PACKAGE SPECIFICATION

HSL

1 SUMMARY

This set of subroutines compute the solution to an extended system of n+m real linear equations in n+m unknowns,

$$\begin{pmatrix} \mathbf{A} & \mathbf{B} \\ \mathbf{C} & \mathbf{D} \end{pmatrix} \begin{pmatrix} \mathbf{x}_1 \\ \mathbf{x}_2 \end{pmatrix} = \begin{pmatrix} \mathbf{b}_1 \\ \mathbf{b}_2 \end{pmatrix},\tag{1}$$

in the case where the n by n matrix A is nonsingular and solutions to the systems

$$\mathbf{A}\mathbf{x} = \mathbf{b}$$
 and $\mathbf{A}^T \mathbf{y} = \mathbf{c}$

may be obtained from an external source, such as an existing factorization. The subroutine uses reverse communication to obtain the solution to such smaller systems. The method makes use of the Schur complement matrix

$$S = D - C A^{-1}B.$$

The Schur complement is stored and factorized as a dense matrix and the subroutine is thus only appropriate if there is sufficient storage for this matrix. Special advantage is taken of symmetry and definiteness in the coefficient matrices. Provision is made for introducing additional rows and columns to, and removing existing rows and columns from, the extended matrix.

ATTRIBUTES — **Version:** 1.0.0. (12 July 2004) **Types:** Real (single, double). **Original date:** March, 2001. **Origin:** N.I.M. Gould, Rutherford Appleton Laboratory. **Remark:** This is a thread-safe version of MA39 and supersedes it.

2 HOW TO USE THE PACKAGE

2.1 Calling sequence

To solve the extended system, the user must first make a call to MA69A/AD to form and factorize the Schur complement matrix S and then call MA69B/BD to compute the solution to the extended system. The solution of additional extended systems, with the same coefficient matrix but different right-hand sides, may be found by further calls to MA69B/BD.

The solution of further-extended systems of the form

$$\begin{pmatrix} \mathbf{A} & \mathbf{B} & \mathbf{c}_1 \\ \mathbf{C} & \mathbf{D} & \mathbf{c}_2 \\ \mathbf{r}_1^T & \mathbf{r}_2^T & d \end{pmatrix} \begin{pmatrix} \mathbf{x}_1 \\ \mathbf{x}_2 \\ x_{n+m+1} \end{pmatrix} = \begin{pmatrix} \mathbf{b}_1 \\ \mathbf{b}_2 \\ b_{n+m+1} \end{pmatrix}$$

may be found by firstly calling MA69C/CD to update the existing factorization of S (obtained from MA69A/AD) to give that of the Schur complement of A in the further-extended coefficient matrix and then by calling MA69B/BD. Likewise, the solution of extended systems of the form

$$\begin{pmatrix} \mathbf{A} & \bar{\mathbf{B}} \\ \bar{\mathbf{C}} & \bar{\mathbf{D}} \end{pmatrix} \begin{pmatrix} \mathbf{x}_1 \\ \mathbf{x}_2 \end{pmatrix} = \begin{pmatrix} \mathbf{b}_1 \\ \mathbf{b}_2 \end{pmatrix},$$

in which a row and column are removed from the coefficient matrix of (1), may be found by firstly calling MA69D/DD to update the existing factorization of S (obtained from MA69A/AD) to give that of the Schur complement of A in the new extended coefficient matrix and then once again by calling MA69B/BD.

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2.2 The factorization stage

Call MA69A/AD to factorize the Schur complement matrix.

The single precision version

```
CALL MA69A ( N, M, ICLASS, LBD, BD, IRNBD, IPBD, LCD, CD, JCNCD,

* IPCD, R, LR, Q, LQ, W, VECTOR, ISAVE, INFORM )
```

The double precision version

```
CALL MA69AD( N, M, ICLASS, LBD, BD, IRNBD, IPBD, LCD, CD, JCNCD, IPCD, R, LR, Q, LQ, W, VECTOR, ISAVE, INFORM )
```

- N is an INTEGER variable set by the user to the dimension of the matrix A. It is unchanged by the subroutine. **Restriction:** $N \ge 0$.
- M is an INTEGER variable set by the user to the dimension of the matrix \mathbf{D} . It is unchanged by the subroutine. **Restriction:** $M \ge 0$.

ICLASS is an INTEGER variable set by the user to indicate the type of matrix used. The permitted values are:

- 1 the extended matrix is unsymmetric,
- 2 the extended matrix is symmetric,
- 3 the extended matrix is symmetric and the Schur complement matrix S is known to be positive definite.
- 4 the extended matrix is symmetric and the Schur complement matrix **S** is known to be negative definite.

It is unchanged by the subroutine. **Restriction:** $1 \le ICLASS \le 4$.

LBD is an INTEGER variable which must be set by the user to be at least as large as the number of nonzero entries in the partitioned matrix

$$\begin{pmatrix} \mathbf{B} \\ \mathbf{D}_U \end{pmatrix}$$
,

where \mathbf{D}_U is the upper triangular part of \mathbf{D} , ie, $(\mathbf{D}_U)_{ij} = (\mathbf{D})_{ij}$ if $i \le j$ and zero otherwise. It is unchanged by the subroutine.

BD is a REAL (DOUBLE PRECISION in the D version) array of length LBD which must be set by the user to the value of the entries in the partitioned matrix

$$\binom{\mathbf{B}}{\mathbf{D}_U}$$
,

where \mathbf{D}_U is the upper triangular part of \mathbf{D} . The entries must be ordered by columns, with the entries in each column contiguous and those of column j preceding those of column j+1 (j=1,...,M). The ordering within each column is unimportant. Any element in BD below the diagonal of \mathbf{D} will be removed by MA69A/AD.

