporate element ordering within the MA62 package. However, the Harwell Subroutine Library routine MC43 (Duff et al., 1989) can be used to preorder the elements for MA62.

3 The software package MA62

In this section, we describe the user interface to MA62, its internal data structures, and its use of BLAS kernels. We highlight how it has been possible to take advantage of symmetry and positive definiteness when designing the code.

3.1 The user interface

An initial decision when designing MA62 was that it should have a user interface which was similar to that of the unsymmetric frontal solver MA42. This was not only because we felt the flexibility of the reverse communication interface used by MA42 remained appropriate for the symmetric positive-definite case, but because we wanted to make it straightforward for a user who was familiar with MA42 to use MA62. The MA62 package has six entries which may be called directly by the user. Each of the subroutines are named according to the naming convention of the Harwell Subroutine Library, with the single precision version having names commencing with MA62 plus one more letter, and double precision versions with the additional sixth letter D. For simplicity, we will use the single precision names throughout this report. The user-callable entries are:

Initialization : MA62I initializes the parameters which control the execution of the package. A single call must be made to MA62I before any other routines in the MA62 package are called.

Prepass: MA62A determines in which element each variable appears for the last time and thus when a variable is fully summed and can be eliminated. MA62A must be called once for each element.

Symbolic factorization : MA62J uses the information from MA62A to determine the amount of real and integer storage required for the factorization. MA62J must be called once for each element, in the same order as in the calls to MA62A.

Direct access files : MA62P sets up direct access files for holding the matrix factors. Use of MA62P is optional. If direct access files are used, a single call to MA62P must be made.

Numerical factorization : MA62B uses the information generated by MA62A and MA62J in the factorization of the matrix (1.2) and, if element right-hand sides $\mathbf{B}^{(l)}$ are specified, MA62B solves the equations (1.1) with right-hand side(s) $\mathbf{B} = \sum_{k=1}^{m} \mathbf{B}^{(l)}$. MA62B must be called once for each element, in the same order as in the calls to MA62A and MA62J.

Solve : MA62C uses the factors produced by MA62B to rapidly solve for further right-hand sides. Use of MA62C is optional. If used, a single call to MA62C will solve for the number of right-hand sides specified by the user.

We briefly discuss each of these subroutines. Full details of their argument lists and their calling sequences are given in the Specification Sheets (see Appendix).

3.1.1 Initialization

The user must make a single call to MA62I prior to calling any of the other routines in the MA62 package. MA62I assigns default values to the control parameters held in the arrays ICNTL and CNTL. These parameters control the action of the subroutines within the MA62 package. They include parameters to control the level of diagnostic printing and parameters which specify the number of bytes for a real and an integer word. Full details of the control parameters and their default values are included in the Specification Sheets. Should the user want a control parameter to have a value other than its default, the appropriate parameter should be reset after the call to MA62I. MA62I also initializes the array ISAVE, which is used to hold variables that must be preserved between calls to routines in the MA62 package but are unlikely to be of interest to the user. The array ISAVE is also used both to check the data input by the user and to ensure that the user has called the routines in the MA62 package in the correct sequence.

3.1.2 Prepass

MA62A must be called for each element to specify the variable indices associated with it. This subroutine records, in the array LAST of length ndf (where ndf is the largest integer used to index a variable), the call at which each variable appears for the last time (becomes fully summed). This information must be passed unchanged to the symbolic factorization and numerical factorization subroutines (MA62J and MA62B, respectively). The elements must be presented to the symbolic and numerical factorization routines in exactly the same order as to MA62A.

3.1.3 Symbolic factorization

One of the difficulties facing the user of a frontal code is the need to specify file sizes for the factors and the maximum front sizes required before the computation begins. A symbolic factorization works only with the variable indices associated with the elements and, by assuming each variable may be eliminated as soon as it is fully summed, it determines the maximum order of the frontal matrix and the file sizes needed for the factors. For general unsymmetric matrices, the need to incorporate pivoting means the statistics returned by the symbolic factorization are only lower bounds on the front size and file sizes actually needed. But for positive-definite

matrices a variable can always be eliminated once it is fully summed and, since the symbolic factorization is inexpensive, we decided to require the user to perform a symbolic factorization before the numerical factorization commences. The symbolic factorization is performed by calling the subroutine MA62J for each element in the same order as they were presented to MA62A. An entry in ISAVE is flagged so that a check can be made at the start of the numerical factorization that MA62J has been called. The real and the integer storage required by the factorization are returned to the user after the last element has been input in the information array INFO. If the user provides the numerical factorization with less space than that determined by MA62J, it can be detected immediately and the computation terminated with an error message.

MA62 allows the user to specify (using the control parameter ICNTL(5)) the minimum number of pivots that will be selected at any stage. Delaying performing eliminations until the number of fully summed variables is at least ICNTL(5) (ICNTL(5) $\geq$ 1) increases the Level 3 BLAS component of the factorization (see Section 3.3), albeit at the cost of more floating-point operations, increased storage for the reals in the factor, and, in general, an increase in the maximum front size and consequently in the in-core storage required. Since the symbolic factorization is cheap to perform, the user may want to look at the effect on the maximum front size and the file sizes of different values of ICNTL(5) before starting the numerical factorization. MA62 has been designed so that this can be done in a straightforward way. Provided the user has performed a complete sequence of calls to MA62J, the user may reset ICNTL(5) and then repeat the sequence of calls to MA62J **without** making any further changes to the input parameters. Having chosen the minimum pivot block size, the calls to the numerical factorization routine MA62B must immediately follow a sequence of calls to MA62J with the **same** value of ICNTL(5). A component of ISAVE is used to check this.

3.1.4 Direct access files

A key feature of MA62 (and of MA42 and the earlier code MA32) is that it offers the user the option of holding the matrix factors in direct access files. MA62 optionally uses two direct access files, one for the reals in the factors and one for the indices of the variables in the factors. A single call to the subroutine MA62P sets up the direct access files. The user must specify the stream numbers for the direct access files and may optionally name the files.

Corresponding to each direct access file is an in-core buffer (or workspace). Eliminations are performed during the numerical factorization whenever the number of fully summed variables KR is at least ICNTL(5). The eliminations generate KR columns of the matrix factor **(PL)D**. The columns are written to the real in-core buffer and each time columns are written, the following integer data is written (in order) to the integer buffer:

1. The number of integers being written.
2. The number KR of eliminations (that is, the number of columns being written to the real buffer).
3. The current front size FRNT.

4. A list of the indices of the FRNT variables in the current front.

5. The number of integers being written.

The number of integers is held as the first and last entry to allow the real and integer data to be scanned both in the order in which it is written and in reverse order. Reverse order is needed when performing the back substitution (2.4). Once either a buffer is full or all the elimination operations are complete, the contents of the buffer are output to the associated direct access file. Use of direct access files is unnecessary if there is sufficient in-core space for the factors. Numerical results given in Sections 4.5 and 4.6 show that, on some machines, the overheads which result from using direct access files can be considerable, particularly during the solve phase.

We remark that the unsymmetric frontal code MA42 uses three direct access files since it stores the **L** and **U** factors of **A** separately. Moreover, since the unsymmetric code uses off-diagonal pivoting to maintain stability, it is necessary to hold both row and column indices of the variables in the frontal matrix. Therefore, in addition to the saving in real storage, if the minimum pivot block size ICNTL(5) is set to 1, MA62 uses approximately half the integer storage of MA42, and if ICNTL(5) > 1, the savings are even greater. This is illustrated in Table 4.12 in Section 4.5.

3.1.5 Numerical factorization and optional solve

The numerical factorization subroutine MA62B accepts the element matrices $\mathbf{A}^{(l)}$ and, optionally, the corresponding element right-hand sides $\mathbf{B}^{(l)}$, one at a time. Only the upper triangular part of $\mathbf{A}^{(l)}$ needs to be specified by the user but, to facilitate the assembly process, MA62B copies the upper triangular part into the lower triangle. If any variables in the incoming element are internal to the element, they are eliminated within the element and the columns of the matrix factor which are generated are written to the buffers before contributions from the remaining variables are assembled into the frontal matrix. These internal variables are termed *static condensation variables* and the number of such variables is returned to the user in the information array INFO at the end of the numerical factorization. As the element is being assembled, the number KR of variables in the front which are now fully summed is counted. If this number is at least as large as the control parameter ICNTL(5), KR eliminations are performed (see Section 3.3). Otherwise, as long as elements remain to be assembled, control is returned to the user for the next element to be input.

Since the space required by the numerical factorization can not exceed that determined by the symbolic factorization, on the assumption that the user supplies consistent data (and using the array ISAVE we have incorporated many checks for this in the program), the only way MA62 can terminate before the factorization is complete is if the matrix **A** is found not to be positive definite. In MA62, each pivot candidate (that is, each fully summed variable) is checked to see that it is of absolute value at least as large as the control parameter CNTL(1) (with default value zero). If a pivot is found to be too small, an error flag is set and control returned to the user. Note that although the factorization will not proceed, it need not be the case that the matrix is singular. If a pivot is found to be negative, the matrix

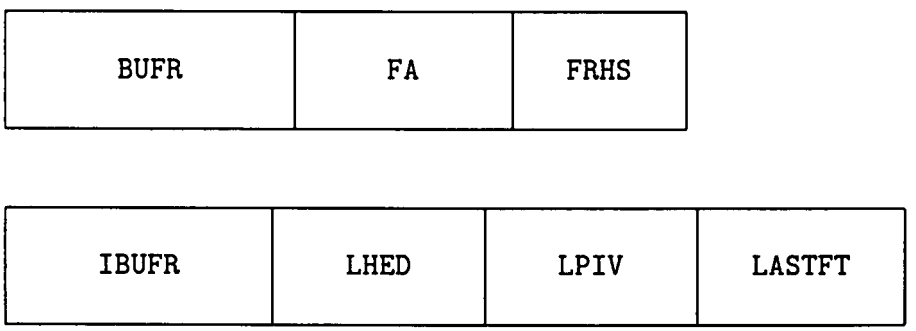
is not positive definite, but provided it is of absolute value at least CNTL(1), the computation continues and the number of negative pivots is returned to the user in the information array INFO at the end of the computation.

3.1.6 Further solves

In common with many other sparse direct codes, MA62 offers the option of solving for further right-hand side matrices **B**, without recalling the numerical factorization routine. On each call to the solve routine MA62C, the number of right-hand sides (columns of **B**) must be specified in nrhs. In contrast to MA62A, MA62J, and MA62B, there is no input by elements to MA62C and the right-hand sides must be input in assembled form. This gives MA62C a straightforward interface. In MA62, the forward elimination and diagonal solution ((2.2) and (2.3)) are combined. For the forward elimination, the real and integer data for the factors is read in the order in which it was written and, for the back substitution, the data is read in reverse order. When nrhs > 1, both the forward elimination and back substitution steps use _GEMM, the Level 3 BLAS matrix-matrix multiplication kernel (see Section 3.3). When there is only one right-hand side (nrhs $= 1$), Level 2 BLAS are used. It should be noted that **B** is involved in this matrix-matrix product and that _GEMM becomes more efficient with an increased number of columns in **B**. This is illustrated in Section 4.5 (Tables 4.13 to 4.15).

3.2 Internal data structures

The internal data structures used by MA62 are simplified and modified versions of those used by MA42 and, earlier, by MA32 (see Duff, 1981, for a detailed description of the internal arrays used by MA32). The user must supply both a real workspace array and an integer workspace array, which are subdivided as follows:



We first discuss the real workspace.

BUFR is the in-core buffer for the reals in the factor **(PL)D**. The length of BUFR is chosen by the user. On exit from the symbolic factorization, the required length of the file for the reals in the factor is given by INFO(7). If the user calls the numerical factorization MA62B with nrhs right-hand sides, the total real storage for the factors and the right-hand sides is INFO(7) + nrhs $\times$ ndf (ndf is the largest integer used to index a variable). If direct access files are not being used, BUFR must be at least this length. Otherwise, for efficiency,

BUFR should be chosen so that INFO(7)+nrhs×ndf = k_1×BUFR with $k_1 \geq 1$ as small as available space permits. After the eliminations following an element assembly, the columns of (**PL**)**D** which have been generated are written to BUFR (see Subsection 3.1.4).

FA holds the current frontal matrix. On exit from the symbolic factorization, the maximum front size is given by INFO(3). The frontal matrix is held as a square matrix of order INFO(3) but only the data in the upper triangular part is meaningful. Storage for both upper and lower triangular parts is needed to permit the use of Level 3 BLAS (see Section 3.3).

FRHS holds the right-hand sides corresponding to the current frontal matrix. FRHS is a matrix of size INFO(3) by nrhs, where nrhs is the number of right-hand sides to be solved for at the same time as the factorization. FRHS is not needed if nrhs = 0.

We now turn our attention to the integer workspace.

IBUFR is the in-core buffer for the integer data for the factors. The length of IBUFR is chosen by the user. On exit from the symbolic factorization, the required length of the file for the integer data is given by INFO(8). If direct access files are not being used, IBUFR must be at least this length. Otherwise, for efficiency, IBUFR should be chosen so that INFO(8) = k_2×IBUFR with $k_2 \geq 1$ as small as available space permits. After the eliminations following an element assembly, the indices of the columns of (**PL**)**D** which have been generated by the eliminations are written to IBUFR (see Subsection 3.1.4).

The remaining integer arrays LHED, LPIV, and LASTFT are each of length INFO(3) (the maximum frontsize). To discuss these arrays we need some terminology. The *global* index of a variable is the integer given to it by the user in the calls to the subroutines in the package (if the variables are numbered contiguously then the global index of a variable is its index in the assembled matrix **A**). The *local* index of a fully or partially summed variable refers to its location in the current frontal matrix. During the factorization, the array LAST (which was set by the prepass MA62A to hold the call at which each variable becomes fully summed) is used as workspace and it, together with the internal arrays LHED, LPIV, and LASTFT, are used to provide an efficient mapping between global and local indices as follows:

LHED holds the global indices of the variables in the current frontal matrix.

LPIV holds the local indices of the fully summed variables in the current frontal matrix.

LAST is used to hold the local indices of the variables in the current frontal matrix. If the variable with global index JVAR is partially summed, its local index is -LAST(JVAR). Otherwise, LAST(JVAR) is the assembly step at which JVAR becomes fully summed.

LASTFT is used to hold the assembly step at which variables in the front become fully summed (the information which was originally held in LAST). For each partially summed variable JVAR in the front, LASTFT(-LAST(JVAR)) holds the assembly step at which JVAR is fully summed.

To summarize the use of LHED, LAST and LASTFT, suppose on the first call to MA42B that LAST(JVAR) = KELL. If, at some stage before the assembly of the element KELL, JVAR is partially summed with local index L, then LHED(L) = JVAR, LASTFT(L) = KELL, and LAST(JVAR) = −L. The use of LASTFT to hold information which was originally held in LAST avoids the use of a second array of length ndf.

