



## 1 SUMMARY

The module HSL\_MP42 uses the multiple front method to solve sets of finite-element equations  $\mathbf{AX}=\mathbf{B}$  that have been divided into non-overlapping subdomains. The HSL routines MA42 and MA52 are used with MPI for message passing.

The coefficient matrix  $\mathbf{A}$  must be of the form

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

where the summation is over finite elements. The element matrix  $\mathbf{A}^{(k)}$  is nonzero only in those rows and columns which correspond to variables in the  $k$ -th element. The right-hand side(s)  $\mathbf{B}$  may optionally be in the form

$$\mathbf{B} = \sum_{k=1}^m \mathbf{B}^{(k)} \quad (2)$$

where  $\mathbf{B}^{(k)}$  is nonzero only in those rows which correspond to variables in element  $k$ .

In the multiple front method, a frontal decomposition is performed on each subdomain separately. Thus, on each subdomain,  $L$  and  $U$  factors are computed. Once all possible eliminations have performed within a subdomain, there remain the interface variables that are shared by more than one subdomain together with any variables that are not eliminated because of stability or efficiency considerations. If  $\mathbf{F}_i$  is the remaining frontal matrix for subdomain  $i$ , and  $\mathbf{C}_i$  is the corresponding right-hand side matrix, then the remaining problem is

$$\mathbf{FY} = \mathbf{C}, \quad (3)$$

where  $\mathbf{F} = \sum_i \mathbf{F}_i$  and  $\mathbf{C} = \sum_i \mathbf{C}_i$ . By treating each  $\mathbf{F}_i$  as an element matrix, the interface problem (3) is also solved by the frontal method. Once (3) has been solved, back-substitution on the subdomains completes the solution.

The element data and/or the matrix factors may optionally be held in direct-access files.

**ATTRIBUTES** — **Version:** 2.0.0. (18th July 2008) **Types:** Real (single, double). **Remark:** If  $\mathbf{A}$  is symmetric definite, use HSL\_MP62. **Calls:** HSL\_MP01, KB08, MA42, MA52, MC53, MC63. **Language:** Fortran 95 + TR 15581 (allocatable components). **Original date:** September 1999. **Origin:** J.A. Scott, Rutherford Appleton Laboratory.

## 2 HOW TO USE THE PACKAGE

### 2.1 Calling sequences

The module HSL\_MP42 has five separate phases:

- (1) Initialize
- (2) Analyse
- (3) Factorize
- (4) Solve
- (5) Finalize

Prior to calling the first phase, the user must choose the number of processes to run on and must initialize MPI by calling `MPI_INIT` on each process. The processes have rank 0, 1, 2,... The **host** is the process with rank zero. The user must also define an MPI communicator for the package. The communicator defines the set of processes to be used by MP42. Each phase must then be called in order by each process (although the solve phase is optional). Before calling

each phase, the user must have completed all other tasks that he or she was performing with the defined communicator (and with any other communicator that overlaps the MP42 communicator). During the factorize phase, the matrix factors are generated. If element right-hand side matrices are supplied (that is, right-hand sides of the form (2)), the solution is returned to the user at the end of the factorize phase. If the right-hand sides are only available in assembled form, or if the user wishes to use the matrix factors generated by the factorize phase to solve for further right-hand sides, the solve phase should be called. The finalize phase deallocates all arrays that have been allocated by the package and, optionally, deletes all direct-access files used to hold the matrix factors. The user may factorize more than one matrix at the same time by running more than one instance of the package; a instance of the package is terminated by calling the finalize phase. After the finalize phase and once the user has completed any other calls to MPI routines he or she wishes to make, the user should call `MPI_FINALIZE` to terminate the use of MPI. This is illustrated in the simple example code given in Section 5.

Access to the module requires a `USE` statement and the user must declare a structure data of type `MP42_DATA` defined by the module. `HSL_MP42` has a single user-callable subroutine `MP42A/AD` with a single parameter `data` of type `MP42_DATA`. If the user wishes to run more than one instance of the module at once, a separate parameter of type `MP42_DATA` is needed for each instance.

`data` has many components. In the following sections we describe the components of interest to the user. In Section 2.2, we describe the components that must be set by the user and that contain the solution vector, in Section 2.3 we describe the components that control the action, and in Section 2.4 we describe the components that hold information of potential interest to the user.

The following pseudocode illustrates how `MP42A/AD` must be used.

#### *Single precision version*

```
USE HSL_MP42_SINGLE
...
INTEGER ERCODE
TYPE (MP42_DATA) data
...
CALL MPI_INIT(ERCODE)
...
CALL MP42A (data)
...
CALL MPI_FINALIZE(ERCODE)
```

#### *Double precision version*

```
USE HSL_MP42_DOUBLE
...
INTEGER ERCODE
TYPE (MP42_DATA) data
...
CALL MPI_INIT(ERCODE)
...
CALL MP42AD (data)
...
CALL MPI_FINALIZE(ERCODE)
```

## 2.2 Input and output components

Prior to the first call to `MP42A/AD` for the current instance, the user must initialize the following component of `data`:

`data%COMM` is a scalar of type default `INTEGER` that must hold an MPI communicator. `data%COMM` must be initialized

prior to the first call to MP42A/AD to define the set of processes to be used by MP42. Before each phase is called, the user must have completed all other tasks he or she was performing that involved data%COMM (or involved any other communicator that overlaps data%COMM). data%COMM is not altered. Note that the code may be run using a single process.