IRNBD is an INTEGER array of length LBD, which must be set by the user. It must contain the row indices of the corresponding entries in BD. Any element whose index in IRNBD is below the diagonal of **D** will be removed by MA69A/AD.

IPBD is an INTEGER array of length M+1, which must be set by the user. It must be set so that IPBD(j) points to the positions in the arrays BD and IRNBD of the first entry in column j (j = 1,, M). IPBD(M+1) must be set to the number of entries in

$$\begin{pmatrix} \mathbf{B} \\ \mathbf{D}_{II} \end{pmatrix}$$

plus one. This argument may be changed by MA69A/AD to reflect the removal of any subdiagonal entries of $\bf D$ input in BD and IRNBD.

LCD is an INTEGER variable which must be set by the user when ICLASS=1 to be at least as large as the number of

- nonzero entries in the partitioned matrix ($\mathbf{C} \mathbf{D}_L$), where \mathbf{D}_L is the strict lower triangular part of \mathbf{D} , i.e., $(\mathbf{D}_L)_{ii} = (\mathbf{D})_{ii}$ if i > j and zero otherwise. It need not be set if ICLASS > 1 and is unchanged by the subroutine.
- is a REAL (DOUBLE PRECISION in the **D** version) array of length LCD which must be set by the user when ICLASS=1 to the value of the entries in the partitioned matrix ($\mathbf{C} \ \mathbf{D}_L$), where \mathbf{D}_L is the strict lower triangular part of **D**. The entries must be ordered by rows, with the entries in each row contiguous and those of row i preceding those of row i+1 (i=1,...,M). Any element on or to the right of the diagonal of **D** will be removed by MA69A/AD. The ordering within each row is unimportant. This argument need not be set if ICLASS > 1.
- JCNCD is an INTEGER array of length LCD, which must be set by the user when ICLASS=1. It must then contain the column indices of the corresponding entries in CD. Any element whose index is on or to the right of the diagonal of **D** will be removed by MA69A/AD. This argument need not be set if ICLASS > 1.
- IPCD is an INTEGER array of length M+1, which must be set by the user when ICLASS=1. It must then be set so that IPCD(i) points to the positions in the arrays CD and JCNCD of the first entry in row i (i=1,...,M). IPCD(M+1) must be set to the number of entries in (\mathbf{C} \mathbf{D}_L) plus one. This argument may be changed by MA69A/AD to reflect the removal of entries on or to the right of the diagonal of \mathbf{D} input in CD and JCNCD. It need not be set if ICLASS > 1.
- is a REAL (DOUBLE PRECISION in the D version) array of length LR which need not be set by the user. On a successful exit from MA69A/AD, R contains the upper triangular matrix associated with a factorization of the Schur complement matrix \mathbf{S} . The upper triangle of the relevant matrix is stored by columns. If ICLASS=1 or 2, the matrix returned is the matrix \mathbf{R} associated with the $\mathbf{Q}\mathbf{R}$ factorization $\mathbf{S} = \mathbf{Q}\mathbf{R}$ of the Schur complement. If ICLASS=3, R contains the matrix \mathbf{R} associated with the Cholesky factorization $\mathbf{S} = \mathbf{R}^T\mathbf{R}$ of the Schur complement. If ICLASS=4, R contains the matrix \mathbf{R} associated with the Cholesky factorization $-\mathbf{S} = \mathbf{R}^T\mathbf{R}$ of the negative of the Schur complement.
- LR is an INTEGER variable set by the user to the length of the array R. It is unchanged by the subroutine. **Restriction:** $LR \ge M^*(M+1)/2$.
- is a REAL (DOUBLE PRECISION in the D version) two dimensional LQ by M array which need not be set by the user. On a successful exit from MA69A/AD when ICLASS=1 or 2 Q(i,j) ($1 \le i,j \le M$) contains the i,j-th entry of the matrix \mathbf{Q} in the \mathbf{QR} factorization $\mathbf{S} = \mathbf{QR}$ of the Schur complement. Q is not used for other values of ICLASS.
- LQ is an INTEGER variable which must be set by the user to actual size of the first dimension of the two dimensional array Q. It is unchanged by the subroutine. **Restriction:** LQ≥M.
- W is a REAL (DOUBLE PRECISION in the D version) array of length at least M which is used for workspace and which need not be set by the user.
- VECTOR is a REAL (DOUBLE PRECISION in the D version) array of length at least N which need not be set by the user on initial (INFORM=1) entry. If INFORM is greater than 1 on exit, a re-entry must be made with VECTOR set appropriately (see INFORM).
- ISAVE is an INTEGER workspace variable that need not be set by the user on initial (INFORM=1) entry to MA69A/AD, and which must not be changed between this and subsequent calls.
- INFORM is an INTEGER variable which must be set by the user on input to 1. On output, the value of INFORM is used to request additional information, to signal an error in the input data or to indicate a successful call to the subroutine. Possible values of INFORM and their consequences are as follows:
 - 0 The required factorization of the Schur complement S is given in the arrays R and Q.
 - 2,3 The user must obtain the solution to the system of equations Ax = b and re-enter MA69A/AD with INFORM unchanged. The particular vector b is returned in the array VECTOR; the user must calculate x and pass this vector back in VECTOR.
 - 4 The user must obtain the solution to the system of equations $\mathbf{A}^T \mathbf{y} = \mathbf{c}$ and re-enter MA69A/AD with

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INFORM unchanged. The particular vector \mathbf{c} is returned in the array VECTOR; the user must calculate \mathbf{y} and pass this vector back in VECTOR.