3.3 The use of high level BLAS

In this section, we describe the use of the BLAS in performing both the numerical factorization and the forward elimination and back substitution steps. We first consider the factorization. After the assembly of an element, the frontal matrix can be written in the form

$$\mathbf{F} = \begin{pmatrix} \mathbf{F}_T & \mathbf{F}_C^T \\ \mathbf{F}_C & \mathbf{F}_U \end{pmatrix}, \tag{3.1}$$

where the submatrices $\mathbf{F}_T$ and $\mathbf{F}_C$ are fully summed. Since the pivots may be picked from the diagonal of $\mathbf{F}_T$ in order, we can compute the factorization

$$\begin{pmatrix} \mathbf{F}_T & \mathbf{F}_C^T \\ \mathbf{F}_C & \mathbf{F}_U \end{pmatrix} = \begin{pmatrix} \mathbf{F}_{TL} & \mathbf{0} \\ \mathbf{F}_L & \mathbf{I} \end{pmatrix} \begin{pmatrix} \mathbf{D}_T & \mathbf{0} \\ \mathbf{0} & \widehat{\mathbf{F}} \end{pmatrix} \begin{pmatrix} \mathbf{F}_{TL}^T & \mathbf{F}_L^T \\ \mathbf{0} & \mathbf{I} \end{pmatrix}, \tag{3.2}$$

where

$$\mathbf{F}_T = \mathbf{F}_{TL}\mathbf{D}_T\mathbf{F}_{TL}^T, \tag{3.3}$$

$$\mathbf{F}_L = \mathbf{F}_C(\mathbf{D}_T\mathbf{F}_{TL}^T)^{-1} \tag{3.4}$$

and the Schur complement $\widehat{\mathbf{F}}$ is given by

$$\widehat{\mathbf{F}} = \mathbf{F}_U - \mathbf{F}_L\mathbf{D}_T\mathbf{F}_L^T. \tag{3.5}$$

Level 3 BLAS kernels can be used in computing $\mathbf{F}_L$ and $\widehat{\mathbf{F}}$. From (3.4) it follows that

$$\mathbf{F}_L\mathbf{D}_T = \mathbf{F}_C\mathbf{F}_{TL}^{-T}. \tag{3.6}$$

The Level 3 kernel _TRSM can be used to form $\mathbf{F}_L\mathbf{D}_T$ and $\mathbf{F}_L^T$ follows by diagonal scaling. If the number of fully summed variables is KR, the Level 3 kernel _GEMM with internal dimension KR may then be used to compute (3.5). However, since only the upper triangular part of $\widehat{\mathbf{F}}$ is needed, forming the whole of $\widehat{\mathbf{F}}$ involves many unnecessary operations. With a front size of FRNT, the computation (3.5) requires $2 * \mathrm{KR} * (\mathrm{FRNT} - \mathrm{KR})^2$ floating-point operations. We could form only the upper triangle of $\widehat{\mathbf{F}}$ by updating each column using the Level 2 kernel _GEMV. This would

reduce the number of floating-point operations to KR * (FRNT − KR) * (FRNT − KR + 1) but the efficiency gains of using Level 3 BLAS would be lost. To take advantage of Level 3 BLAS while at the same time restricting the number of unnecessary operations, the columns of $\widehat{\mathbf{F}}$ may be computed in blocks. Assuming a block size of NB with FRNT − KR = m*NB then, using Fortran 90 section notation,

$$\begin{aligned}\widehat{\mathbf{F}}(1:\mathtt{K},\mathtt{K}-\mathtt{NB}+1:\mathtt{K}) &= \mathbf{F}_U(1:\mathtt{K},\mathtt{K}-\mathtt{NB}+1:\mathtt{K}) - \\ &(\mathbf{F}_L\mathbf{D}_T)(1:\mathtt{K},1:\mathtt{KR}) * \mathbf{F}_L^T(1:\mathtt{KR},\mathtt{K}-\mathtt{NB}+1:\mathtt{K}) \end{aligned} \tag{3.7}$$

where K = K1 * NB, K1 = $1, 2, \ldots, m$. The update (3.7) can be performed using _GEMM with interior dimension KR (the Level 2 kernel _GEMV is used if KR = 1).

By increasing the minimum number of pivots that are selected at each stage (that is, by increasing the value of the control parameter ICNTL(5)), KR is increased and greater efficiency can be gained from using _GEMM to perform (3.7). This is discussed further by Cliffe, Duff and Scott (1997) (see also Tables 4.8 to 4.11 in Section 4.4).

In MA62, the size of the blocks used in (3.7) is controlled by the parameter ICNTL(7). In general, FRNT − KR = $(m-1)$ * ICNTL(7) + r and the final block will have r columns. As a result of numerical experiments, we have chosen 16 as the default value for both ICNTL(5) and ICNTL(7). The effects of using different values are illustrated in Section 4.4.

The other main use of high level BLAS is in the solution phase. The columns of $\mathbf{PL}$ corresponding to the KR variables eliminated at the same stage are

$$\begin{pmatrix} \mathbf{F}_{TL} \\ \mathbf{F}_L \end{pmatrix}. \tag{3.8}$$

We use direct addressing in the solution phase to exploit this block structure. At each stage of the forward elimination all the active components of the partial solution vector $\mathbf{Y}$ (where $(\mathbf{PL})\mathbf{DY} = \mathbf{B}$) are put into an array $\mathbf{W} = (\mathbf{W}_1, \mathbf{W}_2)^T$, with $\mathbf{W}_1$ of dimension KR by nrhs and $\mathbf{W}_2$ of dimension FRNT-KR by nrhs. The operations

$$\mathbf{W}_1 \leftarrow \mathbf{F}_{TL}^{-1}\mathbf{W}_1 \tag{3.9}$$

followed by

$$\mathbf{W}_2 \leftarrow \mathbf{W}_2 - \mathbf{F}_L\mathbf{W}_1 \tag{3.10}$$

and finally

$$\mathbf{W}_1 \leftarrow \mathbf{D}_T^{-1}\mathbf{W}_1 \tag{3.11}$$

are performed before $\mathbf{W}$ is unloaded into $\mathbf{Y}$. Similarly, during the back substitution, all the active components of the partial solution vector $\mathbf{Y}$ are put into an array $\mathbf{Z}_1$ of leading dimension KR and the active variables of the solution vector $\mathbf{X}$ are put into an array $\mathbf{Z}_2$ of leading dimension FRNT-KR. The operations

$$\mathbf{Z}_1 \leftarrow \mathbf{Z}_1 - \mathbf{F}_L^T\mathbf{Z}_2 \tag{3.12}$$

and then

$$\mathbf{Z}_1 \leftarrow \mathbf{F}_{TL}^{-T}\mathbf{Z}_1 \tag{3.13}$$

are carried out before $\mathbf{Z}_1$ is unloaded into $\mathbf{X}$.

In MA62, $\mathbf{F}_L$ is written to the buffer by columns, and $\mathbf{F}_{TL}$ is written to the buffer in packed form. Provided KR > 1, the forward elimination and back substitutions are performed using the Level 2 BLAS kernels _GEMV and _TPSV if there is only one right-hand side (nrhs = 1), and the Level 3 routine _GEMM and the Level 2 routine _TPSV if there are multiple right-hand sides. We observe that there is no Level 3 BLAS kernel for solving a triangular system of equations with the matrix held in packed form and multiple right-hand sides. We performed some numerical experiments in which we stored $\mathbf{F}_{TL}$ as a full matrix with only the lower triangular part containing meaningful data and, in the forward elimination and back substitutions, we used the Level 2 kernel _TRSV if nrhs = 1 and the corresponding Level 3 kernel _TRSM otherwise. Our results showed that the savings in the real storage which result in storing only the packed lower triangular matrix $\mathbf{F}_{TL}$ are small (generally less than 10 per cent of the real storage requirement). This is illustrated in Table 4.12 in Section 4.5. The triangular solves (3.9) and (3.13) account for a relatively small part of the total solution time. Our experience is that there is little difference in the CPU times when _TRSM is used in place of _TPSV. As a result, we have chosen in MA62 to minimize storage requirements by using the packed triangular form.

Although the factorization and solution stages described above are reasonably straightforward, their implementation within MA62 using Level 3 BLAS kernels is non-trivial. Elements are assembled into the frontal matrix FA until there are at least ICNTL(5) fully summed variables. The fully summed columns are then permuted to the last columns of FA and, if supplied, the corresponding rows of the right-hand side array FRHS are permuted to the end of the array. When an element is assembled into FA, only the upper triangular part of FA contains meaningful data, and symmetry must be exploited to perform the column interchanges. We remark that, by permuting the fully summed columns to the last columns of FA, once the eliminations have been performed and the resulting data written to the in-core buffers BUFR and IBUFR, the last columns of FA can be reset to zero and the next element assembled. If instead we were to permute the fully summed columns to the start of FA, further costly data movement would be required.

After permuting the fully summed columns to the end, the pivots are generated in reverse order on the diagonal of the factors. We now discuss in detail what this means for the forward elimination operation (3.9). As already mentioned, the triangular parts of the factor matrix are held in packed form. We store the lower triangular matrix $\mathbf{F}_{TL}$ by rows and store the negative of the pivot entries at the end of each row. Thus, if KR = 3 and the lower triangular part of the matrix $\mathbf{F}_{TL}$ is given by

$$\begin{pmatrix} piv_3 & & \\ a & piv_2 & \\ b & c & piv_1 \end{pmatrix},$$

it is stored as

$$-piv_3 \;\; a \;\; -piv_2 \;\; b \;\; c \;\; -piv_1.$$

In equation (3.9) we wish to compute

$$\begin{pmatrix} 1 & & \\ c & 1 & \\ b & a & 1 \end{pmatrix}^{-1} \mathbf{W}_1, \tag{3.14}$$

but since we have the pivots in reverse order, we are computing

$$\tilde{\mathbf{P}}\mathbf{L}^{-1}\tilde{\mathbf{P}}^T\tilde{\mathbf{P}}\mathbf{W}_1,$$

where $\tilde{\mathbf{P}}$ is the reverse permutation $\{\mathtt{KR}, \mathtt{KR}-1, ..., 1\}$ and $\mathbf{L}$ is the matrix in (3.14). Our coefficient matrix is therefore of the form

$$\begin{pmatrix} 1 & a & b \\ & 1 & c \\ & & 1 \end{pmatrix}^{-1}.$$

Thus, using the data held in the form above, in MA62 the packed triangular solve Level 2 BLAS routine _TPSV is called with its control parameters set to "Upper", "Unit", and "No transpose".

3.4 Exploiting zeros in the front

During the factorization, the frontal matrix may contain some zero entries. Treating the frontal matrix as a dense matrix results in unnecessary operations being performed with these zeros. As we have shown, high level BLAS are used, so that the cost of these operations may not be prohibitive. If, however, the frontal matrix contains a significant number of zeros, it can be advantageous to exploit these zeros. In particular, there are many zeros in the front if the elements are poorly ordered. To see how we can exploit the zeros, suppose the frontal matrix has been permuted to the form (3.1). By performing further row and column permutations, the frontal matrix can be expressed in the form

$$\mathbf{F} = \begin{pmatrix} \mathbf{F}_T & \mathbf{F}_{C_1}^T & \mathbf{0} \\ \mathbf{F}_{C_1} & \mathbf{F}_{U_1} & \mathbf{F}_{U_2}^T \\ \mathbf{0} & \mathbf{F}_{U_2} & \mathbf{F}_{U_3} \end{pmatrix}, \tag{3.15}$$

where the zero matrix is of order KR by K for some K with $0 \leq \mathtt{K} \leq \mathtt{FRNT} - \mathtt{KR}$ (FRNT is the current front size and KR is the number of fully summed variables). The factorization then becomes

$$\begin{pmatrix} \mathbf{F}_T & \mathbf{F}_{C_1}^T & \mathbf{0} \\ \mathbf{F}_{C_1} & \mathbf{F}_{U_1} & \mathbf{F}_{U_2}^T \\ \mathbf{0} & \mathbf{F}_{U_2} & \mathbf{F}_{U_3} \end{pmatrix} = \begin{pmatrix} \mathbf{F}_{TL} & \mathbf{0} & \mathbf{0} \\ \mathbf{F}_{L_1} & \mathbf{I} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{I} \end{pmatrix} \begin{pmatrix} \mathbf{D}_T & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \widehat{\mathbf{F}_{U_1}} & \mathbf{F}_{U_2}^T \\ \mathbf{0} & \mathbf{F}_{U_2} & \mathbf{F}_{U_3} \end{pmatrix} \begin{pmatrix} \mathbf{F}_{TL}^T & \mathbf{F}_{L_1}^T & \mathbf{0} \\ \mathbf{0} & \mathbf{I} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{I} \end{pmatrix}, \tag{3.16}$$

where

$$\mathbf{F}_{L_1} = \mathbf{F}_{C_1}(\mathbf{D}_T\mathbf{F}_{TL}^T)^{-1}, \tag{3.17}$$

and $\widehat{\mathbf{F}_{U_1}}$ is given by

$$\widehat{\mathbf{F}_{U_1}} = \mathbf{F}_{U_1} - \mathbf{F}_{L_1}\mathbf{D}_T\mathbf{F}_{L_1}^T. \tag{3.18}$$

If KR > 1, the matrix $\mathbf{F}_{L_1}$ may still contain some zeros. However, the experiments which we report in Table 4.3 (Section 4.3) show that, in general, the number of zeros remaining in the factors is small (less than 10 per cent of the total number of entries in the factors). Furthermore, $\mathbf{F}_{L_1}$ rather than $\mathbf{F}_L$ ($\mathbf{F}_L = (\mathbf{F}_{L_1}^T, \mathbf{0})^T$), is written to the buffer, resulting in savings in both the real and integer factor storage.

In MA62, zeros in the front are exploited if the default value ICNTL(9) $= 1$ is used. With this setting, once an element has been assembled and the fully summed columns permuted to the last columns of the frontal matrix, row permutations are performed to collect the zeros in the fully summed columns into a block held in the first rows. We now explain how this is achieved in MA62. The number K of rows with zeros in all the pivotal columns is initially set to 0. Rows 1 to FRNT $-$ KR $+ 1$ of the pivotal columns are scanned in reverse order. Let I be the index of the row currently being scanned. There are two possibilities: either there is a nonzero entry in at least one of the pivotal columns or all the entries in the pivotal columns are zero. In the first case, no action is needed and, assuming I > 1, we now scan row I-1. In the second case, we increment K by one and, starting with row K, we search for a row with index at most I-1 with a nonzero entry in at least one of the pivotal columns. If we find such a row, it is interchanged with row I and we then scan row I-1. Otherwise, there are no more rows to add to the zero block and we are ready to perform the elimination operations.

In general, when zeros in the front are exploited, the real and integer storage used to hold the factors will be less than that predicted by the symbolic factorization, which assumes that the frontal matrices are dense. The information on the storage actually used is returned to the user in the information array INFO. Zeros in the front are not exploited if the control parameter ICNTL(9) is set by the user to 0. Results which demonstrate how beneficial it can be to exploit zeros in the front are given in Section 4.3.

4 Numerical results

4.1 Test problems

In this section, we describe the problems that we use for testing the performance of MA62. In all cases, they arise in real engineering and industrial applications. The problems are all unassembled finite-element problems and a brief description of each is given in Table 4.1. The first seven problems are from the Harwell-Boeing Collection (Duff, Grimes and Lewis, 1992), the RAMAGE01 and RAMAGE02 problems were provided by Alison Ramage of the University of Strathclyde (Ramage and Wathen, 1993), the problem AEAC5081 is from Andrew Cliffe of AEA Technology, and the remaining problems (TRDHEIM, CRPLAT2, OPT1, and TSYL201) were supplied by Christian Damhaug of Det Norske Veritas, Norway. For all the problems, values for the entries of the element matrices were generated using the Harwell Subroutine Library (HSL) random number generator FA01 and

Identifier	Order	Number of elements	Description/discipline
CEGB3306	3222	791	2.5D Framework problem
CEGB2919	2859	128	3D cylinder with flange
CEGB3024	2996	551	2D reactor core section
LOCK1074	1038	323	Lockheed gyro problem
LOCK2232	2208	944	Lockheed tower problem
LOCK3491	3416	684	Lockheed cross-cone problem
RAMAGE01	1476	128	3D Navier-Stokes
AEAC5081	5081	800	Double glazing problem
TRDHEIM	22098	813	Mesh of the Trondheim fjord
CRPLAT2	18010	3152	Corrugated plate field
OPT1	15449	977	Part of oil production platform
TSYL201	20685	960	Part of oil production platform
RAMAGE02	16830	1400	3D Navier-Stokes

Table 4.1: The test problems

each was made symmetric and diagonally dominant. In all the experiments, apart from those reported on in Sections 4.2 and 4.3, the elements were ordered using the direct element reordering algorithm offered by the HSL routine MC43 before the frontal solvers were called.