For each call to MP42A/AD, a job parameter is needed. This parameter determines which phase of the package is to be performed.

data%JOB is a scalar of type default INTEGER that must be initialized on **all** processes before **each** call to MP42A/AD. It must be given the same value on all processes. It is not altered.

JOB = 1 initializes an instance of the module. A call with JOB = 1 must be made before any other calls to the module. On exit, the components of data that control the action contain default values. If the user wishes to use values other than the defaults, the corresponding components of data should be reset after the call with JOB = 1. Full details of the control components of data are given in Section 2.3.

JOB = 2 uses element variable lists to generate lists of interface variables and, optionally, to reorder the elements within each subdomain and allocate subdomains to processes.

JOB = 3 uses the information from the call with JOB = 2 to generate the  $L$  and  $U$  factors in the subdomains, form the  $L$  and  $U$  factors for the interface problem, and, if  $\mathbf{B}^{(k)}$  are specified, to solve the equations

$$\mathbf{A}\mathbf{X}=\mathbf{B} \text{ with right-hand side(s) } \mathbf{B}=\sum_{k=1}^m \mathbf{B}^{(k)}. \text{ A call with JOB = 3 must be preceded by a call with JOB = 2.}$$

JOB = 23 performs JOB = 2 then JOB = 3.

JOB = 4 uses the factors produced by a call with JOB = 3 to rapidly solve further systems of the form  $\mathbf{A}\mathbf{X}=\mathbf{B}$  ( $\mathbf{B}$  in assembled form). A call with JOB = 4 must be preceded by a call with JOB = 3 (or 23) but several calls with JOB = 4 may follow a single call with JOB = 3 (or 23).

JOB = 5 deallocates all arrays that have been allocated by the module and, optionally, deletes all direct-access files that have been used to hold the matrix factors. A call with JOB = 5 should be made after all other calls for the current instance are complete. Note that components of data that are allocated by the user are **not** deallocated.

### 2.2.1 Input components for data%JOB = 2 or 23

Prior to a call with data%JOB = 2 or 23, the following components **must** be set by the user on the host (note that if data%JOB = 23, the input components described in Section 2.2.3 must also be set):

data%NDOM is a scalar of type default INTEGER that must be set to the number of subdomains. This component is not altered. **Restriction:** data%NDOM > 1.

data%NELT is a scalar of type default INTEGER that must be set to the number of elements in the problem. This component is not altered. **Restriction:** data%NELT ≥ data%NDOM.

data%NELTSB is a rank-1 allocatable array of type default INTEGER that must be allocated by the user with size at least data%NDOM. On entry, data%NELTSB(JDOM) must hold the number of elements in subdomain JDOM (JDOM = 1, 2, ..., data%NDOM). This component is not altered. **Restriction:** data%NELTSB(:) > 0.

data%ELTVAR is a rank-1 allocatable array of type default INTEGER that must be allocated by the user and set to contain lists of the variable indices belonging to the finite elements. The lists of the variables in each of the elements belonging to subdomain 1 must precede those for the elements belonging to subdomain 2, and so on. If duplicate indices are detected in an element or variable indices less than 1 are found, the computation terminates with an error. This component is not altered.

data%ELTPTR is a rank-1 allocatable array of type default INTEGER that must be allocated with size at least data%NELT+1. data%ELTPTR(IELT) must contain the position in data%ELTVAR of the first variable in the

IELT-th element in the element variable lists (IELT = 1, 2, ..., data%NELT), and data%ELTPTR(data%NELT+1) must be set to the position after the last variable in the last element. This component is not altered.

Additionally, the following component must be allocated and set if the control component data%ICNTL(10) (see Section 2.3) is nonzero.

data%INV\_LIST is a rank-1 allocatable array of type default INTEGER that must be allocated with size at least data%NDOM. On entry, data%INV\_LIST(JDOM) must hold the rank of the process that is to factorize subdomain JDOM (JDOM = 1, 2, ..., data%NDOM). This component is not altered. **Restriction:**  $0 \leq \text{data\%INV\_LIST}(:) < \text{data\%NPROC}$  (where data%NPROC is the number of processes, see Section 2.4.1).

The following component must be allocated and set if data%ICNTL(9) > 0.

data%NORDER is a rank-2 allocatable array of type default INTEGER that must be allocated with size  $\max_{1 \leq \text{JDOM} \leq \text{data\%NDOM}} \text{data\%NELTSB}(\text{JDOM}) + 1$  by data%NDOM. It is used to hold the element assembly order. Within subdomain JDOM, the elements are locally labelled 1, 2, ..., data%NELTSB(JDOM), according to the order in which the user inputs the variable lists in data%ELTVAR. On subdomain JDOM, the elements will be assembled in the order data%NORDER(1,JDOM), data%NORDER(2, JDOM), ..., data%NORDER(data%NELTSB(JDOM), JDOM). Note that if the user has already used MP42 to factorize a matrix with a given sparsity pattern and wishes to factorize another matrix with the same pattern, savings may be made by setting data%ICNTL(9) to a value greater than 1 and leaving data%NORDER unchanged since the factorization of the original matrix