Negative values of INFORM indicate that some input data has been incorrectly assigned. Possible values of INFORM and some potential remedies are:

- -1 One of the previously mentioned restrictions on the values of M, N, ICLASS, LQ or LR has been violated. Check these values and re-enter with INFORM=1.
- -2 The Schur complement matrix is singular; this has been detected during the **QR** factorization of **S**. Check the matrix entries.
- -3 The Schur complement matrix is not positive definite; this has been detected during the Cholesky factorization of **S**. Check the matrix entries.
- -4 The Schur complement matrix is not negative definite; this has been detected during the Cholesky factorization of -S. Check the matrix entries.
- -5 MA69A/AD has been called with INFORM ≤0. Reset INFORM to 1 and re-enter.

2.3 The solution stage

Call MA69B/BD to solve the extended system of equations using the factorization produced by a previous call to MA69A/AD. MA69B/BD should only be used if the call to MA69A/AD terminated successfully (i.e., with INFORM=0).

The single precision version

```
CALL MA69B ( N, M, ICLASS, LBD, BD, IRNBD, IPBD, LCD, CD, JCNCD, * IPCD, R, LR, Q, LQ, RHS, X, VECTOR, INFORM )
```

The double precision version

```
CALL MA69BD( N, M, ICLASS, LBD, BD, IRNBD, IPBD, LCD, CD, JCNCD, * IPCD, R, LR, Q, LQ, RHS, X, VECTOR, INFORM )
```

Arguments N, M, ICLASS, LCD, CD, JCNCD, IPCD, LBD, BD, IRNBD, IPBD R, LR, Q, LQ are the same as those of the same name in the call to MA69A/AD and must be unchanged since that call. They are not altered by MA69B/BD.

RHS is a REAL (DOUBLE PRECISION in the D version) array of length N+M which must be set on entry to the values of the right-hand-side vector

$$\begin{pmatrix} \mathbf{b}_1 \\ \mathbf{b}_2 \end{pmatrix}$$

of the extended system of equations. RHS is not altered by the subroutine.

X is a REAL (DOUBLE PRECISION in the D version) array of length N+M which need not be set on entry. On final exit, X contains the values of the solution

$$\begin{pmatrix} \mathbf{x}_1 \\ \mathbf{x}_2 \end{pmatrix}$$

to the extended system of equations.

VECTOR is a REAL (DOUBLE PRECISION in the D version) array of length at least N which need not be set by the user on initial (INFORM=1) entry. If INFORM is greater than 1 on exit, a re-entry must be made with VECTOR set appropriately (see INFORM).

INFORM is an INTEGER variable which must be set by the user on input to 1. On output, the value of INFORM is used to request additional information or to indicate a successful call to the subroutine. Possible values of INFORM and their consequences are as follows:

0 The required solution of the extended system of equations is given in the array X.

2,3 The user must obtain the solution to the system of equations Ax = b and re-enter MA69A/AD with INFORM unchanged. The particular vector b is returned in the array VECTOR; the user must calculate x and pass this vector back in VECTOR.

4 The user must obtain the solution to the system of equations $\mathbf{A}^T \mathbf{y} = \mathbf{c}$ and re-enter MA69A/AD with INFORM unchanged. The particular vector \mathbf{c} is returned in the array VECTOR; the user must calculate \mathbf{y} and pass this vector back in VECTOR.

2.4 The updating stage

Call MA69C/CD to extend the factorization of the Schur complement when a new row and column are appended to the extended matrix. Subsequent systems of equations with the larger coefficient matrix may then be solved by calls to MA69B/BD. Note in particular that the arrays CD, JCNCD, IPCD, BD, IRNBD and IPBD must be expanded to allow for the incoming row and column.

The single precision version

```
CALL MA69C ( N, M, ICLASS, LBD, BD, IRNBD, IPBD, LCD, CD, JCNCD, * IPCD, R, LR, Q, LQ, W, VECTOR, RSAVE, INFORM )
```

The double precision version

```
CALL MA69CD( N, M, ICLASS, LBD, BD, IRNBD, IPBD, LCD, CD, JCNCD, * IPCD, R, LR, Q, LQ, W, VECTOR, RSAVE, INFORM )
```

Arguments N M, and ICLASS are the same as those of the same name in the call to MA69A/AD. They are not altered by MA69C/CD. ICLASS must not have been changed since previous calls to MA69A/AD.

LBD is an INTEGER variable which must be set by the user to be at least as large as the number of nonzero entries in the matrix

$$\begin{pmatrix} \mathbf{B} & \mathbf{c}_1 \\ \mathbf{D}_U & \mathbf{c}_2 \\ d \end{pmatrix},$$

where \mathbf{D}_{U} is the upper triangular part of \mathbf{D} . This argument is unchanged by the subroutine.

BD is a REAL (DOUBLE PRECISION in the D version) array of length LBD which must be set by the user to the value of the entries in the partitioned matrix

$$\begin{pmatrix} \mathbf{B} & \mathbf{c}_1 \\ \mathbf{D}_U & \mathbf{c}_2 \\ & d \end{pmatrix},$$

where \mathbf{D}_U is the upper triangular part of \mathbf{D} . The entries must be ordered by columns, with the entries in each column contiguous and those of column j preceding those of column j+1 (j=1,...,M+1). Any element below the diagonal of \mathbf{D} will be ignored. The ordering within each column is unimportant. Any element below the diagonal of \mathbf{D} will be removed by MA69C/CD.