All the HSL linear equation solvers used in our numerical experiments have control parameters with default values. Unless stated otherwise, we use these defaults in each case.

The experimental results given in this paper were obtained using 64-bit floating-point arithmetic on the following platforms:

- A single processor of a CRAY J932 using the CRAY Fortran compiler cf77-7 with compiler option -Zv for the Fortran 77 codes and f90 with default options for the Fortran 90 codes.
- An IBM RS/6000 3BT using the IBM Fortran compilers xlf and xlf90, with compiler option -O.
- A DEC 7000 3BT using the DEC Fortran compilers f77 and f90, with default compiler options.

On each machine the vendor-supplied BLAS were used. All times are CPU times in seconds and include the i/o overhead for the codes which use direct access files. In all the tables in which the number of floating-point operations ("ops") are quoted, we count all operations (+, -, *, /) equally.

4.2 The effect of ordering

As explained in Section 2, the order in which the elements are presented to the frontal solver has a significant effect on its performance. If we denote by f_l the number of variables in the front before the lth elimination, then an important measure,

particularly for computing the amount of in-core storage required, is the maximum front size

$$\max_{l=1,n} f_l.$$

A prediction of the work involved in the frontal algorithm can be obtained from the root-mean squared front size (rms front size) defined by

$$\left(\sum_{l=1}^{n} f_l^2/n\right)^{1/2}.$$

In Table 4.2, we show the results of using the element ordering code MC43 with

Identifier	Max front size in MA62		rms front size in MA62		Number of ops ($*10^7$)		Factorize time (seconds)	
	Before	After	Before	After	Before	After	Before	After
CEGB3306	366	90	248.3	65.5	3.1	1.7	0.6	0.4
CEGB2919	357	306	216.5	191.0	8.3	10.2	0.9	1.0
CEGB3024	162	146	113.7	90.0	2.7	2.6	0.5	0.5
LOCK1074	822	138	519.2	84.1	6.6	0.9	0.7	0.2
LOCK2232	1278	84	749.2	56.2	5.1	0.8	1.1	0.3
LOCK3491	846	231	582.6	138.7	51.2	5.3	3.9	0.8
RAMAGE01	470	377	345.6	279.3	18.3	12.1	1.4	1.1
AEAC5081	163	170	125.7	98.1	12.4	7.7	1.5	1.1
TRDHEIM	288	360	184.2	174.4	51.8	50.2	5.9	5.7
CRPLAT2	1570	550	1183.6	378.6	1918.9	262.4	124.4	20.3
OPT1	2688	995	2070.9	610.9	857.2	552.4	57.2	37.0
TSYL201	1209	549	862.7	511.6	1528.4	554.2	97.1	38.8
RAMAGE02	1730	1457	1498.1	1295.0	3811.9	2852.3	231.5	175.7

Table 4.2: The results of using the MC43 ordering with MA62 (CRAY J932). The root mean-squared front size is denoted by "rms front size".

our symmetric positive-definite frontal solver, MA62 (default settings are used for all control parameters). We note that the original order is the one provided by the application which, in most instances, the originator of the problem believed to be a "good" element ordering. For some problems, reordering with MC43 gives a significant reduction in the maximum and rms front sizes and this is reflected in the reduced factorize times and operation counts. Having generated a new ordering, MC43 compares the maximum front size of the new ordering with that of the original ordering, and then returns to the user the ordering with the smallest maximum front size. However, it is possible that by doing this MC43 rejects the ordering with the smallest rms front size (which is generally the ordering that gives the smallest operation count and factorize time when used with the frontal solver). In all our experiments we have therefore made a minor alteration to MC43 so that the ordering with the smallest rms front size is selected, even if the maximum front size is increased. We see the effect of this on test problems AEAC5081 and TRDHEIM. We note that the effect of using Level 3 BLAS means that the poorer orderings have a higher Megaflop rate so that the ratio of times, before and after ordering, is not as

high as the operation count ratio. For the problem CEGB2919, the maximum and rms front sizes are reduced by using MC43 but the operation count and the factorize time are smaller for the original element ordering. This is because for this problem more zeros are exploited in the front for the original ordering than for the MC43 ordering. If zeros are not exploited (ICNTL(9) is set to 0), the element ordering generated by MC43 is more efficient than the original ordering (see Table 4.3 below).

4.3 The effect of exploiting zeros

We discussed, in Section 3.4, the option offered by MA62 of exploiting zeros within the front. Zeros are ignored if ICNTL(9) = 0 and are exploited if ICNTL(9) = 1. In Table 4.3, we show the effect of exploiting zeros. We have chosen some of the test problems which were initially not well ordered (see Table 4.2) and have run these problems with ICNTL(9) = 0 and 1, both with and without preordering using MC43. We see that, in general, if the elements are not well ordered, substantial savings are achieved in the factor storage, the number of operations, and the factorize time by exploiting zeros in the front. Once the elements have been ordered, the savings which result form exploiting zeros are much smaller. Indeed, if the savings in the factor storage and operation counts are very small, the overheads of searching for zeros and increased data movement to accumulate the zeros into blocks can increase the factorize time. On the DEC 7000, we found that for the problem TSYL201 the factorize time without exploiting zeros was 95 seconds but this increased to 101 seconds when zeros were exploited. However, in general, the factorize and solve times are reduced by taking advantage of zeros, so we have chosen the default setting to be ICNTL(9) = 1.

4.4 The effect of blocking parameters

In this section, we examine how the performance of the frontal code MA62 is affected by the parameters which control the minimum pivot block size and the size of the blocks used in updating the frontal matrix (ICNTL(5) and ICNTL(7), respectively). In Tables 4.4 to 4.7 results are given for a subset of our test problems for a range of values of ICNTL(7). In these tests we use minimum pivot block sizes of 1 (so that variables are eliminated as soon as they become fully summed) and 16. Zeros in the front are exploited (ICNTL(9) = 1). The timings quoted confirm that it is generally advantageous to exploit Level 3 BLAS, albeit at the cost of an increased operation count. As a result of our numerical experiments, we have chosen the default value for ICNTL(7) in MA62 to be 16.

In Tables 4.8 to 4.11 results are given for the test problems CEGB3306, AEAC5081, CRPLAT2, and OPT1 for a range of values of ICNTL(5) (ICNTL(7) = 16). It is apparent that modest increases in the minimum pivot block size have little effect on the size of the largest pivot block and on the maximum front size, and that the real storage requirement and the operation count grow slowly with ICNTL(5). The factor times indicate that, in general, modest savings can be achieved by allowing ICNTL(5) to be greater than 1 but the precise choice of the minimum pivot block size parameter does not appear crucial. This is important from a practical point of view since it is possible to get good performance without having to optimize

Identifier	Ordered	ICNTL(9)	Real Storage (Kwords)		Integer Storage (Kwords)	Number of ops ($*10^7$)	Factorize time (seconds)
CEGB3306	N	0	765	(661)	45	21.5	1.8
	N	1	218	(113)	14	3.1	0.6
	Y	0	207	(51)	14	1.7	0.4
	Y	1	204	(47)	14	1.7	0.4
CEGB2919	N	0	582	(99)	37	12.5	1.1
	N	1	403	(5)	17	8.3	0.9
	Y	0	467	(4)	24	10.2	1.0
	Y	1	446	(4)	20	10.2	1.0
LOCK1074	N	0	486	(324)	22	29.5	2.0
	N	1	219	(57)	10	6.6	0.7
	Y	0	86	(8)	5	0.9	0.2
	Y	1	85	(6)	5	0.9	0.2
LOCK2232	N	0	1418	(1282)	78	127.3	8.5
	N	1	206	(71)	13	5.1	1.1
	Y	0	122	(22)	8	0.9	0.3
	Y	1	114	(13)	8	0.8	0.3
LOCK3491	N	0	1804	(808)	100	118.4	8.1
	N	1	1062	(69)	59	51.3	3.9
	Y	0	456	(97)	27	7.3	0.9
	Y	1	380	(22)	23	5.3	0.8
CRPLAT2	N	0	20734	(3822)	1125	2545.9	163.3
	N	1	17053	(131)	940	1918.9	124.4
	Y	0	6556	(124)	37	267.4	20.4
	Y	1	6490	(59)	37	262.4	20.3
OPT1	N	0	29331	(19865)	1124	6357.8	384.8
	N	1	9628	(207)	355	857.2	57.2
	Y	0	8142	(214)	358	571.1	37.8
	Y	1	7984	(90)	341	552.4	37.0
TSYL201	N	0	16693	(248)	709	1546.3	97.9
	N	1	16521	(88)	701	1528.4	97.1
	Y	0	10416	(48)	485	554.2	38.6
	Y	1	10405	(48)	483	554.2	38.8

Table 4.3: The effect of exploiting zeros in the front (CRAY J932). If ICNTL(9) = 0, zeros are not exploited; if ICNTL(9) = 1, zeros are exploited. The figures in parentheses are the number of zeros (in thousands) which are held explicitly in the factors.

Identifier	ICNTL(7) (ICNTL(5) = 1)			
	1	8	16	32
CEGB3306	11.0	12.3	13.8	17.0
LOCK2232	4.3	4.9	5.8	7.7
LOCK3491	40.4	42.9	46.1	53.7
RAMAGE01	110.3	112.9	116.2	123.3
AEAC5801	60.9	64.7	69.5	80.4
TRDHEIM	458.7	473.1	491.5	532.2
CRPLAT2	2447.3	2492.2	2545.6	2658.0
	(ICNTL(5) = 16)			
CEGB3306	14.1	15.8	17.0	20.3
LOCK2232	6.4	7.1	8.0	10.3
LOCK3491	47.5	50.0	53.4	61.6
RAMAGE01	115.1	117.8	121.0	128.8
AEAC5801	68.7	72.5	77.3	88.3
TRDHEIM	46937	483.6	502.1	542.7
CRPLAT2	2525.8	2570.7	2624.2	2736.6

Table 4.4: The number of operations required to perform the numerical factorization for different values of the blocking parameter ICNTL(7). The operation counts are in millions of floating-point operations.

Identifier	ICNTL(7) (ICNTL(5) = 1)			
	1	8	16	32
CEGB3306	0.59	0.52	0.51	0.53
LOCK2232	0.43	0.39	0.37	0.40
LOCK3491	1.21	1.03	1.01	1.01
RAMAGE01	1.39	1.21	1.19	1.21
AEAC5801	1.71	1.48	1.40	1.44
TRDHEIM	6.32	5.72	5.72	5.83
CRPLAT2	33.31	27.84	27.34	27.60
	(ICNTL(5) = 16)			
CEGB3306	0.49	0.48	0.45	0.48
LOCK2232	0.38	0.35	0.34	0.36
LOCK3491	0.93	0.85	0.84	0.88
RAMAGE01	1.21	1.08	1.08	1.09
AEAC5801	1.30	1.17	1.20	1.23
TRDHEIM	6.72	6.01	6.07	6.17
CRPLAT2	24.01	21.12	20.91	21.14

Table 4.5: The time in seconds for the numerical factorization for different values of the blocking parameter ICNTL(7) (CRAY J932).

Identifier	ICNTL(7) (ICNTL(5) = 1)			
	1	8	16	32
CEGB3306	0.41	0.33	0.30	0.27
LOCK2232	0.20	0.16	0.16	0.13
LOCK3491	1.17	0.88	0.93	0.94
RAMAGE01	1.78	1.82	1.79	1.79
AEAC5801	1.69	1.30	1.30	1.39
TRDHEIM	7.12	7.35	6.82	7.02
CRPLAT2	40.67	40.55	38.90	37.68

Table 4.6: The time in seconds for the numerical factorization for different values of the blocking parameter ICNTL(7) (IBM RS/6000).

Identifier	ICNTL(7) (ICNTL(5) = 1)			
	1	8	16	32
CEGB3306	0.84	0.82	0.78	0.80
LOCK2232	0.46	0.43	0.44	0.46
LOCK3491	1.89	1.79	1.77	1.80
RAMAGE01	3.07	2.65	2.47	2.50
AEAC5801	2.78	2.59	2.51	2.60
TRDHEIM	16.32	14.07	13.40	13.71
CRPLAT2	77.19	64.83	60.32	62.13

Table 4.7: The time in seconds for the numerical factorization for different values of the blocking parameter ICNTL(7) (DEC 7000).

Identifier	ICNTL(5)	Largest pivot block	Maximum front size	Factor flops ($*10^6$)	Storage (Kwords) Real	Integer
CEGB3306	1	6	78	14	179	33
	8	12	84	15	191	19
	16	18	90	17	204	14
	32	36	108	22	236	8
	40	42	114	24	246	8
AEAC5081	1	10	156	69	530	90
	8	17	161	71	537	48
	16	25	170	77	562	33
	32	41	185	88	600	20
	40	49	195	95	626	18
CRPLAT2	1	24	544	2546	6383	1050
	8	24	544	2583	6435	540
	16	24	550	2624	6491	370
	32	42	568	2751	6655	195
	40	50	574	2795	6708	170
OPT1	1	38	983	5470	7971	503
	8	38	983	5473	7974	490
	16	39	995	5524	8019	353
	32	67	1009	5657	8137	226
	40	67	1009	5729	8195	193

Table 4.8: Storage statistics and operation counts for different values of the minimum pivot block size (ICNTL(5)).

the parameter from run to run. In general, the solve times are reduced by using ICNTL(5) > 1. This is because, by increasing ICNTL(5), the integer data written to and read from the buffers is reduced and, as a result, the amount of data which must be copied from the partial solution matrix into the arrays used for direct addressing is reduced. Since the amount of data copied is related to the number of right-hand sides, the time saved increases with the number nrhs of right-hand sides. On the basis of our numerical experiments on the different machines, in MA62 the default value for ICNTL(5) is 16. However, we note that if the user is going to perform a large number of solves, it may be beneficial to choose a value of ICNTL(5) larger than this default. However, since using ICNTL(5) > 1 reduces the repetition of the storage of the variable indices, increasing ICNTL(5) can give substantial savings in the integer storage used.