### 2.2.2 Output components for data%JOB = 2 or 23

The following component is allocated on each process.

data%INV\_LIST is a rank-1 allocatable array of type default INTEGER of size data%NDOM. On exit, data%INV\_LIST(JDOM) holds the rank of the process that is to factorize subdomain JDOM (JDOM = 1, 2, ..., data%NDOM).

data%IENT is a rank-1 allocatable array of type default INTEGER of size data%NDOM. On exit, data%IENT(L) holds the number of variable indices for subdomain L (L = 1, 2, ..., data%NDOM).

data%ENTRIES is a rank-1 allocatable array of type default INTEGER of size data%NDOM. On exit, data%ENTRIES(L) holds the number of nonzero matrix entries for subdomain L (L = 1, 2, ..., data%NDOM).

data%ICOUNT is a rank-1 allocatable array of type default INTEGER of dimension 0:data%NPROC-1. On exit, data%ICOUNT(IPROC) holds the number of subdomains assigned to process IPROC (IPROC = 0, 1, ..., data%NPROC-1).

data%IDOM is a rank-1 allocatable array of type default INTEGER. On exit, on process IPROC, data%IDOM(J) holds the index of the J th subdomain that is to be factorized by the process (J = 1, 2, ..., data%ICOUNT(IPROC)).

### 2.2.3 Input components for data%JOB = 3 or 23

Prior to a call with data%JOB = 3 or 23 the following component must be set on the host (note that if data%JOB = 23, the input components described in Section 2.2.1 must also be set):

data%NRHS is a scalar of type default INTEGER that must be set to the number of right-hand sides. This component is not altered. **Restriction:** data%NRHS ≥ 0.

The remaining components of data that must be set depend on the settings for the control components.

The following component must be set on the host if data%ICNTL(7) = 0 (the default).

data%MFRELT is a scalar of type default INTEGER that must be at least as large as the maximum number of variables per element. data%MFRELT determines the record length given in the RECL= specifier of the OPEN statements for the direct-access files for the element data (see data%ICNTL(7) in Section 2.3). This component is not altered.

The following components must be allocated and set on the host if  $\text{data\%ICNTL}(7) = 0$  (the default), 1, or 2.

$\text{data\%VALNAM}$  is a rank-1 allocatable array of type default CHARACTER\*128 that must be allocated with size at least  $\text{data\%NDOM}$ . On entry,  $\text{data\%VALNAM}(\text{JDOM})$  must contain the name of the file holding the element matrices  $\mathbf{A}^{(k)}$  belonging to subdomain JDOM ( $\text{JDOM} = 1, 2, \dots, \text{data\%NDOM}$ ).  $\text{data\%VALNAM}$  is not accessed if  $\text{data\%ICNTL}(7) \geq 3$ . This component is not altered.

$\text{data\%RHSNAM}$  is a rank-1 allocatable array of type default CHARACTER\*128. If  $\text{data\%NRHS} > 0$ ,  $\text{data\%RHSNAM}$  must be allocated with size at least  $\text{data\%NDOM}$ . On entry,  $\text{data\%RHSNAM}(\text{JDOM})$  must contain the name of the file holding the element right-hand side matrices  $\mathbf{B}^{(k)}$  belonging to subdomain JDOM ( $\text{JDOM} = 1, 2, \dots, \text{data\%NDOM}$ ). This component is not altered.

The following components must be allocated set on the host only if  $\text{data\%ICNTL}(7) = 3$  and on each process if  $\text{data\%ICNTL}(7) = 4$ .

$\text{data\%VALUES}$  is a rank-1 allocatable array of type default REAL (or double precision REAL in the double version) that must be allocated and must contain the element matrices  $\mathbf{A}^{(k)}$ . The element matrices must be in the order given by  $\text{data\%ELTVAR}$  and each must be held as a full matrix, stored by columns. This component is not altered.

$\text{data\%RHS}$  is a rank-1 allocatable array of type default REAL (or double precision REAL in the double version). If  $\text{data\%NRHS} > 0$ ,  $\text{data\%RHS}$  must be allocated and must contain the element right-hand side matrices  $\mathbf{B}^{(k)}$ . The  $\mathbf{B}^{(k)}$  matrices must be in the order given by  $\text{data\%ELTVAR}$  and each must be held as a full matrix, stored by columns (so that multiple right hand sides are stored as consecutive columns). This component is not altered.

The following component must be allocated and set on each process IPROC if  $\text{data\%ICNTL}(7) = 5$ .

$\text{data\%RVAL}$  is a rank-1 allocatable array of type default REAL (or double precision REAL in the double version) that must be allocated and must contain the element matrix entries  $\mathbf{A}^{(k)}$  for the subdomains assigned to process IPROC. The element matrices for subdomain  $\text{data\%IDOM}(1)$  must precede those for  $\text{data\%IDOM}(2)$ , and so on, and within each subdomain, the element matrices must be in the order given by  $\text{data\%ELTVAR}$ . The size of  $\text{data\%RVAL}$  on process IPROC must be at least  $\sum \text{data\%ENTRIES}(L)$  where the summation is over the subdomains L assigned to IPROC. This component is not altered.