IRNBD is an INTEGER array of length LBD, which must be set by the user. It must contain the row indices of the corresponding entries in BD. Any element whose index is below the diagonal of \mathbf{D} will be removed by MA69C/CD.

IPBD is an INTEGER array of length M+2, which must be set by the user. It must be set so that IPBD(j) points to the positions in the arrays BD and IRNBD of the first entry in column j (j = 1, ..., M+1). IPBD(M+2) must be set to the number of entries in

$$\begin{pmatrix} \mathbf{B} & \mathbf{c}_1 \\ \mathbf{D}_U & \mathbf{c}_2 \\ & d \end{pmatrix}$$

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plus one. This argument may be changed by MA69C/CD to reflect the removal of any subdiagonal entries of $\bf D$ input in BD and IRNBD.

LCD is an INTEGER variable set by the user when ICLASS=1 to be at least as large as the number of nonzero entries in the partitioned matrix

$$\begin{pmatrix} \mathbf{C} & \mathbf{D}_L \\ \mathbf{r}_1 & \mathbf{r}_2 \end{pmatrix}$$
,

where \mathbf{D}_L is the strict lower triangular part of \mathbf{D} . It need not be set if ICLASS > 1 and is unchanged by the subroutine.

CD is a REAL (DOUBLE PRECISION in the D version) array of length LCD which must be set by the user to the value of the entries in the partitioned matrix

$$\begin{pmatrix} \mathbf{C} & \mathbf{D}_L \\ \mathbf{r}_1 & \mathbf{r}_2 \end{pmatrix}$$

where \mathbf{D}_L is the strict lower triangular part of \mathbf{D} . The entries must be ordered by rows, with the entries in each row contiguous and those of row i preceding those of row i+1 (i=1,...,M+1). Any element on or to the right of the diagonal of \mathbf{D} will be removed by MA69C/CD. The ordering within each row is unimportant. This argument need not be set if ICLASS > 1.

JCNCD is an INTEGER array of length LCD, which must be set by the user when ICLASS=1. It must then contain the column indices of the corresponding entries in CD. Any element whose index is on or to the right of the diagonal of $\bf D$ will be removed by MA69C/CD. This argument need not be set if ICLASS > 1.

IPCD is an INTEGER array of length M+2, which must be set by the user when ICLASS=1. It must then be set so that IPCD(i) points to the positions in the arrays CD and JCNCD of the first entry in row i (i=1,...,M+1). IPCD(M+2) must be set to the number of entries in

$$\begin{pmatrix} \mathbf{C} & \mathbf{D}_L \\ \mathbf{r}_1 & \mathbf{r}_2 \end{pmatrix}$$

plus one. This argument may be changed by MA69C/CD to reflect the removal of entries on or to the right of the diagonal of $\bf D$ input in CD and JCNCD. It need not be set if ICLASS > 1.

R is a REAL (DOUBLE PRECISION in the D version) array of length LR which serves the same purpose as that of the same name in MA69A/AD. On entry to MA69C/CD, the array must be unchanged from that output from the most recent call to MA69A/AD, MA69C/CD or MA69D/DD excepting that, if M=0, R need not have been set. On exit, R contains the relevant factor of the Schur complement of **A** in the further-extended matrix.

LR is an INTEGER variable set by the user to the length of the array R. It is unchanged by the subroutine. **Restriction:** $LR \ge (M+1)*(M+2)/2$.

is a REAL (DOUBLE PRECISION in the D version) two dimensional LQ by M+1 array which serves the same purpose as that of the same name in MA69A/AD. On entry to MA69C/CD, the array must be unchanged from that output from the most recent call to MA69A/AD, MA69C/CD or MA69D/DD excepting that, if M=0, Q need not have been set. On exit, Q contains the relevant factor of the Schur complement of A in the further-extended matrix. Q is only used for ICLASS=1, 2.

LQ is an INTEGER variable which must be set by the user to actual size of the first dimension of the two dimensional array Q. It is unchanged by the subroutine. **Restriction:** LQ≥M+1.

W is a REAL (DOUBLE PRECISION in the D version) array of length at least M+1 which is used for workspace and which need not be set by the user. The contents of W must not be changed between the initial and subsequent calls to MA69C/CD or MA69D/DD.

VECTOR is a REAL (DOUBLE PRECISION in the D version) array of length at least N which need not be set by the user on initial (INFORM=1) entry. If INFORM is greater than 1 on exit, a re-entry must be made with VECTOR set appropriately (see INFORM).

RSAVE is an REAL (DOUBLE PRECISION in the D version) workspace variable that need not be set by the user on initial (INFORM=1) entry to MA69C/CD, and which must not be changed between this and subsequent calls.

INFORM is an INTEGER variable which must be set by the user on input to 1. On output, the value of INFORM is used to request additional information, to signal an error in the input data or to indicate a successful call to the subroutine. Possible values of INFORM and their consequences are as follows:

- 0 The required factorization of the Schur complement S is given in the arrays R and Q.
- 2,3 The user must obtain the solution to the system of equations Ax = b and re-enter MA69C/CD with INFORM unchanged. The particular vector b is returned in the array VECTOR; the user must calculate x and pass this vector back in VECTOR.
 - 4 The user must obtain the solution to the system of equations $\mathbf{A}^T \mathbf{y} = \mathbf{c}$ and re-enter MA69C/CD with INFORM unchanged. The particular vector \mathbf{c} is returned in the array VECTOR; the user must calculate \mathbf{y} and pass this vector back in VECTOR.