Identifier	ICNTL(5)	Factor Time (seconds)	Solve Time (seconds) nrhs=1	nrhs=2	nrhs=10
CEGB3306	1	0.5	0.07	0.10	0.28
	8	0.5	0.04	0.06	0.18
	16	0.4	0.03	0.05	0.14
	32	0.5	0.03	0.04	0.12
	40	0.6	0.03	0.04	0.12
AEAC5081	1	1.4	0.13	0.18	0.55
	8	1.1	0.09	0.12	0.37
	16	1.1	0.07	0.10	0.31
	32	1.3	0.06	0.08	0.27
	40	1.3	0.06	0.08	0.26
CRPLAT2	1	27.3	1.06	1.39	4.66
	8	22.9	0.76	0.98	3.20
	16	20.5	0.62	0.84	2.60
	32	21.1	0.56	0.72	2.24
	40	20.3	0.55	0.71	2.18
OPT1	1	39.2	0.81	1.02	3.27
	8	38.9	0.79	1.02	3.25
	16	37.0	0.70	0.91	2.80
	32	36.5	0.66	0.85	2.58
	40	36.4	0.63	0.82	2.55

Table 4.9: Factor and solve times for different minimum pivot block sizes on the CRAY J932. nrhs denotes the number of right-hand sides.

Identifier	ICNTL(5)	Factor Time (seconds)	Solve Time (seconds) nrhs=1	nrhs=2	nrhs=10
CEGB3306	1	0.3	0.02	0.08	0.25
	8	0.3	0.01	0.06	0.16
	16	0.3	0.03	0.03	0.17
	32	0.4	0.03	0.03	0.18
	40	0.4	0.06	0.06	0.18
AEAC5081	1	1.3	0.10	0.13	0.49
	8	1.2	0.09	0.13	0.41
	16	1.2	0.08	0.11	0.33
	32	1.4	0.09	0.10	0.38
	40	2.0	0.07	0.11	0.36
CRPLAT2	1	38.9	1.13	1.54	7.94
	8	42.1	1.12	1.62	6.09
	16	32.2	0.95	1.46	4.60
	32	32.2	0.92	1.33	4.04
	40	32.2	0.87	1.44	3.82
OPT1	1	81.2	1.12	1.93	6.11
	8	81.4	1.17	1.80	5.89
	16	75.7	1.23	1.82	5.16
	32	75.6	0.94	1.74	4.65
	40	75.1	1.08	1.51	4.64

Table 4.10: Factor and solve times for different minimum pivot block sizes on the IBM RS/6000. nrhs denotes the number of right-hand sides.

Identifier	ICNTL(5)	Factor Time (seconds)	Solve Time (seconds) nrhs=1	nrhs=2	nrhs=10
CEGB3306	1	0.7	0.36	0.40	0.60
	8	0.7	0.31	0.34	0.49
	16	0.8	0.34	0.38	0.50
	32	0.9	0.38	0.40	0.52
	40	0.9	0.38	0.40	0.52
AEAC5081	1	2.5	1.01	1.14	1.64
	8	2.3	0.88	0.99	1.34
	16	2.3	0.91	1.01	1.31
	32	2.4	0.94	1.03	1.31
	40	2.7	0.99	1.07	1.35
CRPLAT2	1	60.3	14.7	16.4	20.7
	8	51.5	13.6	14.9	17.5
	16	50.1	13.2	14.0	16.9
	32	50.0	12.8	14.9	16.6
	40	51.4	13.2	14.3	16.6
OPT1	1	97.6	16.4	18.6	21.5
	8	97.0	16.3	17.8	21.3
	16	94.6	15.9	17.7	20.7
	32	90.5	15.9	17.4	20.3
	40	90.2	16.4	17.4	20.1

Table 4.11: Factor and solve times for different minimum pivot block sizes on the DEC 7000. nrhs denotes the number of right-hand sides.

4.5 The performance of MA62 compared with MA42

Our aim in designing and developing MA62 was to produce a code that would be much more efficient than the general unsymmetric frontal solver MA42 when used to solve symmetric positive finite-element systems. To assess how successful we have been, in Table 4.12 we compare the storage requirements and the operation counts

Identifier	Code	Factor Storage (Kwords) Real		Integer	Factor ops ($*10^6$)
CEGB3306	MA42	375		68	22.6
	MA62	204	(231)	14	17.2
CEGB2919	MA42	1012		72	181.1
	MA62	445	(477)	20	101.9
CEGB3024	MA42	477		110	38.2
	MA62	236	(261)	15	26.3
LOCK1074	MA42	159		27	12.7
	MA62	85	(94)	5	8.9
LOCK2232	MA42	219		40	10.8
	MA62	114	(133)	8	8.9
LOCK3491	MA42	882		151	119.5
	MA62	380	(411)	23	73.1
RAMAGE01	MA42	759		68	219.6
	MA62	388	(406)	17	121.0
AEAC5801	MA42	1065		183	120.4
	MA62	562	(610)	32	77.3
TRDHEIM	MA42	6663		533	866.5
	MA62	2154	(2318)	110	502.1
CRPLAT2	MA42	12915		2116	4980.1
	MA62	6490	(6644)	370	2674.6
OPT1	MA42	16674		1194	11047.1
	MA62	7984	(8165)	341	5710.9
TSYL201	MA42	20905		1020	10723.5
	MA62	10405	(10630)	483	5542.2
RAMAGE02	MA42	41792		3495	55870.1
	MA62	20996	(21204)	851	28523.2

Table 4.12: A comparison of the operation count and storage requirements for MA42 and MA62 on symmetric positive-definite unassembled finite-element systems. The numbers in parentheses are the real storage needed if packed form for $\mathbf{F}_{TL}$ is not used.

for the two codes. For MA62, we give the real storage requirements for storing the lower triangular matrix $\mathbf{F}_{TL}$ in packed form and as a full matrix in which only the lower triangular entries are meaningful (see Section 3.3). In Tables 4.13, 4.14, and 4.15 we compare the timings for MA62 with those for MA42 on the CRAY J932, the IBM RS/6000, and the DEC 7000, respectively. The timings quoted for MA42 were obtained using the option of restricting pivoting to the diagonal. Without this option, the code checks more entries when searching for pivots but in our experiments, it had no significant effect on the factorization time. MA62 was run with the default settings for all the control parameters. Throughout the remainder

of this paper, the 'Analyse' times quoted for both MA42 and MA62 include the time to order the elements using MC43, to perform the prepass of the integer data and to perform the symbolic factorization. The analyse times for both codes are essentially the same since both codes work only with the integer data.

Identifier	Code	Time (seconds)			
		Analyse	Factorize	Solve	
				nrhs = 1	nrhs = 10
CEGB3306	MA42	0.2	0.7	0.07	0.28
	MA62	0.2	0.4	0.03	0.14
CEGB2919	MA42	0.1	1.7	0.07	0.26
	MA62	0.1	1.0	0.05	0.21
CEGB3024	MA42	0.2	0.8	0.09	0.36
	MA62	0.2	0.5	0.04	0.17
LOCK1074	MA42	0.1	0.3	0.02	0.10
	MA62	0.1	0.2	0.01	0.05
LOCK2232	MA42	0.3	0.5	0.05	0.18
	MA62	0.3	0.3	0.02	0.09
LOCK3491	MA42	0.2	1.6	0.11	0.43
	MA62	0.2	0.8	0.05	0.20
RAMAGE01	MA42	0.1	1.8	0.05	0.20
	MA62	0.1	1.0	0.04	0.14
AEAC5801	MA42	0.3	1.9	0.14	0.59
	MA62	0.3	1.1	0.07	0.30
TRDHEIM	MA42	0.6	8.8	0.49	2.00
	MA62	0.6	5.7	0.33	1.42
CRPLAT2	MA42	1.2	45.3	1.13	4.78
	MA62	1.2	20.3	0.62	2.60
OPT1	MA42	0.8	76.0	0.91	3.65
	MA62	0.8	37.0	0.70	2.80
TSYL201	MA42	0.7	71.8	1.00	3.88
	MA62	0.7	38.8	0.90	3.60
RAMAGE02	MA42	1.4	389.6	2.29	9.32
	MA62	1.4	175.7	1.66	6.58

Table 4.13: A comparison of MA42 and MA62 on symmetric positive-definite unassembled finite-element systems (CRAY J932)

For the factorization phase, we see from these tables that MA62 is always significantly faster than MA42 and, for the larger problems, MA62 can be more than twice as fast as MA42. The solve times for MA62 are almost always less than for MA42, particularly for a large number of right-hand sides. This reduction is a result of using a minimum pivot block size of 16 in MA62 (ICNTL(5) = 16) and also of exploiting zeros in the front. If we set ICNTL(5) = 1 and ICNTL(9) = 0 (zeros not exploited), the solve times for the two codes are similar. We remark that the HSL Release 12 version of MA42 does not have an option for specifying the minimum pivot block size, although a version of MA42 used by AEA Technology in their code NAMMU for groundwater flow calculations (Hartley, Jackson and Watson, 1996) does include this option. The current version of MA42 does not take advantage of zeros in the front but recent experiments (Scott, 1997) have shown that the performance of MA42,

particularly in terms of the factor storage and operation count, can be enhanced by exploiting zeros. For example, for the problem LOCK3491, by exploiting the zeros, the real factor storage is cut from 882 to 751 Kwords; the integer storage is reduced from 151 to 123 Kwords; and the operation count is cut from $120*10^6$ to $79*10^6$.

Identifier	Code	Time (seconds)			
		Analyse	Factorize	Solve	
				nrhs = 1	nrhs = 10
CEGB3306	MA42	0.03	0.4	0.05	0.25
	MA62	0.04	0.3	0.03	0.17
CEGB2919	MA42	0.03	2.2	0.11	0.37
	MA62	0.01	1.6	0.04	0.23
CEGB3024	MA42	0.04	0.6	0.07	0.28
	MA62	0.03	0.4	0.01	0.17
LOCK1074	MA42	0.03	0.2	0.01	0.08
	MA62	0.02	0.1	0.01	0.05
LOCK2232	MA42	0.07	0.3	0.03	0.16
	MA62	0.05	0.2	0.02	0.08
LOCK3491	MA42	0.04	1.7	0.06	0.39
	MA62	0.05	1.0	0.04	0.23
RAMAGE01	MA42	0.02	2.6	0.07	0.28
	MA62	0.02	1.7	0.04	0.21
AEAC5801	MA42	0.07	1.8	0.11	0.53
	MA62	0.06	1.2	0.08	0.38
TRDHEIM	MA42	0.11	10.8	0.54	2.8
	MA62	0.12	7.4	0.32	1.7
CRPLAT2	MA42	0.26	58.3	1.5	8.4
	MA62	0.24	33.0	1.0	4.6
OPT1	MA42	0.18	113.6	1.4	7.4
	MA62	0.18	77.2	1.2	5.1
TSYL201	MA42	0.14	107.4	1.6	8.2
	MA62	0.16	68.5	1.6	7.6
RAMAGE02	MA42	0.28	508.4	3.8	19.7
	MA62	0.28	347.3	2.7	12.9

Table 4.14: A comparison of MA42 and MA62 on symmetric positive-definite unassembled finite-element systems (IBM RS/6000)

We also observe that the solution phase of the frontal solvers is much slower on the DEC 7000 than on the other machines. Further investigation shows that, on this machine, the overheads for out-of-core working are considerable and reading the factors from the direct access files accounts for most of the solve time. If direct access files are not used, the MA62 solve time for a single right-hand side for TRDHEIM is cut from 5.3 to 0.6 seconds. For TSYL201, the corresponding times are 22.5 and 2.4 seconds, respectively. On the DEC, the use of direct access files also has a significant effect on the factor time. If we hold the factors in-core, then the MA62 factor time for TRDHEIM reduces from 13.4 to 9.0 seconds and for TSYL201 it is cut from 101 to 70 seconds. Similarly, without the use of direct access files, the MA42 factorization time for TRDHEIM reduces from 26 to 14 seconds and for TSYL201 it is cut from 173 to 116 seconds.

Identifier	Code	Time (seconds)			
		Analyse	Factorize	Solve	
				nrhs = 1	nrhs = 10
CEGB3306	MA42	0.04	1.0	0.4	0.6
	MA62	0.04	0.7	0.3	0.5
CEGB2919	MA42	0.02	4.2	0.9	1.2
	MA62	0.02	2.4	0.7	1.0
CEGB3024	MA42	0.04	1.6	0.5	0.9
	MA62	0.04	1.0	0.4	0.6
LOCK1074	MA42	0.02	0.6	0.2	0.3
	MA62	0.02	0.4	0.1	0.2
LOCK2232	MA42	0.05	0.8	0.2	0.4
	MA62	0.05	0.5	0.2	0.3
LOCK3491	MA42	0.05	3.5	0.9	1.4
	MA62	0.05	1.6	0.6	0.9
RAMAGE01	MA42	0.02	4.1	0.7	1.0
	MA62	0.02	2.4	0.6	0.8
AEAC5801	MA42	0.06	4.0	1.0	1.7
	MA62	0.06	2.2	0.9	1.3
TRDHEIM	MA42	0.10	26.2	7.0	9.4
	MA62	0.11	13.4	5.3	6.8
CRPLAT2	MA42	0.25	105.3	15.3	22.4
	MA62	0.26	50.1	13.2	16.9
OPT1	MA42	0.15	176.4	18.6	24.7
	MA62	0.15	94.6	15.9	21.7
TSYL201	MA42	0.12	173.4	23.1	30.0
	MA62	0.12	101.8	22.5	27.3
RAMAGE02	MA42	0.28	863.4	49.2	65.6
	MA62	0.28	435.6	46.1	57.8

Table 4.15: A comparison of MA42 and MA62 on symmetric positive-definite unassembled finite-element systems (DEC 7000)

4.6 A comparison of the frontal code MA62 with other HSL codes

In this section, we compare the performance of the frontal code MA62 with other codes in the Harwell Subroutine Library that are also designed for solving symmetric positive-definite systems, namely the multifrontal code MA27 and the code VBAN, which is a development version of a new HSL code MA55.

The code MA27 uses the multifrontal algorithm of Duff and Reid (1982). In the analyse phase, pivots are selected from the diagonal using the minimum degree criterion. During the factorization, this pivot sequence may be modified to maintain numerical stability, and 2×2 diagonal block pivots can also be used. By this means, MA27 can stably factorize symmetric indefinite problems. However, if the matrix is known to be positive definite, the user can set a parameter in the calling sequence so that a logically simpler path in the code is followed. In all our tests using MA27, this option was used.

Our colleague John Reid at the Rutherford Appleton Laboratory is currently developing a variable-band code for the solution of systems of equations whose matrix is symmetric and positive-definite. It does no interchanges and takes advantage of variation in bandwidth. The code optionally uses a direct access file to store the matrix factor. The intention is that the new code MA55 will replace an older HSL code MA36. At present, the development code is written in Fortran 90 and it only uses Level 1 BLAS. A Fortran 77 version of MA55 will be made available in the future. It is intended that the MA55 code will use blocking and Level 3 BLAS. We have called the development code used in our experiments VBAN in the tables and in the following text.

The codes are compared on the CRAY J932, the IBM RS/6000, and the DEC 7000 in Tables 4.16 to 4.18. We were unable to run VBAN and MA27 on the largest problems on the IBM RS/6000 because of insufficient memory. The elemental matrices are assembled before MA27 and VBAN are called. The cost of this preprocessing is not included. Since the efficiency of VBAN depends upon the equations being ordered for a small profile, the assembled matrix is ordered using the HSL profile reducing code MC40 prior to calling VBAN, and the time taken to do this is given as the "Analyse" time for VBAN. For MA27, the "Analyse" time is that taken to select the pivot sequence using the minimum degree criterion and prepare the data structures for the subsequent numerical factorization. It is interesting that this more complicated MA27 analyse is usually faster than the reordering for VBAN. This highlighted for us some deficiencies in the MC40 ordering code which we are now attempting to rectify. Similar deficiencies are also present in the MC43 code but are masked because the direct element reordering algorithm works with the connectivity pattern of elements rather than variables.