$\text{data\%RHS\_VAL}$  is a rank-1 allocatable array of type default REAL (or double precision REAL in the double version) that must be allocated and must contain the element right-hand side matrices  $\mathbf{B}^{(k)}$  for the subdomains assigned to process IPROC. The element right-hand side matrices for subdomain  $\text{data\%IDOM}(1)$  must precede those for  $\text{data\%IDOM}(2)$ , and so on, and within each subdomain, the element right-hand side matrices must be in the order given by  $\text{data\%ELTVAR}$  and each must be held as a full matrix, stored by columns (so that multiple right hand sides are stored as consecutive columns). The size of  $\text{data\%RHS\_VAL}$  on process IPROC must be at least  $\text{data\%NRHS} * \sum \text{data\%IENT}(L)$  where the summation is over the subdomains L assigned to IPROC. This component is not altered.

The following component must be allocated and set if  $\text{data\%ICNTL}(13)$  is nonzero.

$\text{data\%LENBUF}$  is a rank-2 allocatable array of type default INTEGER that must be allocated with size 3 by  $\text{data\%NDOM} + 1$ . It is used to hold the sizes (in words) of the buffers (workspace arrays) used by the frontal solver MA42 for the matrix factors. On entry,  $\text{data\%LENBUF}(J, \text{JDOM})$ ,  $J = 1, 2, 3$ , must hold, respectively, the buffer size for the  $U$  factor (including the corresponding right-hand sides), the  $L$  factor, and the row and column indices for the factors on subdomain JDOM ( $\text{JDOM} = 1, 2, \dots, \text{data\%NDOM}$ ).  $\text{data\%LENBUF}(J, \text{data\%NDOM} + 1)$ ,  $J = 1, 2, 3$ , must hold the corresponding buffer sizes for the interface problem, which is solved on the host.  $\text{data\%LENBUF}(2, :)$  is set to zero if the user has reset  $\text{data\%ICNTL}(11)$  to a nonzero value (see Section 2.3). Note that the workspace required by MP42 is dependent on the size of the buffers and for efficiency the buffers should be chosen as large as space permits. If direct-access files are not being used ( $\text{data\%ICNTL}(14) = 0$ ), the buffers must be large enough to hold the matrix factors. On exit,  $\text{data\%LENBUF}$  holds the buffer sizes used by MP42. These differ from the input values if the user-supplied values are too large to enable the required workspace to be allocated, or if direct-access files are not being used and one or more of the buffer sizes

supplied by the user is too small (see warning +4). **Restriction:**  $\text{data}\%LENBUF(:, :) \geq 1$ .

The following component must be allocated and set if  $\text{data}\%ICNTL(14) < 0$ .

$\text{data}\%FILES1$  is a rank-2 allocatable array of type default CHARACTER\*128 that must be allocated with size 3 by  $\text{data}\%NDOM+1$ . On entry,  $\text{data}\%FILES1(J, JDOM)$ ,  $J = 1, 2, 3$ , must hold the names of the direct-access files for the  $U$  factor, the  $L$  factor, and the row and column indices for the factors on subdomain  $JDOM$  ( $JDOM = 1, 2, \dots, \text{data}\%NDOM$ ) and for the interface problem when  $JDOM = \text{data}\%NDOM+1$ . If the user wishes to run further instances of the module before the final call for the first instance ( $\text{data}\%JOB = 5$ ), for each instance  $\text{data}\%ICNTL(14)$  must be set to a nonzero value and file names provided by the user in  $\text{data}\%FILES1$ .

The following component must be allocated and set if  $\text{data}\%ICNTL(15) < 0$ .

$\text{data}\%FILES2$  is a rank-2 allocatable array of type default CHARACTER\*128 that must be allocated with size 2 by  $\text{data}\%NDOM$ . On entry,  $\text{data}\%FILES2(1, JDOM)$  must hold the name of the sequential file for holding the data that remains in the frontal matrix once the factorization on subdomain  $JDOM$  is complete ( $JDOM = 1, 2, \dots, \text{data}\%NDOM$ ). If  $\text{data}\%NRHS > 0$ ,  $\text{data}\%FILES2(2, JDOM)$  must hold the name of the sequential file for the corresponding right-hand sides.  $\text{data}\%FILES2(2, JDOM)$  is not accessed if  $\text{data}\%NRHS = 0$ .

#### 2.2.4 Output components for $\text{data}\%JOB = 3$ or 23

The following component is allocated if  $\text{data}\%NRHS > 0$  and is used to hold the solution vector.

$\text{data}\%X$  is a rank-2 allocatable array of type default REAL (or double precision REAL in the double version) of size  $\text{data}\%LARGEST\_INDEX$  (see Section 2.4) by  $\text{data}\%NRHS$ . On exit, if  $ICNTL(17) = 0$ , if  $I$  has been used to index a variable, then on the host  $\text{data}\%X(I, J)$  holds the solution for variable  $I$  to the  $J$ -th system and is set to zero otherwise ( $J = 1, 2, \dots, \text{data}\%NRHS$ ). If  $ICNTL(17) \neq 0$ , if the solution for variable  $I$  has been computed by the process with rank  $IPROC$ , then on process  $IPROC$   $\text{data}\%X(I, J)$  holds the solution for variable  $I$  to the  $J$ -th system and is set to zero otherwise ( $IPROC = 0, 1, \dots, \text{data}\%NPROC$ ).