Negative values of INFORM indicate that some input data has been incorrectly assigned. Possible values of INFORM and some potential remedies are:

- -1 One of the previously mentioned restrictions on the values of M, N, ICLASS, LQ or LR has been violated. Check these values and re-enter with INFORM=1.
- -2 The Schur complement matrix is singular; this has been detected during the QR factorization of the further-extended Schur complement. Check the matrix entries.
- -3 The Schur complement matrix is not positive definite; this has been detected during the Cholesky factorization of the further-extended Schur complement. Check the matrix entries.
- -4 The Schur complement matrix is not negative definite; this has been detected during the Cholesky factorization of the negative of the further-extended Schur complement. Check the matrix entries.
- -5 MA69C/CD has been called with INFORM ≤ 0 . Reset INFORM to 1 and re-enter.

2.5 The deletion stage

Call MA69D/DD to extend the factorization of the Schur complement when a row and column of the existing extended matrix are to be removed. Subsequent systems of equations with the smaller coefficient matrix may then be solved by calls to MA69B/BD. The data structures for holding B, C and D may be automatically updated if required.

The single precision version

```
CALL MA69D ( N, M, ICLASS, NEWDS, LBD, BD, IRNBD, IPBD, JCDROP,

LCD, CD, JCNCD, IPCD, IRDROP, R, LR, Q, LQ,

W, VECTOR, INFORM )
```

The double precision version

```
CALL MA69DD( N, M, ICLASS, NEWDS, LBD, BD, IRNBD, IPBD, JCDROP,

* LCD, CD, JCNCD, IPCD, IRDROP, R, LR, Q, LQ,

* W, VECTOR, INFORM )
```

Arguments N M, and ICLASS are the same as those of the same name in the call to MA69A/AD. They are not altered by MA69C/CD. ICLASS must not have been changed since previous calls to MA69A/AD.

NEWDS is a LOGICAL variable which must be set on entry. If the user wishes the subroutine to update the data structures required to store the extended matrix (i.e., the arrays BD, IRNBD, IPBD and, if ICLASS = 1, CD, JCNCD and IPCD) to account for the impending row and column removal NEWDS must be set to .TRUE. If the call to MA69D/DD is to be followed by further calls to any of the MA69 subroutines, NEWDS should be set .TRUE. If the user is unconcerned about the data structures, NEWDS should be set .FALSE. We recommend that NEWDS is always set .TRUE. NEWDS is unchanged by the subroutine.

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LBD is an INTEGER variable which must be set by the user to be at least as large as the number of nonzero entries in the partitioned matrix

$$\begin{pmatrix} \mathbf{B} \\ \mathbf{D}_U \end{pmatrix}$$

plus M, where \mathbf{D}_U is the upper triangular part of \mathbf{D} , ie, $(\mathbf{D}_U)_{ij} = (\mathbf{D})_{ij}$ if $i \le j$ and zero otherwise. It is unchanged by the subroutine.

is a REAL (DOUBLE PRECISION in the D version) array of length LBD which must be set by the user to the value of the entries in the partitioned matrix

$$\begin{pmatrix} \mathbf{B} \\ \mathbf{D}_{II} \end{pmatrix}$$
,

as described in §2.2. The required entries of BD will have been set in a previous call to MA69A/AD, MA69C/CD or MA69DD and must not have been altered since. If NEWDS is .TRUE., BD will be altered by MA69D/DD to contain the entries of the partitioned matrix after the required row and column have been removed. If NEWDS is .FALSE., BD will not be altered by the subroutine.

IRNBD is an INTEGER array of length LBD, which must be set by the user. It must contain the row indices of the corresponding entries in BD as described in §2.2 The required values of IRNBD will have been set in a previous call to MA69A/AD, MA69C/CD or MA69DD and must not have been altered since. If NEWDS is .TRUE., IRNBD will be altered by MA69D/DD to contain the row indices of the entries of the partitioned matrix after the required row and column have been removed. If NEWDS is .FALSE., IRNBD will not be altered by the subroutine.

IPBD is an INTEGER array of length M+1, which must be set by the user on input as described in §2.2. The required values of IPBD will have been set in a previous call to MA69A/AD, MA69C/CD or MA69DD and must not have been altered since. If NEWDS is .TRUE., IPBD will be altered by MA69D/DD to contain the pointers to the start of each column of the partitioned matrix after the required row and column have been removed. If NEWDS is .FALSE., IPBD will not be altered by the subroutine.

JCDROP is an INTEGER variable which must be set by the user to the index of the column of

$$\binom{\mathbf{B}}{\mathbf{D}}$$

which is to be removed. It is unchanged by the subroutine. **Restriction:** $1 \le JCDROP \le M$.

LCD is an INTEGER variable which must be set by the user when ICLASS=1 to be at least as large as the number of nonzero entries in the partitioned matrix ($\mathbf{C} \ \mathbf{D}_L$) plus M, where \mathbf{D}_L is the strict lower triangular part of \mathbf{D} , i.e., $(\mathbf{D}_L)_{ii} = (\mathbf{D})_{ii}$ if i > j and zero otherwise. It need not be set if ICLASS > 1 and is unchanged by the subroutine.

is a REAL (DOUBLE PRECISION in the D version) array of length LCD which must be set by the user when ICLASS=1 to the value of the entries in the partitioned matrix ($\mathbf{C} \ \mathbf{D}_L$), as described in §2.2. The required entries of CD will then have been set in a previous call to MA69A/AD, MA69C/CD or MA69DD and must not have been altered since. If NEWDS is .TRUE. and ICLASS=1, BD will be altered by MA69D/DD to contain the entries of the partitioned matrix after the required row and column have been removed. If NEWDS is .FALSE., CD will not be altered by the subroutine. This argument need not be set if ICLASS>1 and is unchanged by the subroutine.