Note that the "In-core" storage figures quoted in Table 4.16 are the minimum in-core storage requirements for performing the matrix factorization and solving the linear system $\mathbf{Ax} = \mathbf{b}$. This figure includes both real and integer storage. On the CRAY, both integers and reals are stored in 64-bit words, so the storage statistics given in Table 4.16 are just the sum of the number of real and the number of integer words needed. We remark that if this minimum in-core storage is used, the performance of the codes will often be considerably degraded since either a large

Identifier	Code	Time (seconds)			Factor ops ($*10^6$)	Storage (Kwords)	
		Analyse	Factorize	Solve		In-core	Factors
CEGB3306	MA27	0.4	0.6	0.03	2.1	114	81
	VBAN	0.5	1.2	0.05	11.6	133	187
	MA62	0.2	0.5	0.03	17.0	8	218
CEGB2919	MA27	1.9	3.6	0.04	57.3	590	384
	VBAN	2.6	4.0	0.08	110.6	402	526
	MA62	0.1	1.0	0.05	101.9	94	465
CEGB3024	MA27	0.6	1.0	0.04	7.1	175	146
	VBAN	0.8	1.3	0.05	17.7	106	219
	MA62	0.2	0.5	0.04	26.3	21	252
LOCK1074	MA27	0.3	0.5	0.01	4.9	109	71
	VBAN	0.4	0.5	0.02	6.0	29	77
	MA62	0.1	0.2	0.01	8.7	19	90
LOCK2232	MA27	0.4	0.6	0.02	2.7	133	83
	VBAN	0.5	0.6	0.03	4.6	11	99
	MA62	0.3	0.3	0.02	8.0	7	122
LOCK3491	MA27	0.9	2.0	0.04	20.2	336	254
	VBAN	1.3	3.0	0.07	65.4	322	428
	MA62	0.2	0.8	0.05	53.3	53	403
RAMAGE01	MA27	1.3	4.0	0.03	94.0	549	345
	VBAN	2.6	3.3	0.05	122.7	243	401
	MA62	0.1	1.0	0.04	121.0	142	405
AEAC5081	MA27	1.3	3.1	0.08	44.4	526	430
	VBAN	1.5	3.7	0.10	69.8	95	564
	MA62	0.3	1.1	0.07	77.3	29	594
TRDHEIM	MA27	10.8	17.7	0.27	211.0	2893	2002
	VBAN	15.3	19.6	0.46	459.0	798	2958
	MA62	0.6	5.6	0.33	502.1	130	2262
CRPLAT2	MA27	5.3	40.2	0.30	1623.8	4554	3815
	VBAN	9.4	54.9	0.77	2475.8	2276	6406
	MA62	1.2	20.3	0.62	2624.2	302	6527
OPT1	MA27	11.9	77.1	0.32	3648.9	7741	5975
	VBAN	20.7	74.2	0.86	4116.5	3315	7215
	MA62	0.8	37.0	0.70	5523.8	990	8325
TSYL201	MA27	13.6	90.0	0.40	4285.0	8922	7069
	VBAN	22.3	96.4	1.18	5262.0	2079	10231
	MA62	0.7	38.8	0.90	5542.2	301	10888
RAMAGE02	MA27	20.4	783.0	1.05	44988.9	30569	21297
	VBAN	39.1	338.3	2.16	29922.7	3692	21787
	MA62	1.4	175.6	1.66	28523.2	2123	21847

Table 4.16: A comparison of MA27, VBAN and MA62 on symmetric positive-definite finite-element systems (CRAY J932).

Identifier	Code	Time (seconds)		
		Analyse	Factorize	Solve
CEGB3306	MA27	0.09	0.15	0.01
	VBAN	0.14	1.60	1.28
	MA62	0.04	0.33	0.06
CEGB2919	MA27	0.31	2.54	0.05
	VBAN	0.49	6.14	2.97
	MA62	0.01	1.56	0.04
CEGB3024	MA27	0.11	0.30	0.02
	VBAN	0.17	1.80	1.23
	MA62	0.03	0.42	0.01
LOCK1074	MA27	0.04	0.16	0.01
	VBAN	0.07	0.75	0.54
	MA62	0.02	0.12	0.01
LOCK2232	MA27	0.08	0.18	0.02
	VBAN	0.11	0.73	0.58
	MA62	0.05	0.23	0.02
LOCK3491	MA27	0.16	0.82	0.04
	VBAN	0.30	4.32	2.50
	MA62	0.05	0.99	0.04
RAMAGE01	MA27	0.18	3.95	0.04
	VBAN	0.43	5.55	2.42
	MA62	0.02	1.68	0.04
AEAC5081	MA27	0.24	1.80	0.07
	VBAN	0.38	5.33	3.17
	MA62	0.06	1.35	0.08
TRDHEIM	MA27	2.02	10.83	0.28
	MA62	0.12	7.41	0.32
CRPLAT2	MA27	1.15	65.4	0.49
	MA62	0.24	33.0	1.06
OPT1	MA27	2.37	146.3	0.76
	MA62	0.18	77.2	1.19
TSYL201	MA27	2.27	169.3	0.89
	MA62	0.16	68.5	1.63
RAMAGE02	MA62	0.25	347.3	2.67

Table 4.17: A comparison of MA27, VBAN and MA62 on symmetric positive-definite finite-element systems (IBM RS/6000).

Identifier	Code	Time (seconds)		
		Analyse	Factorize	Solve
CEGB3306	MA27	0.07	0.14	0.01
	VBAN	0.10	0.64	0.11
	MA62	0.04	0.78	0.35
CEGB2919	MA27	0.30	1.99	0.05
	VBAN	0.36	4.05	0.31
	MA62	0.02	2.40	0.75
CEGB3024	MA27	0.09	0.30	0.02
	VBAN	0.13	0.85	0.16
	MA62	0.04	0.98	0.40
LOCK1074	MA27	0.04	0.19	0.01
	VBAN	0.05	0.29	0.06
	MA62	0.02	0.41	0.15
LOCK2232	MA27	0.06	0.16	0.01
	VBAN	0.08	0.27	0.06
	MA62	0.05	0.48	0.19
LOCK3491	MA27	0.15	0.78	0.03
	VBAN	0.22	2.50	0.26
	MA62	0.05	1.60	0.62
RAMAGE01	MA27	0.18	3.11	0.05
	VBAN	0.31	4.15	0.23
	MA62	0.02	2.41	0.65
AEAC5081	MA27	0.21	1.51	0.06
	VBAN	0.27	2.81	0.34
	MA62	0.06	2.28	0.92
TRDHEIM	MA27	1.98	9.3	0.43
	VBAN	2.40	18.8	2.06
	MA62	0.11	13.4	5.31
CRPLAT2	MA27	1.03	49.1	0.91
	VBAN	2.12	129.1	4.56
	MA62	0.26	52.1	13.2
OPT1	MA27	2.15	140.0	1.49
	VBAN	3.64	212.8	5.44
	MA62	0.15	93.7	15.9
TSYL201	MA27	2.43	167.9	1.78
	VBAN	4.62	212.7	7.24
	MA62	0.12	100.8	22.5
RAMAGE02	MA27	3.56	2970.0	5.81
	VBAN	8.58	2008.4	17.6
	MA62	0.28	435.7	46.1

Table 4.18: A comparison of MA27, VBAN and MA62 on symmetric positive-definite finite-element systems (DEC 7000).

number of data compressions must be performed or a large number of records written to direct access files. The length (in real words) of the in-core files used by both MA62 and VBAN was 25000.

Our experiments show that, with the exception of some of the smaller problems on the DEC 7000, MA62 requires less time for the factorization than VBAN although it needs more floating-point operations. In most cases, we see that the minimum degree ordering as expected performs a much better job of reducing the number of entries in the factors than our "band" orderings; sometimes the factor storage for MA27 is about half that of the better of the other two codes. In general, the number of entries in the factors is slightly less for VBAN than for MA62. Both VBAN and MA62 store their factors in direct access files and so, as expected, usually require much less "In-core" storage than MA27. However, VBAN sometimes requires a lot more in-core storage than MA62. This will happen if there is just a single row of high bandwidth towards the end of the reordered matrix. For the simple variable-band scheme used by VBAN, this would require that many previous rows needed to update this be held in memory. The frontal code does not suffer from this problem; the only effect is to add one to the front size for most of the computation. One possible remedy is to develop better orderings for the variable-band scheme and this is currently being studied.

We again observe that on the DEC 7000 the overheads for out-of-core working are high. Since MA27 does not have these overheads, on this machine if the factors are held in direct access files, for some of the test problems (particularly the smaller problems) MA27 has the fastest factorize time and for all the problems it has the fastest solve time for a single right-hand side. We remark that MA27 is designed for assembled problems; we are not aware of any software which implements a multifrontal algorithm for symmetric problems and which accepts matrices in elemental form.

5 Conclusions

We have designed and developed a frontal code for solving systems of symmetric positive-definite unassembled finite-element equations. The code optionally uses direct access files to hold the matrix factors and makes full use of Level 3 BLAS in its innermost loop and in the solution phase. We have shown that, as well as needing approximately half the real storage for the matrix factors as the general frontal code MA42, the code can be more than twice as fast as MA42. Compared with other HSL codes, we have seen that the frontal method can provide a very powerful approach for the solution of large sparse systems. We notice that, although other approaches may result in much less fill-in, if the factors are held in direct access files, the frontal code generally requires far less main memory. The performance of the factorization and solution phases of the frontal codes is significantly affected by the efficiency of the i/o. If the i/o does not add a large overhead, the frontal scheme is generally faster than other the approaches considered, although this conclusion may have to be modified when multifrontal and variable band codes for positive definite systems that exploit the Level 3 BLAS become available.

6 Availability of the code

MA62 is written in standard Fortran 77. The code will be included in Release 13 of the Harwell Subroutine Library. MA27 and MA42, as well as the ordering routines MC40 and MC43, are available in Release 12 of the HSL. Anybody interested in using any of these codes should contact the HSL Manager: Scott Roberts, AEA Technology, Building 552 Harwell, Didcot, Oxfordshire OX11 0RA, England, tel. +44 (0) 1235 434988, fax +44 (0) 1235 434136, email Scott.Roberts@aeat.co.uk, who will provide licencing information.

7 Acknowledgements

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References

K. A. Cliffe, I. S. Duff, and J. A. Scott. Performance issues for frontal schemes on a cache-based high performance computer. Technical Report RAL-TR-97-001, Rutherford Appleton Laboratory, 1997.

J. J. Dongarra, J. DuCroz, I. S. Duff, and S. Hammarling. A set of Level 3 Basic Linear Algebra Subprograms. *ACM Trans. Mathematical Software*, **16**(1), 1–17, 1990.

I. S. Duff. MA32 - a package for solving sparse unsymmetric systems using the frontal method. Report AERE R10079, Her Majesty's Stationery Office, London, 1981.

I. S. Duff. Enhancements to the MA32 package for solving sparse unsymmetric equations. Report AERE R11009, Her Majesty's Stationery Office, London, 1983.

I. S. Duff. Design features of a frontal code for solving sparse unsymmetric linear systems out-of-core. *SIAM J. Scientific and Statistical Computing*, **5**, 270–280, 1984.

I. S. Duff and J. K. Reid. MA27 – A set of Fortran subroutines for solving sparse symmetric sets of linear equations. Report AERE R10533, Her Majesty's Stationery Office, London, 1982.

I. S. Duff and J. A. Scott. MA42 – a new frontal code for solving sparse unsymmetric systems. Technical Report RAL-TR-93-064, Rutherford Appleton Laboratory, 1993.

I. S. Duff and J. A. Scott. The design of a new frontal code for solving sparse unsymmetric systems. *ACM Trans. Mathematical Software*, **22**(1), 30–45, 1996.

I. S. Duff, R. G. Grimes, and J. G. Lewis. Users' guide for the Harwell-Boeing sparse matrix collection (Release I). Technical Report RAL-TR-92-086, Rutherford Appleton Laboratory, 1992.

I. S. Duff, J. K. Reid, and J. A. Scott. The use of profile reduction algorithms with a frontal code. *Inter. Journal on Numerical Methods in Engineering*, **28**, 2555–2568, 1989.

L.J. Hartley, C.P. Jackson, and S.P. Watson. NAMMU (Release 6.3) User Guide. Technical Report AEA-ES-0138, AEA Technology, 1996.

Harwell Subroutine Library. *A Catalogue of Subroutines (Release 12).* Advanced Computing Department, AEA Technology, Harwell Laboratory, Oxfordshire, England, 1996.

P. Hood. Frontal solution program for unsymmetric matrices. *Inter. Journal on Numerical Methods in Engineering*, **10**, 379–400, 1976.

B. M. Irons. A frontal solution program for finite-element analysis. *Inter. Journal on Numerical Methods in Engineering*, **2**, 5–32, 1970.

A. Ramage and A. J. Wathen. Iterative solution techniques for the Navier-Stokes equations. Technical Report AM-93-01, School of Mathematics, University of Bristol, 1993.

J. A. Scott. Exploiting zeros in frontal solvers. Technical Report to appear, Rutherford Appleton Laboratory, 1997.

A Appendix: Specification Sheets

1 SUMMARY

To solve one or more sets of sparse symmetric linear unassembled finite-element equations, AX=B, by the frontal method, optionally holding the matrix factor out-of-core in direct access files. The package is primarily designed for positive-definite matrices since numerical pivoting is not performed. Use is made of high-level BLAS kernels. The coefficient matrix **A** must of the form

$$\mathbf{A}=\sum_{k=1}^{m}\mathbf{A}^{(k)}, \tag{1}$$

with $\mathbf{A}^{(k)}$ nonzero only in those rows and columns that correspond to variables in the k-th element.

The frontal method is a variant of Gaussian elimination and involves the factorization

$$\mathbf{A}=\mathbf{PLD(PL)}^{\mathrm{T}},$$

where **P** is a permutation matrix, **D** is a diagonal matrix, and **L** is a unit lower triangular matrix. MA62 stores the reals of the factors and their indices separately. A principal feature of MA62 is that, by holding the factors out-of-core, large problems can be solved using a predetermined and relatively small amount of in-core memory. At an intermediate stage of the solution, l say, the 'front' contains those variables associated with one or more of $\mathbf{A}^{(k)}$, $k=1,2,...,l$, which are also present in one or more of $\mathbf{A}^{(k)}$, $k=l+1,...,m$. For efficiency, the user should order the $\mathbf{A}^{(k)}$ so that the number of variables in the front (the 'front size') is small. For example, a very rectangular grid should be ordered pagewise parallel to the short side of the rectangle. The elements may be preordered using the Harwell Subroutine Library routine MC43.

ATTRIBUTES — Versions: MA62A, MA62AD. **Calls:** _AXPY, _GER, _GEMV, _TPSV, _TRSV, _GEMM, _TRSM. **Language:** Fortran 77. **Date:** April 1997. **Origin:** I.S. Duff and J.A. Scott, Rutherford Appleton Laboratory. **Conditions on external use:** (i), (ii), (iii) and (iv).

2 HOW TO USE THE PACKAGE

2.1 Argument lists and calling sequences

There are six entries:

(a) The subroutine MA62I/ID must be called to initialize the parameters that control the execution of the package. This subroutine must be called once prior to calling other routines in the package.

(b) MA62A/AD must be called for each element to specify which variables are associated with it. This subroutine determines in which element each variable appears for the last time.