#### 2.2.5 Input components for $\text{data}\%JOB = 4$

Prior to a call with  $\text{data}\%JOB = 4$  the following components must be set on the host:

$\text{data}\%NRHS$  is a scalar of type default INTEGER that must be set to the number of right-hand sides. This component is not altered. **Restriction:**  $\text{data}\%NRHS \geq 1$ .

$\text{data}\%B$  is a rank-2 allocatable array of type default REAL (or double precision REAL in the double version) that must be allocated with size  $\text{data}\%LARGEST\_INDEX$  (see Section 2.4) by  $\text{data}\%NRHS$ . On entry,  $\text{data}\%B$  must be set by the user so that if  $I$  is used to index a variable,  $\text{data}\%B(I, J)$  is the corresponding component of the right-hand side for the  $J$ -th system ( $J = 1, 2, \dots, \text{data}\%NRHS$ ). This component is altered.

#### 2.2.6 Output components for $\text{data}\%JOB = 4$

The following component is allocated on a call with  $\text{data}\%JOB = 4$  and is used to hold the solution vector.

$\text{data}\%X$  is a rank-2 allocatable array of type default REAL (or double precision REAL in the double version) of size  $\text{data}\%LARGEST\_INDEX$  (see Section 2.4) by  $\text{data}\%NRHS$ . On exit, if  $ICNTL(17) = 0$ , if  $I$  has been used to index a variable, then on the host  $\text{data}\%X(I, J)$  holds the solution for variable  $I$  to the  $J$ -th system and is set to zero otherwise ( $J = 1, 2, \dots, \text{data}\%NRHS$ ). If  $ICNTL(17) \neq 0$ , if the solution for variable  $I$  has been computed by the process with rank  $IPROC$ , then on process  $IPROC$   $\text{data}\%X(I, J)$  holds the solution for variable  $I$  to the  $J$ -th system and is set to zero otherwise ( $IPROC = 0, 1, \dots, \text{data}\%NPROC$ ).

### 2.3 Control components

On exit from the initial call ( $\text{data}\%JOB = 1$ ), the control components of  $\text{data}$  are set to default values. If the user wishes to use values other than the defaults, the corresponding components of  $\text{data}$  should be reset on the host process after the initial call and prior to a call with  $\text{data}\%JOB = 2$  or 23.

`data%ICNTL` is a rank-1 array of type default `INTEGER` and size 30.

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

`ICNTL(2)` is the unit number for warning messages and has the default value 6. Printing of warning messages is suppressed if `ICNTL(2) < 0`.

`ICNTL(3)` is the unit number for diagnostic printing and has the default value 6. Printing is suppressed if `ICNTL(3) < 0`.

`ICNTL(4)` is used to control printing of diagnostic messages (all printing is on the host only). It has default value 1. Possible values are:

$\leq 0$  No printing.

1 Error and warning messages only.

2 As 1, plus some additional diagnostic printing.

3 As 2, but timings of parts of the code (elapsed wall clock times in seconds) are also printed.

`ICNTL(5)` is not currently used. It is given the default value 0.

`ICNTL(6)` controls whether zeros in the front are exploited. Zeros within the front are ignored if `ICNTL(6) = 0`. The default value is 1.

`ICNTL(7)` is used to control how the user wishes to supply the element matrices  $\mathbf{A}^{(k)}$  and the element right-hand side matrices  $\mathbf{B}^{(k)}$  on a call with `data%JOB = 3` or `23`. There are 4 options:

0 The element data and element right-hand sides are held in direct-access files. The data required by the process with rank `IPROC` must be readable by that process (`IPROC = 0, 1, \dots, data%NPROC-1`). For each subdomain, the element data is read in element-by-element as required by the corresponding process. This minimises storage requirements and data movement between processes. After a call with `data%JOB = 2`, `data%INV_LIST(JDOM)` holds the rank of the process that is to factorize subdomain `JDOM`. For each subdomain `JDOM` to be factorized by process `IPROC`, there must be an unformatted direct-access file holding the values of the entries in the element matrices and, if `data%NRHS > 0`, another holding the values of the entries in the element right-hand side matrices, that can be read by process `IPROC`. The record length given in the `RECL=` specifier of the `OPEN` statements for the direct-access files holding the element matrices and element right-hand side matrices must be that required for `REAL` (or double precision `REAL` in the double version) arrays of size `data%MFRELT*data%MFRELT`, and `data%MFRELT*data%NRHS`, respectively. The element matrices and element right-hand side matrices must be written to the direct-access files in the same order as they are held in `data%ELTVAR`. Each element matrix must be held as a full matrix, stored by columns. Each element right-hand side matrix must also be held as a full matrix, stored by columns (so that multiple right hand sides are stored as consecutive columns). The names of the files for subdomain `JDOM` must be given in `data%VALNAM(JDOM)` and `data%RHSNAM(JDOM)`, respectively (`JDOM = 1, 2, \dots, data%NDOM`).

1 As 0, except the element data and element right hand sides are held in unformatted sequential files. In this case, all the element data for a subdomain is read in by the process to which it is assigned at once. This requires more memory.