JCNCD is an INTEGER array of length LCD, which must be set by the user when ICLASS=1. It must then contain the column indices of the corresponding entries in CD as described in §2.2 The required values of JCNCD will have been set in a previous call to MA69A/AD, MA69C/CD or MA69DD and must not have been altered since. If NEWDS is .TRUE. and ICLASS=1, JCNCD will be altered by MA69D/DD to contain the column indices of the entries of the partitioned matrix after the required row and column have been removed. If NEWDS is .FALSE., JCNCD will not be altered by the subroutine. This argument need not be set if ICLASS >1 and is unchanged by the subroutine.

IPCD is an INTEGER array of length M+1, which must be set by the user on input when ICLASS=1 as described in §2.2. The required values of IPCD will then have been set in a previous call to MA69A/AD, MA69C/CD or

MA69DD and must not have been altered since. If NEWDS is .TRUE. and ICLASS=1, IPCD will be altered by MA69D/DD to contain the pointers to the start of each row of the partitioned matrix after the required row and column have been removed. If NEWDS is .FALSE., IPCD will not be altered by the subroutine. This argument need not be set if ICLASS>1 and is unchanged by the subroutine.

- IRDROP is an INTEGER variable which must be set by the user if ICLASS=1 to the index of the row of (C D) which is to be removed. It is unchanged by the subroutine. This argument need not be set if ICLASS > 1. **Restriction:** $1 \le IRDROP \le M$.
- is a REAL (DOUBLE PRECISION in the D version) array of length LR which serves the same purpose as that of the same name in MA69A/AD. On entry to MA69D/DD, the array must be unchanged from that output from the most recent call to MA69A/AD, MA69C/CD or MA69D/DD. On exit, R contains the relevant factor of the Schur complement of **A** in the new extended matrix.
- LR is an INTEGER variable set by the user to the length of the array R. It is unchanged by the subroutine. **Restriction:** $LR \ge M^*(M+1)/2$.
- is a REAL (DOUBLE PRECISION in the D version) two dimensional M by M array which serves the same purpose as that of the same name in MA69A/AD. On entry to MA69D/DD, the array must be unchanged from that output from the most recent call to MA69A/AD, MA69C/CD or MA69D/DD. On exit, Q contains the relevant factor of the Schur complement of $\bf A$ in the new extended matrix. Q is only used for ICLASS=1, 2.
- LQ is an INTEGER variable which must be set by the user to actual size of the first dimension of the two dimensional array Q. It is unchanged by the subroutine. **Restriction:** $LQ \ge M$.
- W is a REAL (DOUBLE PRECISION in the D version) array of length at least M which is used for workspace and which need not be set by the user. The contents of W must not be changed between the initial and subsequent calls to MA69D/DD or MA69C/CD.
- $\label{eq:vector} \mbox{VECTOR} \ \ is \ a \ \mbox{REAL} \ (\mbox{DOUBLE PRECISION} \ in \ the \ D \ version) \ array \ of \ length \ at \ least \ N \ which \ is \ again \ used \ for \ workspace \ and \ which \ need \ not \ be \ set \ by \ the \ user.$
- INFORM is an INTEGER variable which must be set by the user on input to 1. On output, the value of INFORM is used to signal an error in the input data or to indicate a successful call to the subroutine. Possible values of INFORM and their consequences are as follows:
 - 0 The required factorization of the Schur complement S is given in the arrays R and Q.

Negative values of INFORM indicate that some input data has been incorrectly assigned. Possible values of INFORM and some potential remedies are:

- -1 One of the previously mentioned restrictions on the values of M, N, ICLASS, JCDROP, IRDROP, LQ or LR has been violated. Check these values and re-enter with INFORM=1.
- -2 The Schur complement matrix is singular; this has been detected during the QR factorization of the further-extended Schur complement. Check the matrix entries.
- -5 MA69D/DD has been called with INFORM ≤ 0 . Reset INFORM to 1 and re-enter.

2.6 Error returns

If some error in the input data is detected by the subroutines, they return immediately to the calling program with the error flag INFORM having a negative value. See §2.2-2.5 for details.

2.7 Multiple updates

Once MA69C/CD or MA69D/DD (with NEWDS=.TRUE.) has been used to update the factorization of the Schur complement matrix, it is as if the enlarged or reduced matrix were that originally factorized by MA69A/AD. Consequently *sequences* of row and column additions and removals may be performed so long as sufficient storage is available.

MA69

3 GENERAL INFORMATION

Use of common: none.

Workspace: provided by the user through the argument W (REAL (DOUBLE PRECISION in the D version) array of length M).

Other routines called directly: internal subroutines MA69E/ED and MA69F/FD are used by MA69A/AD, MA69B/BD and MA69C/CD and MA69D/DD. The basic linear algebra subprograms (BLAS) SAXPY/DAXPY SCOPY/DCOPY SDOT/DDOT SROT/DROT and SROTG/DROTG are also called.

Input/output: none.

Restrictions: $N \ge 0$, $M \ge 0$ and $1 \le ICLASS \le 4$. Also $LR \ge M^*(M+1)/2$ and $LQ \ge M$ for MA69A/AD, MA69B/BD and MA69D/DD, $LR \ge (M+1)^*(M+2)/2$ and $LQ \ge M+1$ for MA69C/CD and $1 \le IRDROP \le M$ and $1 \le JCDROP \le M$ for MA69D/DD

4 METHOD

The subroutine MA69A/AD forms the Schur complement $S = D - C A^{-1}B$ of A in the extended matrix by repeated reverse communication to obtain the columns of $A^{-1}B$. The Schur complement or its negative is then factorized into its QR or, if possible, Cholesky factors.