(c) MA62J/JD must be called for each element. This subroutine uses the information from MA62A/AD to determine the amount of real and integer storage required for the factorization.

(d) The use of MA62P/PD is optional. If direct access files are to be used, MA62P/PD must be called once prior to calling MA62B/BD and MA62C/CD.

(e) MA62B/BD must be called for each element to specify the nonzeros of $\mathbf{A}^{(k)}$ and, optionally, the corresponding element right-hand side(s) $\mathbf{B}^{(k)}$. MA62B/BD uses the information generated by MA62A/AD and MA62J/JD in the factorization of the matrix (1) and, if $\mathbf{B}^{(k)}$ are specified, MA62B/BD solves the equations $\mathbf{AX}=\mathbf{B}$ with right-hand side(s) $\mathbf{B}=\sum_{k=1}^{m}\mathbf{B}^{(k)}$.

(f) The use of MA62C/CD is optional. MA62C/CD uses the factors produced by MA62B/BD to solve for further right-hand sides.

2.1.1 The initialization subroutine

To initialize control parameters, the user must make a single call of the following form:

The single precision version

```
CALL MA62I(ICNTL,CNTL,ISAVE)
```

The double precision version

```
CALL MA62ID(ICNTL,CNTL,ISAVE)
```

ICNTL is an INTEGER array of length 15 that need not be set by the user. This array is used to hold control parameters. On exit, ICNTL contains default values. If the user wishes to use values other than the defaults, the corresponding entries in ICNTL should be reset after the call to MA62I/ID. Details of the control parameters are given in Section 2.2.1.

CNTL is a REAL (DOUBLE PRECISION in the D version) array of length 5 that need not be set by the user. This array is used to hold control parameters. On exit, CNTL contains default values. If the user wishes to use values other than the defaults, the corresponding entries in CNTL should be reset after the call to MA62I/ID. Details of the control parameters are given in Section 2.2.1.

ISAVE is an INTEGER array of length 50 that need not be set by the user. This array is used to hold parameters that must be unchanged between calls to routines in the MA62 package.

2.1.2 Specification of which variables belong in each element

A call of the following form must be made for each element.

The single precision version

```
CALL MA62A(NVAR,IVAR,NDF,LAST,LENLST,ICNTL,ISAVE,INFO)
```

The double precision version

```
CALL MA62AD(NVAR,IVAR,NDF,LAST,LENLST,ICNTL,ISAVE,INFO)
```

NVAR is an INTEGER variable that must be set by the user to the number of variables in the element. This argument is not changed by the routine. **Restriction:** NVAR $\geq$ 1.

IVAR is an INTEGER array of length NVAR that must be set by the user to contain the indices of the variables associated with the element. These indices need not be in increasing order but must be distinct. This argument is not changed by the routine. **Restrictions:** 1 $\leq$ IVAR(I) $\leq$ LENLST and IVAR(I) $\neq$ IVAR(J), I, J = 1, 2, ..., NVAR.

NDF is an INTEGER variable that need not be set by the user. On each exit, it will be set to the largest integer so far used to index a variable. It must not be changed by the user between calls to MA62A/AD nor prior to subsequent calls to MA62J/JD and MA62B/BD. Note that, if the variables are not indexed contiguously, NDF will exceed the number of variables in the problem (see INFO(3) in Section 2.2.2).

LAST is an INTEGER array of length LENLST that need not be set by the user. On each exit from MA62A/AD, LAST(I) indicates the element in which the variable with index I last appeared or, if it has not appeared, LAST(I) is zero. On exit from the final call, if I has been used to index a variable, LAST(I) is the element at which variable I is fully summed and is zero otherwise. The first NDF entries of this array must not be changed between calls to MA62A/AD nor prior to subsequent calls to MA62J/JD and MA62B/BD.

LENLST is an INTEGER variable that must be set by the user to the dimension of array LAST. LENLST must be at least as large as the largest integer used to index a variable and must not be changed between calls to MA62A/AD. This argument is not changed by the routine. **Restriction:** LENLST $\geq$ 1.

ICNTL is an INTEGER array of length 15 that must be set by the user to hold control parameters. Default values are set by the call to MA62I/ID. Details of the control parameters are given in Section 2.2.1. ICNTL(I), I = 1, 2, and 8, are accessed by the routine. This argument is not changed by the routine.

ISAVE is an INTEGER array of length 50 that is used to hold parameters that must be unchanged between calls to routines in the MA62 package. This argument is changed by the routine.

INFO is an INTEGER array of length 30 that need not be set by the user. On each successful exit, INFO(1) is set to 0. Negative values of INFO(1) indicate a fatal error has been detected (see Section 2.3). If an error is detected, INFO(2) holds additional information concerning the error. INFO(I), I $\geq$ 3, are not accessed by the routine.

2.1.3 Symbolic factorization of A

To determine the amount of real and integer storage required by the factorization, a call of the following form must be made for each element. The elements must have the same index lists and be in exactly the same order as when MA62A/AD was called. All the calls to MA62A/AD must be completed before MA62J/JD is called. Note that the storage is dependent on the control parameter ICNTL(5). If the user wishes to compute the storage required by different values of ICNTL(5), it is not necessary to recall MA62A/AD before repeating the sequence of calls to MA62J/JD.

The single precision version

```
CALL MA62J(NVAR,IVAR,NDF,LAST,ICNTL,ISAVE,INFO)
```

The double precision version

```
CALL MA62JD(NVAR,IVAR,NDF,LAST,ICNTL,ISAVE,INFO)
```

NVAR, IVAR are as in the corresponding calls to MA62A/AD but MA62J/JD does not check IVAR for duplicate indices. NVAR and IVAR are not changed by the routine.

NDF is an INTEGER variable which must be unchanged since the final call to MA62A/AD. This argument is not changed by the routine.

LAST is an INTEGER array of length NDF which must be unchanged since the final call to MA62A/AD. This argument is not changed by the routine.

ICNTL is an INTEGER array of length 15 that must be set by the user to hold control parameters. Default values are set by the call to MA62I/ID. Details of the control parameters are given in Section 2.2.1. ICNTL(I), I = 1, 2, 5, and 8, are accessed by the routine. This argument is not changed by the routine.

ISAVE is an INTEGER array of length 50 that is used to hold parameters that must be unchanged between calls to routines in the MA62 package. This argument is changed by the routine.

INFO is an INTEGER array of length 30 that need not be set by the user. On successful exit, INFO(1) is set to 0. Negative values of INFO(1) indicate a fatal error has been detected (see Section 2.3). If an error is detected, INFO(2) holds additional information concerning the error. On exit from the final call, INFO(I), I = 3, 4,..., 8, contain information about the factorization. Details are given in Section 2.2.2. INFO(I), I ≥ 9, are not accessed by the routine.

2.1.4 To set up direct access files

If the user wishes to keep in-core memory requirements low by using direct access files for the factors, a single call of the following form must be made.

The single precision version

```
CALL MA62P(ISTRM,FILNAM,LENBUF,ICNTL,ISAVE,INFO)
```

The double precision version

```
CALL MA62PD(ISTRM,FILNAM,LENBUF,ICNTL,ISAVE,INFO)
```

ISTRM is an INTEGER array of length 2. ISTRM(1) and ISTRM(2) must be set by the user to specify the unit numbers of the direct access files for the reals in the factors and the indices of the variables in the factors, respectively. This argument is not changed by the routine. **Restrictions:** ISTRM(I) must lie in the range [1,99], ISTRM(I) ≠ 6, ICNTL(1), or ICNTL(2) (I =1, 2), and ISTRM(1) ≠ ISTRM(2).

FILNAM is a CHARACTER*60 array of length 2. If ICNTL(6) is set to a value other than its default value 0, the user must set FILNAM(1) and FILNAM(2) to filenames for the direct access files for the reals in the factors and the indices of the variables in the factors, respectively. If ICNTL(6) = 0, FILNAM is not accessed by the routine. This argument is not changed by the routine.

LENBUF is an INTEGER array of length 2. LENBUF(1) must be set by the user to the length, in REAL (DOUBLE PRECISION in the D version) words, of the in-core buffer (workspace) associated with the direct access file for the reals in the factors (including the corresponding right-hand sides) and LENBUF(2) must be set by the user to the length, in INTEGER words, of the buffer associated with the direct access file for the indices of the variables in the factors. LENBUF(I) (I =1, 2) have a crucial effect on the in-core memory requirements of MA62B/BD and MA62C/CD (see arguments LW and LIW in Sections 2.1.5 and 2.1.6). If *nrhs* is the number of right-hand sides to be input to MA62B/BD, LENBUF should be chosen so that INFO(7) + *nrhs**NDF = k_1*LENBUF(1) and INFO(8) = k_2*LENBUF(2) with $k_1, k_2 \geq 1$ as small as available space permits (INFO(7) and INFO(8) as output from the final call MA62J/JD). LENBUF is not changed by the routine. **Restrictions:** LENBUF(I) > 0, I =1, 2.

ICNTL is an INTEGER array of length 15 that must be set by the user to hold control parameters. Default values are set by the call to MA62I/ID. Details of the control parameters are given in Section 2.2.1. ICNTL(I), I = 1, 2, 3, 4, 6, and 8, are accessed by the routine. This argument is not changed by the routine. **Restrictions:** ICNTL(3) > 0 and ICNTL(4) > 0.

ISAVE is an INTEGER array of length 50 that is used to hold parameters that must be unchanged between calls to routines in the MA62 package. This argument is changed by the routine.

INFO is an INTEGER array of length 30 that need not be set by the user. On successful exit, INFO(1) is set to 0. Negative values of INFO(1) indicate a fatal error has been detected (see Section 2.3). If an error is detected, INFO(2) holds additional information concerning the error. INFO(I), I ≥ 3, are not accessed by the routine.

2.1.5 To factorize A and optionally solve AX = B

A call of the following form must be made for each element. The elements must have the same index lists and be in exactly the same order as when MA62A/AD and MA62J/JD were called.

Note that all the calls to MA62J/JD for a particular problem must be completed before calling MA62B/BD.

The single precision version

```
      CALL MA62B(NVAR,IVAR,NDF,LAST,LAVAR,AVAR,NRHS,RHS,LX,X,
     *           LENBUF,LW,W,LIW,IW,ICNTL,CNTL,ISAVE,INFO,RINFO)
```

The double precision version

```
      CALL MA62BD(NVAR,IVAR,NDF,LAST,LAVAR,AVAR,NRHS,RHS,LX,X,
     *           LENBUF,LW,W,LIW,IW,ICNTL,CNTL,ISAVE,INFO,RINFO)
```

NVAR, IVAR, NDF, LAST are as in the corresponding calls to MA62J/JD. NVAR and NDF are not changed by the routine. On exit, the data in IVAR may have been permuted. Between calls to MA62B/BD, LAST is used as workspace and will be changed but on exit from the final call (or on an error return), LAST will have been restored to its original value.

LAVAR is an INTEGER variable that must be set by the user to the first dimension of the arrays AVAR and RHS. LAVAR must be unchanged between calls to MA62B/BD. This argument is not changed by the routine. **Restriction:** LAVAR ≥ NVAR.

AVAR is a REAL (DOUBLE PRECISION in the D version) array of dimensions LAVAR by NVAR. On entry, AVAR(I,J) must contain the contribution to entry (IVAR(I), IVAR(J)) in the matrix **A** from the current element (I, J = 1, 2,..., NVAR, J ≥ I). Contributions to the same entry from different elements are summed. This argument is changed by the routine.

NRHS is an INTEGER variable that must be set by the user to the number of right-hand sides and must not be changed between calls to MA62B/BD. If the user does not wish to solve for any right-hand sides, NRHS should be set to 0. This argument is not changed by the routine. **Restriction:** NRHS ≥ 0.

RHS is a REAL (DOUBLE PRECISION in the D version) array with leading dimension LAVAR. If NRHS = 0, this array is not accessed. Otherwise on entry, the first NRHS columns of RHS must be set by the user so that RHS(I,J) contains the contribution to component IVAR(I) of the J-th right-hand side from the current element (I = 1, 2,..., NVAR, J = 1, 2,..., NRHS). Contributions to the same component from different elements are summed. This argument is changed by the routine.

LX is an INTEGER variable that must be set by the user to the first dimension of the array X. This argument is not changed by the routine. **Restriction:** If NRHS ≥ 1, LX ≥ NDF.

X is a REAL (DOUBLE PRECISION in the D version) array with leading dimension LX that need not be set by the user. If NRHS = 0, this array is not accessed. Otherwise, the second dimension of X must be at least NRHS and, on successful exit from the final call to MA62B/BD, if I has been used to index a variable, X(I,J) holds the solution for variable I to system J and is set to zero otherwise (I=1,2,...,NDF, J=1,2,..., NRHS).

LENBUF is an INTEGER array of length 2. If the user is using direct access files, LENBUF must be unchanged since the call to MA62P/PD. Otherwise, LENBUF(1) must be set by the user to the length, in REAL (DOUBLE PRECISION in the D version) words, of the file for the reals in the factors (including the corresponding right-hand sides) and LENBUF(2) must be set by the user to the length, in INTEGER words, of the file for the indices of the variables in the factors. This array must not be changed between calls to MA62B/BD. This argument is not changed by the routine. **Restriction:** If direct access files are not being used, LENBUF(1) ≥ INFO(7) + NDF*NRHS, LENBUF(2) ≥ INFO(8) (INFO(7) and INFO(8) as output from the last call to MA62J/JD).

LW is an INTEGER variable that must be set by the user to the dimension of array W. It must be unchanged between calls to MA62B/BD. This argument is not changed by the routine. **Restriction:** LW≥ LENBUF(1) + INFO(6)*(NRHS + INFO(6)) + 3 (INFO(6) as output from the last call to MA62J/JD).

W is a REAL (DOUBLE PRECISION in the D version) array of length LW that is used as workspace by MA62B/BD. This array must be unchanged between calls to MA62B/BD. If direct access files are not being used (MA62P/PD not called), the first LENBUF(1) + 3 entries of W must be unchanged between the last call to MA62B/BD and any subsequent calls to MA62C/CD.

LIW is an INTEGER variable that must be set by the user to the dimension of array IW. It must not be changed between calls to MA62B/BD. This argument is not changed by the routine. **Restriction:** LIW≥ LENBUF(2) +3*INFO(6) (INFO(6) as output from the last call to MA62J/JD).

IW is an INTEGER array of length LIW that is used as workspace by MA62B/BD. This array must be unchanged between calls to MA62B/BD. If direct access files are not being used (MA62P/PD not called), the first LENBUF(2) entries of IW must be unchanged between the final call to MA62B/BD and any subsequent calls to MA62C/CD.

ICNTL is an INTEGER array of length 15 that must be set by the user to hold control parameters. Default values are set by the call to MA62I/ID. Details of the control parameters are given in Section 2.2.1. ICNTL(5) must be unchanged since calling MA62J/JD. ICNTL(I), I = 1, 2, 5, 7, 8, and 9 are accessed by the routine. This argument is not changed by the routine.

CNTL is a REAL (DOUBLE PRECISION in the D version) array of length 5 that must be set by the user to hold control parameters. Default values are set by the call to MA62I/ID. Details of the control parameters are given in Section 2.2.1. Only CNTL(1) is accessed by the routine. This argument is not changed by the routine.

ISAVE is an INTEGER array of length 50 that is used to hold parameters that must be unchanged between calls to routines in the MA62 package. This argument is changed by the routine.