2 As 1, except the host must be able to read all the files. For each subdomain, the data is read by the host and then passed to the process assigned to that subdomain before the factorization begins. This requires the host to have more memory and each process must be able to store the data for all the subdomains assigned to it at once.

3 The user must supply the element data and the element right-hand sides in memory on the host using `data%VALUES` and `data%RHSVAL`. This option avoids reading from direct-access or

sequential files but it does involve more data movement between processes than  $ICNTL(7) = 0$  or 1.

- 4 The user must supply the element data and the element right-hand sides in memory on each process using `data%VALUES` and `data%RHSVAL`. Supplying the data in this way avoids reading from direct-access or sequential files as well as data movement between processes. This option is suitable for shared memory machines.
- 5 On each process, the user must supply the element data and the element right-hand sides for each of the subdomains assigned to it in memory using `data%RVAL` and `data%RHS_VAL`. Supplying the data in this way avoids reading from direct-access or sequential files as well as data movement between processes; the amount of data required to be held on each process is less than for  $ICNTL(7) = 4$  (assuming more than one process is used).

**Restriction:**  $ICNTL(7) = 0, 1, 2, 3, 4,$  or 5.

$ICNTL(8)$  has the default value 0. If the matrix is found to be singular during the decomposition and  $ICNTL(8)$  is equal to 0, an error flag is set and the computation terminates (see error return -12 in Section 2.5). If  $ICNTL(8)$  is nonzero, a warning is given and the computation continues.

$ICNTL(9)$  controls the order in which the elements are assembled in the subdomains. If  $ICNTL(9) = 0$  (the default), the assembly order is generated automatically using MC53 during the analyse phase (`data%JOB = 2`). If  $ICNTL(9) > 0$ , the user must specify the assembly order using the array `data%NORDER`. Otherwise, the elements are assembled in the order in which they are given in `data%ELTVAR`.

$ICNTL(10)$  is used to control whether the user wishes to decide which process is to factorize which subdomain. If  $ICNTL(10) = 0$  (the default), this choice is made automatically during the analyse phase (`data%JOB = 2`). Otherwise, the user must choose a process for each subdomain using `data%INV_LIST`.

$ICNTL(11)$  controls whether the user wishes to call MP42 with `JOB = 4` to solve for further right-hand sides. If  $ICNTL(11) = 0$  (the default), both the  $L$  and  $U$  factors are stored and the solve phase may be called. If  $ICNTL(11)$  is nonzero, the  $L$  factor is not stored. This reduces storage requirements but MP42 may not be called with `JOB = 4`.

$ICNTL(12)$  controls whether the user wants the direct-access files used to hold the matrix factors to be deleted at the end of the computation. If  $ICNTL(12) = 0$  (the default), when the final call is made to MP42 (`data%JOB = 5`), the direct-access files are deleted. Otherwise, the direct-access files are disconnected but not deleted.  $ICNTL(12)$  is not used if  $ICNTL(14)$  is equal to 0.

$ICNTL(13)$  controls the size of the buffers (work arrays) associated with the direct-access files used to hold the matrix factors. If  $ICNTL(13) = 0$  (the default), the buffer sizes are chosen by the code. If  $ICNTL(13)$  is nonzero, the user must set buffer sizes in `data%LENBUF`.

$ICNTL(14)$  controls whether or not direct-access files are used to hold the matrix factors. If  $ICNTL(14) = 0$  (the default), direct-access files are **not** used and the factors are held in main memory. Otherwise, unformatted direct-access files are used. If  $ICNTL(14) > 0$ , the code automatically names the files and they are written to the current directory. The files for the factors on subdomain 1 are called `ufact.0001`, `lfact.0001`, `integ.0001`, on subdomain 2 they are `ufact.0002`, `lfact.0002`, `integ.0002`, and so on. The files for the factors for the interface problem are `ufact_interf`, `lfact_interf`, `integ_interf`. If  $ICNTL(14) < 0$ , the user must supply names for the files in `data%FILES1`. If the user wishes to run a second instance of the module before the final call for the first instance (`data%JOB = 5`), `data%ICNTL(14)` **must** be set to a negative value and file names provided by the user in `data%FILES1`.

$ICNTL(15)$  controls whether or not sequential files are used to hold the data that remains in the frontal matrix and corresponding right-hand side once the factorization on the subdomain is complete. If  $ICNTL(15) = 0$  (the default), files are **not** used. Otherwise, unformatted sequential files are used (using files reduces storage requirements but the extra I/O involved can increase the overall computational time). If  $ICNTL(15) > 0$ , the

code automatically names the files and they are written to the current directory. The remaining data for subdomain 1 is written to files `fvar.0001` and (if `data%NRHS > 0`) `frhs.0001`, for subdomain 2 the files are `fvar.0002` and `frhs.0002`, and so on. If `ICNTL(15) < 0`, the user must supply names for the files for the factors in `data%FILES2`. If the user wishes to run a second instance of the module before the final call for the first instance (call with `JOB = 5`), `data%ICNTL(15)` **must** be set to a negative value and file names provided by the user in `data%FILES2`.