The subroutine MA69B/BD solves the extended system using the following well-known scheme:

- (i) Compute the solution to $\mathbf{A}\mathbf{u} = \mathbf{b}_1$;
- (ii) Compute \mathbf{x}_2 from $\mathbf{S}\mathbf{x}_2 = \mathbf{b}_2 \mathbf{C}\mathbf{u}$;
- (iii) Compute the solution to $Av = Bx_2$; and
- (iv) Compute $\mathbf{x}_1 = \mathbf{u} \mathbf{v}$.

The subroutines MA69C/CD and MA69D/DD compute the factorization of the Schur complement after a row and column have been appended to, and removed from, the extended matrix, respectively. The existing factorization is updated to obtain the new one; this is normally more efficient than forming the factorization from scratch.

5 EXAMPLE OF USE

As a simple example, suppose we wish to solve the system of equations

Notice that the leading 5 by 5 coefficient matrix is diagonal and hence easily invertible. So we might choose n=5, m=2 and use MA69AD/MA69BD to find the required solution. As the matrix is unsymmetric, we must set ICLASS=1.

Now suppose that we have solved this system as described and are now confronted with the further system

Rather than applying MA69AD/MA69BD with n=5, m=3, we note that the new coefficient matrix differs from the old one merely in having an extra row and column. Thus, we can use MA69CD with n=5, m=2 to update the existing factorization and then call MA69BD with n=5, m=3 to calculate the desired solution.

Finally, suppose that we have solved this second system and now wish to solve

$$\begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 1 & 1 \\ 0 & 2 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 3 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 4 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 5 & 1 & 0 \\ 1 & 0 & 1 & 0 & 1 & 3 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \\ x_5 \\ x_6 \\ x_7 \end{pmatrix} = \begin{pmatrix} 3 \\ 5 \\ 4 \\ 5 \\ 6 \\ 6 \\ 2 \end{pmatrix}$$

Again, rather than applying MA69AD/MA69BD with n=5, m=2, we note that this third coefficient matrix is the second one with its n+1-st row and n+2-nd column removed. Thus, we can use MA69DD with n=5, m=3 to update the existing factorization and then call MA69BD with n=5, m=2 to calculate the desired solution.

To carry out these calculations, we might use the following piece of code. Notice how the extra row and column for the second problem are simply introduced at the end of the existing data structures.

```
PROGRAM MAIN
INTEGER I, ICLASS, INFORM, IRDROP, JCDROP, LBD, LCD, LQ, LR
INTEGER M, MPN, MPNP1, MP1, MP2, N, ISAVE
DOUBLE PRECISION RSAVE
PARAMETER ( N = 5, M = 2, ICLASS = 1 )
PARAMETER ( LBD = 15, LCD = 13 )
PARAMETER ( MP1 = M + 1, MP2 = MP1 + 1, MPN = M + N
PARAMETER ( MPNP1 = MP1 + N, LQ = MP1, LR = MP1 * MP2 / ^{2} )
INTEGER IRNBD( LBD ), JCNCD( LCD ), IPBD( MP2 ), IPCD( MP2 )
DOUBLE PRECISION BD( LBD ), CD( LCD ), W( MP1 ),
                 R( LR ), Q( LQ, MP1 ), VECTOR( N ), X1( MPN ),
                 RHS1( MPN ), X2( MPNP1 ), RHS2( MPNP1 ),
                 X3(MPN), RHS3(MPN)
EXTERNAL MA69AD, MA69BD, MA69CD, MA69DD
INTRINSIC DBLE
DATA ( IPBD( I ), I = 1, 3 ) / 1, 7, 10 /
DATA ( IPCD( I ), I = 1, 3 ) / 1, 6, 10 /
DATA ( IRNBD( I ), I = 1, 9 ) / 1, 2, 3, 4, 5, 6, 5, 6, 7
DATA ( BD( I ), I = 1, 9 ) / 1.0D+0, 1.0D+0, 1.0D+0, 1.0D+0,
          1.0D+0, 1.0D+0, 1.0D+0, 2.0D+0, 4.0D+0 /
DATA ( JCNCD( I ), I = 1, 9 ) / 1, 2, 3, 4, 5, 1, 3, 5, 6 /
DATA ( CD( I ), I = 1, 9 ) / 1.0D+0, 1.0D+0, 1.0D+0, 1.0D+0,
          1.0D+0, 1.0D+0, 1.0D+0, 1.0D+0, 3.0D+0
DATA RHS1/ 2.0D+0, 3.0D+0, 4.0D+0, 5.0D+0, 7.0D+0, 8.0D+0, 1.0D+1/
DATA RHS2/ 5.0D+0, 5.0D+0, 4.0D+0, 5.0D+0, 7.0D+0, 1.2D+1,
           1.2D+1, 4.0D+0 /
DATA RHS3/ 3.0D+0, 5.0D+0, 4.0D+0, 5.0D+0, 6.0D+0, 6.0D+0, 2.0D+0/
```