INFO is an INTEGER array of length 20 that need not be set by the user. On successful exit, INFO(1) is set to 0. Negative values indicate a fatal error. For nonzero values of INFO(1), see Section 2.3. For details of the information contained in the other components of INFO, see Section 2.2.2.

RINFO is a REAL (DOUBLE PRECISION in the D version) array of length 10 that need not be set by the user. For details of the information contained in RINFO, see Section 2.2.2.

2.1.6 To solve further systems AX = B

The single precision version

```
CALL MA62C(NRHS,LX,B,X,LW,W,LIW,IW,ICNTL,ISAVE,INFO)
```

The double precision version

```
CALL MA62CD(NRHS,LX,B,X,LW,W,LIW,IW,ICNTL,ISAVE,INFO)
```

NRHS is an INTEGER variable that must be set by the user to the number of systems which are to be solved. This argument is not changed by the routine. **Restriction:** NRHS≥1.

LX is an INTEGER variable that must be set by the user to the first dimension of the arrays B and X. This argument is not changed by the routine. **Restriction:** LX≥NDF (NDF as output from the final call to MA62A/AD).

B is a REAL (DOUBLE PRECISION in the D version) array of dimensions LX by NRHS that must be set by the user so that if I has been used to index a variable, B(I,J) is the corresponding component of the right-hand side for the J-th system (J=1,2,..., NRHS). This argument is changed by the routine.

X is a REAL (DOUBLE PRECISION in the D version) array of dimension LX by NRHS that need not be set by the user. On exit, if I has been used to index a variable, X(I,J) holds the solution for variable I to system J and is set to zero otherwise (J=1,2,..., NRHS).

LW is an INTEGER variable that must be set by the user to the dimension of the array W. A sufficient value for LW is L1+L2, where L1 = LENBUF(1)+NRHS*INFO(6). If direct access files are not being used (MA62P/PD was not called), L2 = 3, otherwise, L2 = INFO(6)*INFO(6). This argument is not changed by the routine. **Restriction:** LW≥L1+L2.

W is a REAL (DOUBLE PRECISION in the D version) array of length LW. If direct access files are not being used (MA62P/PD was not called), the first LENBUF(1) + 3 entries of W must be unchanged since the last call to MA62B/BD and these entries are unchanged by MA62C/CD. Otherwise, W is used by MA62C/CD as workspace.

LIW is an INTEGER variable that must be set by the user to the dimension of the array IW. If direct access files are not

being used (MA62P/PD was not called), LIW must be at least L1 = LENBUF(2). Otherwise, LIW must be at least L1 = LENBUF(2) + INFO(6) + 4. This argument is not changed by the routine. **Restriction:** LIW≥L1.

IW is an INTEGER array of length LIW. If direct access files are not being used (MA62P/PD was not called), the first LENBUF(2) entries of IW must be unchanged since the last call to MA62B/BD and these entries are unchanged by MA62C/CD. Otherwise, IW is used by MA62C/CD as workspace.

ICNTL is an INTEGER array of length 15 that must be set by the user to hold control parameters. Default values are set by the call to MA62I/ID. Details of the control parameters are given in Section 2.2.1. ICNTL(I), I = 1, 2, and 8, are accessed by the routine. This argument is not changed by the routine.

ISAVE is an INTEGER array of length 50 that is used to hold parameters that must be unchanged between calls to routines in the MA62 package. This argument is changed by the routine.

INFO is an INTEGER array of length 30 that need not be set by the user. On successful exit, INFO(1) is set to 0. Negative values of INFO(1) indicate a fatal error has been detected (see Section 2.3). If an error is detected, INFO(2) holds additional information concerning the error. INFO(I), I≥3, are not accessed by the routine.

2.2 Arrays for control and information

2.2.1 Control parameters

The elements of the arrays ICNTL and CNTL control the action of MA62A/AD, MA62J/JD, MA62P/PD, MA62B/BD, and MA62C/CD. Default values are set by MA62I/ID.

ICNTL(1) is the stream number for error messages and has the default value 6. Printing of error messages is suppressed if ICNTL(1) < 0.

ICNTL(2) is the stream number for warning messages and diagnostic printing. It has the default value 6. Printing of such messages is suppressed if ICNTL(2) < 0.

ICNTL(3) is the number of bytes for a real word. ICNTL(3) has the default value 4 (8 for the D version).

ICNTL(4) is the number of bytes for an integer word. ICNTL(4) has the default value 4.

ICNTL(5) has the default value 16. ICNTL(5) controls the minimum number of variables which are eliminated at any one stage (except the last stage, when fewer than ICNTL(5) variables may remain). ICNTL(5) is only accessed on the first call to MA62J/JD and the first call to MA62B/BD. The value of ICNTL(5) on the first call to MA62B/BD should be the same as on the first call to MA62J/JD. Increasing ICNTL(5) in general increases the number of floating-point operations and real storage requirements but allows greater advantage to be taken of Level 3 BLAS.

ICNTL(6) has the default value 0. If it is set to a value other than 0, the user must supply names for the direct access data sets in the parameter FILNAM when calling MA62P/PD.

ICNTL(7) is the block size for the numerical factorization of the frontal matrix. It controls the trade-off between Level 2 and Level 3 BLAS. If ICNTL(7) = 1, Level 2 BLAS is used to form the Schur complement. If ICNTL(7) ≥ 1, the Level 3 BLAS routine _GEMM is used with internal dimension ICNTL(7). Increasing ICNTL(7) increases the number of flops since symmetry is not exploited as well. The optimal value for ICNTL(7) depends on the computer being used. A value of ICNTL(7) less than one is treated as one and, if at some stage of the factorization, ICNTL(7) has a value which is larger than the current front size, ICNTL(7) is treated as the front size. Typical range: 16 to 64. Default value: 16.

ICNTL(8) is used to control the printing of error, warning, and diagnostic messages in MA62. It has default value 2. Possible values are:

- 0 No messages are output.
- 1 Only error messages are output.
- 2 Error and warning messages output.
- 3 As for 2, plus scalar parameters, arrays of length 2, and the control parameters on the first entry to MA62A/AD, MA62J/JD, MA62P/PD, and MA62B/BD, and scalar parameters on entry to MA62C/CD.
- 4 As for 3, plus INFO(I, (I = 1, 2,..., 8) on exit from final call to MA62J/JD, and the arrays INFO and RINFO on on exit from final call to MA62B/BD.

ICNTL(9) controls whether or not zeros within the frontal matrix are exploited. If ICNTL(9) = 0, the frontal matrix is treated as a dense matrix and zeros within the front are ignored. If ICNTL(9) = 1, the code will look for zeros

occurring within the frontal matrix and will try to avoid unnecessary operations using zeros. This option can increase the amount of data movement but can also give worthwhile savings in the computation and in the number of entries in the factors if some variables are involved in only a few elements and these elements are well separated in the element order. The default value is 1.

ICNTL(10) to ICNTL(15) are currently not used but may be used in a later release of the code.

CNTL(1) has the default value zero. If, during the factorization, the absolute value of any pivot is less than or equal to CNTL(1), the computation terminates and the matrix is declared to be not positive definite (see INFO(1) = −12).

CNTL(2) to CNTL(5) are currently not used but may be used in a later release of the code.

2.2.2 Information arrays

The entries of the arrays INFO and RINFO provide information on the action of MA62A/AD, MA62J/JD, MA62P/PD, MA62B/BD, and MA62C/CD.

INFO(1) is used as an error flag. If a call to a routine in the MA62 package is successful, on exit INFO(1) has value 0. A negative value of INFO(1) indicates an error has been detected and a value greater than zero indicates a warning has been issued (see Section 2.3). If an error is detected during a call to MA62J/JD, the information contained in INFO(I), $3 \leq I \leq 8$ will be incomplete. Likewise, if an error is detected during a call to MA62B/BD, the information contained in INFO(I), $I \geq 9$ and in RINFO will be incomplete.

INFO(2) holds additional information concerning the error (see Section 2.3).

INFO(3) holds, on successful exit from the final call to MA62J/JD, the total number of variables in the problem.

INFO(4) holds, on successful exit from the final call to MA62J/JD, the number of static condensation variables (a static condensation variable is one which appears in only one element).

INFO(5) holds, on successful exit from the final call to MA62J/JD, the largest number of variables eliminated at a single stage (that is, the maximum order of a pivot block).

INFO(6) holds, on successful exit from the final call to MA62J/JD, the maximum front size.

INFO(7) holds, on successful exit from the final call to MA62J/JD, the length in REAL (DOUBLE PRECISION in the D version) words of the file required by the numerical factorization for the reals in the factors (no allowance is made for right-hand sides).

INFO(8) holds, on successful exit from the final call to MA62J/JD, the length in INTEGER words of the file required by the numerical factorization for the indices of the variables in the factors.

INFO(9) holds, on successful exit from the final call to MA62B/BD, the number of negative pivots.

INFO(10) holds, on successful exit from the final call to MA62B/BD, the number of buffers used for the reals in the factors.

INFO(11) holds, on successful exit from the final call to MA62B/BD, the number of buffers used for the indices of the variables in the factors.

INFO(12) holds, on successful exit from the final call to MA62B/BD, the maximum number of buffers required to hold the reals in a block of pivot rows.

INFO(13) holds, on successful exit from the final call to MA62B/BD, the maximum number of buffers required to hold the indices of the variables in a block of pivot rows.

INFO(14) holds, on successful exit from the final call to MA62B/BD, the length in REAL (DOUBLE PRECISION in the D version) words of the file actually used during the factorization for the reals in the factors and the corresponding right-hand sides. If NRHS = 0 and ICNTL(9) = 0, INFO(14) = INFO(7).

INFO(15) holds, on successful exit from the final call to MA62B/BD, the number of entries in the factors that have value zero. If there a large number of zeros in the factors and zeros in the front have not been exploited (ICNTL(9) = 0), the user should either set ICNTL(9) = 1 or reorder the elements.

INFO(16) holds, on successful exit from the final call to MA62B/BD, the number of entries (including zero entries) stored in the factors. If zeros in the front are not exploited (ICNTL(9) = 0), INFO(16) = INFO(7).

INFO(17) holds, on successful exit from the final call to MA62B/BD, the number of integers actually used during the factorization to store the factors. If zeros in the front are not exploited (ICNTL(9) = 0), INFO(17) = INFO(8).

INFO(18) to INFO(30) are currently not used but may be used in a later release of the code.

RINFO(1) holds, on successful exit from the final call to MA62B/BD, the natural logarithm of the modulus of the determinant of the matrix **A**.

RINFO(2) holds, on successful exit from the final call to MA62B/BD, the number of floating-point operations to perform the factorization. This count includes operations performed during static condensation.

RINFO(3) holds, on successful exit from the final call to MA62B/BD, the root-mean-squared front size.

RINFO(4) to RINFO(10) are currently not used but may be used in a later release of the code.

2.3 Error diagnostics

On successful completion, the subroutines in the MA62 package will exit with the parameter INFO(1) set to 0. Other values for INFO(1) and the reasons for them are given below.

A negative value for INFO(1) is associated with a fatal error. If ICNTL(8) > 0 and ICNTL(1) > 0, a self-explanatory message is, in each case, output on unit ICNTL(1) (see Section 2.2.1). The negative values for INFO(1) are:

–1 LENLST ≤ 0 on entry to MA62A/AD. (MA62A/AD first entry only).

–2 NVAR ≤ 0 in the current element. (MA62A/AD, MA62J/JD, and MA62B/BD entries). This error is also returned if NVAR is greater than LAVAR (MA62B/BD entries only).

–3 A index of a variable in the current element is out of range. INFO(2) holds the index which is out of range. (MA62A/AD, MA62J/JD, and MA62B/BD entries).

–4 Duplicate occurrences of the same variable index found in the current element. INFO(2) holds the duplicated index. (MA62A/AD entries only).

–5 NRHS ≥ 1 and the defined first dimension LX of the array X (and the array B) is less than NDF as output from the final call to MA62A/AD. INFO(2) holds the value of NDF output from MA62A/AD. (MA62B/BD first entry only and MA62C/CD entry).

–6 Defined length LW of the real workspace array W violates the restrictions on LW. LW must be increased to at least INFO(2). (MA62B/BD first entry only and MA62C/CD entry).

–7 Defined length LIW of the integer workspace array IW violates the restrictions on LIW. LIW must be increased to at least INFO(2). (MA62B/BD first entry only and MA62C/CD entry).

–8 MA62J/JD has been called without MA62A/AD having been called. (MA62J/JD first entry only).

–9 The number of right-hand sides NRHS is out of range. Either NRHS < 0 (MA62B/BD first entry only) or NRHS < 1 (MA62C/CD entry). This error is also returned if the user has changed the number of right-hand sides between calls to MA62B/BD. If this error is returned by MA62B/BD, INFO(2) holds the value of NRHS on the first call to MA62B/BD.

–10 The order of the elements or one or more of the elements themselves has been changed since the calls to MA62J/JD. (MA62B/BD entries only).

–11 A variable appears again after it has been fully summed (this happens if an index list for an element has been changed since MA62A/AD was called, or the order of the elements has been changed, or more elements have been entered than were entered to MA62A/AD). INFO(2) holds the index of the fully summed variable. (MA62J/JD and MA62B/BD entries).

–12 Attempt to use pivot of absolute value less than or equal to CNTL(1). INFO(2) holds the call on which this error was encountered. (MA62B/BD entries only).

–13 The value of NDF has been changed since the final call to MA62A/AD. INFO(2) holds the value of NDF output from MA62A/AD. (MA62J/JD and MA62B/BD first entries only).

–14 The number of calls made to MA62J/JD was different from the number of calls made to MA62A/AD. This error is also returned if MA62B/BD is called without MA62J/JD being called. INFO(2) holds the number of calls made to MA62J/JD. (MA62B/BD first entry only).

–15 LENBUF(1) or LENBUF(2) violates the restrictions on it.
LENBUF(I) ≤ 0, I = 1 or 2. (MA62P/PD entry only), or
LENBUF(1) < INFO(7) + NDF*NRHS, or LENBUF(2) < INFO(8), (MA62B/BD first entry only, direct access files not in use), or
LENBUF(I), I = 1 or 2, has been changed between the call to MA62P/PD and the first call to MA62B/BD.

–16 ISTRM(1)=ISTRM(2) or ISTRM(I), I = 1 or 2, lies out of range, or is equal to 6, ICNTL(1), or ICNTL(2). (MA62P/PD entry only).

–17 Error encountered in Fortran OPEN statement. INFO(2) holds the IOSTAT parameter (the IOSTAT parameter is a parameter which, after an input/output operation is completed, is set to zero if no error was detected and to a positive integer otherwise). (MA62P/PD entry only).

–18 ICNTL(I) ≤ 0 for I = 3 or 4. (MA62P/PD entry only).

–19 Error detected when reading a direct access file. INFO(2) holds the IOSTAT parameter. (MA62B/BD and MA62C/CD entries).

–20 Error detected when writing to a direct access file. INFO(2) holds the IOSTAT parameter (MA62B/BD entries only).

Warning messages are associated with a positive value for INFO(1). If ICNTL(8) > 1 and ICNTL(2) > 0, a self-explanatory message is, in each case, output on unit ICNTL(2) (see Section 2.2.1). The warnings are:

+1 On entry to MA62J/JD, ICNTL(5) is less than or equal to zero. The default value 16 is used. (MA62J/JD first entry only).

+2 On entry to MA62B/BD, ICNTL(5) is not equal to the value used by MA62J/JD. The value used by MA62J/JD is used. (MA62B/BD first entry only).