`ICNTL(16)` has the default value 32. `ICNTL(16)` is the minimum number of variables that are eliminated at each stage of the factorization. Increasing `ICNTL(16)` in general increases the number of floating-point operations and real storage requirements but allows greater advantage to be taken of Level 3 BLAS and reduces integer storage.

`ICNTL(17)` controls whether or not the solution vector is assembled on the host. If `ICNTL(17) = 0` (the default), the solution is assembled in `data%X` on the host. Otherwise, on exit, each process holds the part of the solution vector that it computed.

`ICNTL(18)` to `ICNTL(30)` are not currently used but are set to zero.

`data%CNTL` is a rank-1 array of type default REAL (or double precision REAL in the double version) and size 10.

`CNTL(1)` has the default value zero. The matrix is declared singular if, during the factorization, the entry of largest absolute value in any column is less than or equal to `CNTL(1)`.

`CNTL(2)` has the default value 0.01. An element of a frontal matrix is only considered suitable for use as a pivot if it is of absolute value at least as large as `CNTL(2)` times the entry of largest absolute value in its column.

`CNTL(3)` to `CNTL(10)` are not currently used but are set to zero.

## 2.4 Information components

The components of `data` described in this section are used to hold information that may be of interest to the user. Some of the information is available on each process and some only on the host.

### 2.4.1 Information on each process

The following information is significant on each process. The information is available after a call to MP42 with `data%JOB = 1, 2, 3, 23, 4, 5`.

`data%ERROR` is a variable of type default INTEGER that is used as an error and a warning flag. A nonzero value indicates an error has been detected or a warning has been issued (see Section 2.5). If an error is detected, the information contained in the other components of `data` described in this section may be incomplete.

`data%NPROC` is a variable of type default INTEGER that is set to the number of processes used by MP42. `data%NPROC` is the number of processes associated with the communicator `data%COMM` and is set by a call within MP42 to `MPI_COMM_SIZE`.

`data%RANK` is a variable of type default INTEGER that holds the rank of the process in the global communicator `data%COMM`. The host is defined to be the process with `data%RANK = 0`.

### 2.4.2 Information available on the host

The following information is available **only** on the host. If an error is detected (see Section 2.5), the information may be incomplete.

**Information available on exit from a call with `data%JOB = 2` or `23`.**

`data%LARGEST_INDEX` is a variable of type default INTEGER that holds the largest integer used to index a variable in the finite element domain.

`data%MAX_NDF` is a variable of type default INTEGER that holds the maximum number of variables per element.

`data%NGUARD` is a rank-1 allocatable array of type default INTEGER of size `data%NDOM`. `data%NGUARD(JDOM)` holds the number of interface variables for subdomain `JDOM` (`JDOM = 1, 2, ..., data%NDOM`).

`data%FLAG_52` is a rank-1 allocatable array of type default INTEGER of size `data%NDOM`. `data%FLAG_52(JDOM)` holds the MA52A/AD error flag for subdomain `JDOM` (`JDOM = 1, 2, ..., data%NDOM`).

`data%NDF` is a rank-1 allocatable array of type default INTEGER of size `data%NDOM`. `data%NDF(JDOM)` holds the number of variables in subdomain `JDOM` (`JDOM = 1, 2, ..., data%NDOM`).

`data%NFRONT` is a rank-1 allocatable array of type default INTEGER of size `data%NDOM`. `data%NFRONT(JDOM)` holds a lower bound on the maximum frontsizes for the frontal elimination on subdomain `JDOM` (`JDOM = 1, 2, ..., data%NDOM`).

`data%RMS` is a rank-1 allocatable array of type default REAL (or double precision REAL in the double version) of size `data%NDOM`. `data%RMS(JDOM)` holds a lower bound on the root mean squared frontsize for the frontal elimination on subdomain `JDOM` (`JDOM = 1, 2, ..., data%NDOM`).

`data%OPS` is a rank-1 allocatable array of type default REAL (or double precision REAL in the double version) of size `data%NDOM`. `data%OPS(JDOM)` holds an estimate of the number of floating-point operations (flops) in the innermost loops for the frontal elimination on subdomain `JDOM` (`JDOM = 1, 2, ..., data%NDOM`).

`data%FLSIZE` is a rank-2 allocatable array of type default REAL of size 2 by `data%NDOM`. `data%FLSIZE(J, JDOM)`, `J = 1, 2` hold, respectively, the estimated storage needed for the real and integer data for the matrix factors on subdomain `JDOM` (`JDOM = 1, 2, ..., data%NDOM`). Note that, if `data%NRHS` right-hand sides are to be solved on the subsequent call with `data%JOB = 3` then, since the right-hand side vectors are stored with the  $U$  factor, the estimated storage needed for the  $U$  factor (including right-hand sides) is  $data%FLSIZE(1, JDOM)/2 + data%NRHS * (data%NDF(JDOM) - data%NGUARD(JDOM))$  and for  $L$  factor it is  $data%FLSIZE(1, JDOM)/2$ .