С

MA69 HSL

```
FIRST PROBLEM.
C
      INFORM = 1
   10 CONTINUE
     CALL MA69AD( N, M, ICLASS, LBD, BD, IRNBD, IPBD, LCD, CD, JCNCD,
                  IPCD, R, LR, Q, LQ, W, VECTOR, ISAVE, INFORM )
     IF ( INFORM .GT. 0 ) THEN
         DO 20 I
                       = 1, N
           VECTOR( I ) = VECTOR( I ) / DBLE( I )
   20
         CONTINUE
        GO TO 10
      END IF
      WRITE(6, 2000) INFORM
      IF ( INFORM .LT. 0 ) STOP
      INFORM = 1
   30 CONTINUE
     CALL MA69BD( N, M, ICLASS, LBD, BD, IRNBD, IPBD, LCD, CD, JCNCD,
                  IPCD, R, LR, Q, LQ, RHS1, X1, VECTOR, INFORM)
      IF ( INFORM .GT. 0 ) THEN
        DO 40 I
                       = 1, N
           VECTOR( I ) = VECTOR( I ) / DBLE( I )
         CONTINUE
        GO TO 30
      END IF
      WRITE(6, 2010) INFORM
      IF ( INFORM .LT. 0 ) STOP
      WRITE(6, 2020) (X1(I), I = 1, MPN)
  SECOND PROBLEM.
С
      IRNBD(10) = 1
      BD(10) = 1.0D+0
      IRNBD( 11 ) = 6
      BD( 11 )
                 = 1.0D+0
      IRNBD( 12 ) = 8
      BD( 12 )
                = 1.0D+0
      IPBD( 4 )
                 = 13
      JCNCD(10) = 1
      CD( 10 )
                 = 1.0D+0
      IPCD(4)
                = 11
      INFORM
                 = 1
  110 CONTINUE
     CALL MA69CD( N, M, ICLASS, LBD, BD, IRNBD, IPBD, LCD, CD, JCNCD,
                  IPCD, R, LR, Q, LQ, W, VECTOR, RSAVE, INFORM )
      IF ( INFORM .GT. 0 ) THEN
         DO 120 I
                       = 1, N
           VECTOR( I ) = VECTOR( I ) / DBLE( I )
  120
         CONTINUE
        GO TO 110
      END IF
      WRITE( 6, 2030 ) INFORM
      IF ( INFORM .LT. 0 ) STOP
      INFORM = 1
  130 CONTINUE
     CALL MA69BD( N, MP1, ICLASS, LBD, BD, IRNBD, IPBD, LCD, CD, JCNCD,
        IPCD, R, LR, Q, LQ, RHS2, X2, VECTOR, INFORM ) ( INFORM .GT. 0 ) THEN
        DO 140 I
                       = 1, N
           VECTOR( I ) = VECTOR( I ) / DBLE( I )
         CONTINUE
  140
         GO TO 130
```

```
END IF
      WRITE(6, 2010) INFORM
      IF ( INFORM .LT. 0 ) STOP
      WRITE(6, 2040) (X2(I), I = 1, MPNP1)
   THIRD PROBLEM.
      IRDROP = 1
      JCDROP = 2
      INFORM = 1
      CALL MA69DD( N, MP1, ICLASS, .TRUE., LBD, BD, IRNBD, IPBD, JCDROP,
                    LCD, CD, JCNCD, IPCD, IRDROP, R, LR, Q, LQ,
                    W, VECTOR, INFORM)
      WRITE( 6, 2050 ) INFORM
      IF ( INFORM .LT. 0 ) STOP
      INFORM = 1
  210 CONTINUE
      CALL MA69BD( N, M, ICLASS, LBD, BD, IRNBD, IPBD, LCD, CD, JCNCD,
                    IPCD, R, LR, Q, LQ, RHS3, X3, VECTOR, INFORM )
         ( INFORM .GT. 0 ) THEN
         DO 220 I
                         = 1, N
            VECTOR( I ) = VECTOR( I ) / DBLE( I )
  220
         CONTINUE
         GO TO 210
      END IF
      WRITE(6, 2010) INFORM
      IF ( INFORM .LT. 0 ) STOP
      WRITE( 6, 2060 ) ( X3( I ), I = 1, MPN )
 2000 FORMAT( /, ' ON EXIT FROM MA69A, INFORM = ', I3 )
 2010 FORMAT( 'ON EXIT FROM MA69B, INFORM = ', I3 )
 2020 FORMAT( /, ' SOLUTION (FIRST EQUATIONS)', /, ( 1P, 8D9.2 ) )
 2030 FORMAT( /, 'ON EXIT FROM MA69C, INFORM = ', I3 )
2040 FORMAT( /, 'SOLUTION (SECOND EQUATIONS)', /, ( 1P, 8D9.2 ) )
2050 FORMAT( /, 'ON EXIT FROM MA69D, INFORM = ', I3 )
 2060 FORMAT( /, ' SOLUTION (THIRD EQUATIONS)', /, ( 1P, 8D9.2 ) )
      END
This produces the following output:
 ON EXIT FROM MA69A, INFORM =
 ON EXIT FROM MA69B, INFORM =
 SOLUTION (FIRST EQUATIONS)
 1.00D+00 1.00D+00 1.00D+00 1.00D+00 1.00D+00 1.00D+00 1.00D+00
 ON EXIT FROM MA69C, INFORM =
 ON EXIT FROM MA69B, INFORM =
 SOLUTION (SECOND EQUATIONS)
 3.00D+00 2.00D+00 1.00D+00 1.00D+00 1.00D+00 1.00D+00 1.00D+00 1.00D+00
 ON EXIT FROM MA69D, INFORM =
 ON EXIT FROM MA69B, INFORM =
 SOLUTION (THIRD EQUATIONS)
 1.00D+00 2.00D+00 1.00D+00 1.00D+00 1.00D+00 1.00D+00 1.00D+00
```