+3 On entry to MA62B/BD or MA62C/CD, ICNTL(1) (or ICNTL(2)) has a value equal to ISTRM(1) or ISTRM(2). The default value 6 is used. (MA62B/BD first entry only and MA62C/CD entry). This warning can only be issued if MA62P/PD has been called.

3 GENERAL INFORMATION

Use of common: None.

Other routines called directly: The BLAS routines SAXPY/DAXPY, SGER/DGER, SGEMV/DGEMV, STPSV/DTPSV, STRSV/DTRSV, SGEMM/DGEMM, STRSM/DTRSM. Subroutines internal to the package are MA62D/DD, MA62E/ED, MA62F/FD, MA62G/GD, MA62H/HD, MA62L/LD, MA62M/MD, MA62N/ND, MA62O/OD.

Workspace: Workspace is provided by the arrays:
W(LW) (MA62B/BD and MA62C/CD).
IW(LIW) (MA62B/BD, and MA62C/CD).
LAST(NDF) is used locally as workspace (MA62B/BD only).
ISAVE(50) is a work array that must be unchanged between calls to routines in the MA62 package.

Input/output: In the event of errors, diagnostic messages are printed. The output streams for these messages are controlled by the variables ICNTL(1) and ICNTL(2), and the level of printing is controlled by ICNTL(8) (see Section 2.2.1). Stream ICNTL(1) is used for error messages (INFO(1) < 0) and stream ICNTL(2) for warnings (INFO(1) > 0) and diagnostic printing.

Restrictions:

MA62A/AD:

NVAR ≥ 1.

LENLST ≥ 1.

1 ≤ IVAR(I) ≤ LENLST and IVAR(I) ≠ IVAR(J), I, J, = 1, 2, ..., NVAR.

MA62J/JD:

NVAR ≥ 1.

1 ≤ IVAR(I) ≤ NDF, I = 1, 2, ..., NVAR.

MA62P/PD:

ISTRM(1) and ISTRM(2) lie in the range [1, 99] and do not equal 6, ICNTL(1), or ICNTL(2).

ISTRM(1) ≠ ISTRM(2).

ICNTL(I) > 0, I = 3, 4.

LENBUF(I) > 0, I = 1, 2.

MA62B/BD:

NVAR ≥ 1.

1 ≤ IVAR(I) ≤ NDF, I = 1, 2, ..., NVAR.

LAVAR ≥ NVAR.

NRHS ≥ 0.

If NRHS ≥ 1, LX ≥ NDF.

If MA62P/PD is not called, LENBUF(1) ≥ INFO(7)+NDF*NRHS, LENBUF(2) ≥ INFO(8).

LW ≥ LENBUF(1) + INFO(6)*(INFO(6) + NRHS) + 3

LIW ≥ LENBUF(2) + 3*INFO(6).

MA62C/CD:

NRHS ≥ 1.

LX ≥ NDF.

If MA62P/PD is not called,
LW ≥ LENBUF(1) + INFO(6)*NRHS + 3
LIW ≥ LENBUF(2) + INFO(6) + 4
otherwise,
LW ≥ LENBUF(1) + INFO(6)*(INFO(6) + NRHS).
LIW ≥ LENBUF(2).

4 METHOD

The method used is a modification of the unsymmetric frontal code of Duff and Scott (1993, 1996).

The elements are assembled into an in-core frontal matrix one at a time. A variable which has appeared for the last time (i.e. does not occur in future elements) is fully summed and is used as a pivot in Gaussian elimination, provided it is of absolute value at least CNTL(1) and there are at least ICNTL(5) fully summed variables. Once all possible eliminations for the current element have been performed, the pivot columns are written to in-core buffers and later, if requested, to direct access files. To prevent the amount of in-core memory required becoming too large, the user should order the elements so that the same variable does not occur in elements that are widely apart in the ordering. Thus, for example, in a problem with a narrow pipe geometry, the elements should be ordered across the cross-section of the pipe rather than along its length. An efficient element ordering can be obtained using the Harwell Subroutine Library routine MC43.

References.

Duff, I.S. and Scott, J.A. (1993). MA42 – A new frontal code for solving sparse unsymmetric systems. Report RAL-93-064, Rutherford Appleton Laboratory.

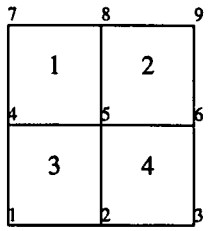
Duff, I.S. and Scott, J.A. (1996). The design of a new frontal code for solving sparse unsymmetric systems. *ACM Trans. Math. Softw.*, **22**, 30-45.

Duff, I.S. and Scott, J.A. (1997). MA62 – A frontal code for sparse positive-definite symmetric systems. Technical Report RAL-TR-97-012, Rutherford Appleton Laboratory.

5 EXAMPLE OF USE

We give an example of the code required to solve a set of symmetric finite-element equations using the MA62 package. The example illustrates the full calling sequence for the MA62 package. In this example, we wish to solve $\mathbf{AX}=\mathbf{B}$. We supply one right-hand side with the elements and then use MA62C/CD to solve for a further two right-hand sides. Direct access files are used to hold the factors.

We wish to solve the following simple finite-element problem in which the finite-element mesh comprises four 4-noded quadrilateral elements with one degree of freedom at each node i, $1 \le i \le 6$ (the nodes 7, 8, and 9 are assumed constrained).



The four element matrices $\mathbf{A}^{(k)}$ $(1 \le k \le 4)$ are

$$\begin{array}{c} 4 \\ 5 \end{array}\begin{pmatrix} 2. & 1. \\ 1. & 7. \end{pmatrix} \qquad \begin{array}{c} 5 \\ 6 \end{array}\begin{pmatrix} 3. & 2. \\ 2. & 8. \end{pmatrix} \qquad \begin{array}{c} 4 \\ 5 \\ 1 \\ 2 \end{array}\begin{pmatrix} 4. & 3. & 2. & 3. \\ 3. & 1. & 3. & 2. \\ 2. & 3. & 6. & 1. \\ 3. & 2. & 1. & 5. \end{pmatrix} \qquad \begin{array}{c} 5 \\ 6 \\ 2 \\ 3 \end{array}\begin{pmatrix} 2. & 1. & 8. & 3. \\ 1. & 3. & 2. & 2. \\ 8. & 2. & 2. & 5. \\ 3. & 2. & 5. & 4. \end{pmatrix},$$

where the variable indices are indicated by the integers before each matrix (columns are identified symmetrically to rows). The corresponding element vectors $\mathbf{b}^{(k)}$ $(1 \le k \le 4)$ are

$$\begin{pmatrix} 3. \\ 8. \end{pmatrix} \qquad \begin{pmatrix} 5. \\ 10. \end{pmatrix} \qquad \begin{pmatrix} 12. \\ 9. \\ 12. \\ 11. \end{pmatrix} \qquad \begin{pmatrix} 14. \\ 8. \\ 17. \\ 14. \end{pmatrix}.$$

The following program is used to solve this problem. In this program, we read the element data into arrays ELTPTR (location of first entry of element), ELTVAR (variable indices), VALUE (numerical values), and RHSVAL (right-hand sides). This method of storing the element data is used here for illustrative purposes; the user may prefer, for example, to read in the element data from a direct access file.

```
C Example to illustrate the use of MA62.
C
C     .. Parameters ..
      INTEGER MAXE,LIWMAX,LRHS,NZMAX,MELT,LENLST,LWMAX,MAXVL,MAXRVL,
     +        NFMAX,NDFMAX
      PARAMETER (MAXE=4,LIWMAX=120,LRHS=2,NZMAX=30,MELT=4,LENLST=6,
     +          LWMAX=120,MAXVL=30,MAXRVL=15,NFMAX=6,NDFMAX=9)
C     ..
C     .. Local Scalars ..
      INTEGER I,IELT,J,JSTRT,K,KSTRT,LIW,LW,LX,NDF,NELT,NFRONT,LAVAR,
     +        NRHS,NVAR,NZ,RHSCRD,VALCRD
C     ..
C     .. Local Arrays ..
      DOUBLE PRECISION AVAR(MAXE,MAXE),B(NDFMAX,LRHS),CNTL(5),
     +                 RHS(MAXE,LRHS),RHSVAL(MAXRVL),RINFO(10),
     +                 VALUE(MAXVL),W(LWMAX),X(NDFMAX,LRHS)
      INTEGER ELTPTR(MELT+1),ELTVAR(NZMAX),ICNTL(15),
     +        INFO(20),ISAVE(50),ISTRM(2),IVAR(MAXE),IW(LIWMAX),
     +        LAST(LENLST),LENBUF(2)
      CHARACTER FILNAM(2)*60
C     ..
C     .. External Subroutines ..
      EXTERNAL MA62AD,MA62BD,MA62CD,MA62ID,MA62JD,MA62PD
C     ..
C
C*** Call to MA62ID
      CALL MA62ID(ICNTL,CNTL,ISAVE)

C Read in the element data.
C NELT is number of elements.
C ELTVAR contains lists of the variables belonging to the finite
C elements, with those for element 1 preceding those for element
C 2, and so on. ELTPTR points to the position in ELTVAR
C of the first variable in element I. NZ is the total number
C of entries in the element lists.

      READ (5,FMT=*) NELT
      READ (5,FMT=*) (ELTPTR(I),I=1,NELT+1)
      NZ = ELTPTR(NELT+1) - 1
      READ (5,FMT=*) (ELTVAR(I),I=1,NZ)
```

```
C Calls to MA62AD to establish when each variable is fully assembled
      DO 20 IELT = 1,NELT
         NVAR = ELTPTR(IELT+1) - ELTPTR(IELT)
         JSTRT = ELTPTR(IELT)
         DO 10 J = 1,NVAR
            IVAR(J) = ELTVAR(JSTRT+J-1)
   10    CONTINUE
C*** Call to MA62AD
         CALL MA62AD(NVAR,IVAR,NDF,LAST,LENLST,ICNTL,ISAVE,INFO)
         IF (INFO(1).LT.0) GO TO 100
   20 CONTINUE

C Calls to MA62JD to determine file sizes
      DO 40 IELT = 1,NELT
         NVAR = ELTPTR(IELT+1) - ELTPTR(IELT)
         JSTRT = ELTPTR(IELT)
         DO 30 J = 1,NVAR
            IVAR(J) = ELTVAR(JSTRT+J-1)
   30    CONTINUE
C*** Call to MA62JD
         CALL MA62JD(NVAR,IVAR,NDF,LAST,ICNTL,ISAVE,INFO)
         IF (INFO(1).LT.0) GO TO 100
   40 CONTINUE

C Call to MA62PD to open direct access data sets.
C Choose stream numbers and file sizes.
      ISTRM(1) = 8
      ISTRM(2) = 9
      LENBUF(1) = 30
      LENBUF(2) = 30
C*** Call to MA62PD
      CALL MA62PD(ISTRM,FILNAM,LENBUF,ICNTL,ISAVE,INFO)
      IF (INFO(1).LT.0) GO TO 100

C VALCRD is the number of numerical values to be input.
C VALUE contains lists of the numerical values in the element
C matrices, with element 1 preceding element 2, and so on.
C Since the element matrices are symmetric only the upper
C triangular part is stored.

      READ (5,FMT=*) VALCRD
      READ (5,FMT=*) (VALUE(I),I=1,VALCRD)
C
C RHSCRD is the number of right-hand side numerical values to
C be input.
C RHSVAL contains lists of the right-hand side numerical values
C corresponding to each of the elements in order.
C
      READ (5,FMT=*) RHSCRD
      READ (5,FMT=*) (RHSVAL(I),I=1,RHSCRD)
C
C Prepare to call MA62BD.
      LAVAR = MAXE
      NRHS = 1
      LX = NDFMAX
      NFRONT = INFO(6)
      LW = 3 + LENBUF(1) + NFRONT* (NFRONT+NRHS)
      LIW = LENBUF(2) + 3*NFRONT
      IF (LW.GT.LWMAX .OR. LIW.GT.LIWMAX) GO TO 110
C
      KSTRT = 1
      DO 70 IELT = 1,NELT
         NVAR = ELTPTR(IELT+1) - ELTPTR(IELT)
         JSTRT = ELTPTR(IELT)
         DO 60 J = 1,NVAR
            IVAR(J) = ELTVAR(JSTRT+J-1)
            DO 50 K = J,NVAR
               AVAR(J,K) = VALUE(KSTRT)
               KSTRT = KSTRT + 1
   50       CONTINUE
            RHS(J,1) = RHSVAL(JSTRT+J-1)
```

```
   60    CONTINUE
C*** Call to MA62BD
         CALL MA62BD(NVAR,IVAR,NDF,LAST,LAVAR,AVAR,NRHS,RHS,LX,X,
     +               LENBUF,LW,W,LIW,IW,ICNTL,CNTL,ISAVE,INFO,RINFO)
         IF (INFO(1).LT.0) GO TO 100
   70 CONTINUE
C
C  Solution is in first NDF locations of X
      WRITE (6,FMT=9000)
      WRITE (6,FMT=9010) (X(I,1),I=1,NDF)
      WRITE (6,FMT=9040) (INFO(I),I=1,14)

C Now read in further right-hand sides
C
      NRHS = 2
      DO 80 J = 1,2
         READ (5,FMT=*) (B(I,J),I=1,NDF)
   80 CONTINUE
      LW = LENBUF(1) + NFRONT* (NFRONT+NRHS)
      LIW = LENBUF(2) + NFRONT + 4
      IF (LW.GT.LWMAX .OR. LIW.GT.LIWMAX) GO TO 100
C*** Call to MA62CD
      CALL MA62CD(NRHS,NDFMAX,B,X,LW,W,LIW,IW,ICNTL,ISAVE,INFO)
      IF (INFO(1).LT.0) GO TO 100
C
C  Solution for J-th right-hand side is in X(.,J), J=1,NRHS
      DO 90 J = 1,NRHS
         WRITE (6,FMT=9060) J
         WRITE (6,FMT=9010) (X(I,J),I=1,NDF)
   90 CONTINUE
      GO TO 110
C Print appropriate fatal error diagnostic
  100 WRITE (6,FMT=9020)
      WRITE (6,FMT=9030) INFO(1)
  110 STOP
C
 9000 FORMAT (/3X,'The MA62BD solution is:')
 9010 FORMAT (/6G12.4)
 9020 FORMAT (/3X,'Error return')
 9030 FORMAT (3X,'INFO(1) = ',I3)
 9040 FORMAT (/' INFO    = ',/14I5)
 9060 FORMAT (/3X,'The solution for rhs number',I2,' is:')
      END
```

The input data used for this problem is:

```
 4
 1   3   5   9  13
 4   5   5   6   4   5   1   2   5   6   2   3
26
 2.  1.  7.  3.  2.  8.  4.  3.  2.  3.  1.  3.
 2.  6.  1.  5.  2.  1.  8.  3.  3.  2.  2.  2.
 5.  4.
12
 3.  8.  5. 10. 12.  9. 12. 11. 14.  8. 17. 14.
-6. -4.  0.  3. -2.  8.
31. 104. 49. 52. 131. 91.
```

This produces the following output:

```
 The MA62BD solution is:

 1.000       1.000       1.000       1.000       1.000       1.000

INFO    =
  0    0    6    2    3    5   19   33   25    1    2    1    2    1

 The solution for rhs number 1 is:

-1.000       1.000      -1.000       1.000      -1.000       1.000

 The solution for rhs number 2 is:

 1.000       2.000       3.000       4.000       5.000       6.000
```