`data%NORDER` is a rank-2 allocatable array of type default INTEGER of size  $\max_{1 \leq JDOM \leq data%NDOM} data%NELTSB(JDOM) + 1$  by `data%NDOM`. Within subdomain `JDOM`, the elements are locally labelled 1, 2, ..., `data%NELTSB(JDOM)`, according to the order in which the user inputs the variable lists in `data%ELTVAR`. On subdomain `JDOM`, the elements will be assembled during the factorize phase in the order `data%NORDER(1, JDOM)`, `data%NORDER(2, JDOM)`, ..., `data%NORDER(data%NELTSB(JDOM), JDOM)`.

**Information available on exit from a call with `data%JOB = 3` or 23.**

`data%STATIC` is a variable of type default INTEGER that holds the total number of static condensations performed.

`data%SINGULAR` is a variable of type default LOGICAL that is set to `.TRUE.` if the matrix is found to be singular.

`data%FLOPS` is a variable of type default REAL (or double precision REAL in the double version) that holds the total number of floating-point operations (flops) in the innermost loops of the factorization (this is the total for all the subdomains and the interface).

`data%NZL` is a variable of type default REAL (or double precision REAL in the double version) that holds the total number of entries in the  $L$  factors.

`data%NZU` is a variable of type default REAL (or double precision REAL in the double version) that holds the total number of entries in the  $U$  factors, plus the right-hand sides (if `data%NRHS = 0`, `data%NZU = data%NZL`).

`data%STORINT` is a variable of type default REAL (or double precision REAL in the double version) that holds the total storage for the row and column indices in INTEGER words.

`data%NLEFT` is a rank-1 allocatable array of type default INTEGER of size `data%NBLOCK`. `data%NLEFT(JDOM)` holds the number of variables left in the front at the end of the elimination process for subdomain `JDOM` (`JDOM = 1, 2, ..., data%NDOM`). Note that, because of stability and efficiency considerations, `data%NLEFT(JDOM)` may be larger than `data%NGUARD(JDOM)`.

`data%INFO_42` is a rank-2 allocatable array of type default INTEGER of size 23 by `data%NDOM+1`. `data%INFO_42(1:23, JDOM)` holds the MA42B/BD integer information array for subdomain `JDOM` (`JDOM = 1,`

2,..., data%NDOM) and for JDOM = data%NDOM+1 it holds the MA42B/BD integer information array for the interface problem. Note that on the subdomains the information in data%INFO\_42 is incomplete since the factorization on the subdomain is a partial factorization (interface variables not eliminated).

data%RINFO\_42 is a rank-2 allocatable array of type default REAL (or double precision REAL in the double version) of size 2 by data%NDOM+1. data%RINFO\_42(:, JDOM) holds the MA42B/BD real information array for subdomain JDOM (JDOM = 1, 2,..., data%NDOM) and for JDOM = data%NDOM+1, it holds the MA42B/BD real information array for the interface problem. Note that on the subdomains the information in data%RINFO\_42 is incomplete since the factorization on the subdomain is a partial factorization (interface variables not eliminated).

data%INFO\_63 is a rank-1 array of type default INTEGER of size 15. data%INFO\_63 holds the MC63A/AD integer information array for the interface problem.

data%RINFO\_63 is a rank-1 array of type default REAL (or double precision REAL in the double version) of size 6. data%RINFO\_63 holds the MC63A/AD real information array for the interface problem.

## 2.5 Error diagnostics

On successful completion, a call to MP42 will exit with the component data%ERROR set to 0. Other values for data%ERROR and the reasons for them are given below.

### 2.5.1 Error diagnostics for data%JOB = 1

- 1 MPI has not been initialized by the user. Immediate return. An error message is printed on the default output unit.

### 2.5.2 Error and warning diagnostics for data%JOB = 2 or 23

A negative value for data%ERROR is associated with a fatal error. Error messages are output on unit data%ICNTL(1). Possible negative values are:

- 2 Either data%NDOM ≤ 1 or data%NDOM > data%NELT.
- 4 Either data%ELTVAR is not allocated or has been allocated with size less than data%ELTPTR(data%NELT+1)-1. This error is also returned if one or more variable indices in data%ELTVAR is out of range (ie. is less than 1) or there are duplicate entries in a row. data%IOUT and data%IDUP hold, respectively, the number of out of range and duplicate entries.
- 5 Error detected in data%ELTPTR. Either data%ELTPTR has not been allocated or has been allocated with size less than data%NELT+1, or the entries of data%ELTPTR are not monotonic increasing.
- 6 data%ICNTL(7) out of range (ie. data%ICNTL(7) ≠ 0, 1, 2, 3, 4, or 5).
- 7 Either the array data%NELTSB has not been allocated or has been allocated with size less than data%NDOM, or data%NELTSB(JDOM) < 1 for one or more subdomain JDOM (1 ≤ JDOM ≤ data%NDOM).
- 8 One or more subdomain have no interface variables.
- 9 Either the array data%INV\_LIST has not been allocated or has been allocated with size less than data%NBLOCK, or an entry in data%INV\_LIST is out of range (data%ICNTL(10) nonzero).
- 11 Error in Fortran ALLOCATE statement. The STAT parameter is returned in data%STAT. If the user is not using direct-access files (data%ICNTL(14)=0), it may be possible to avoid this error by rerunning with data%ICNTL(14) ≠ 0, or if data%ICNTL(13) is nonzero, by reducing the buffer sizes held in data%LENBUF.
- 13 data%JOB does not have the same value on all processes or has an invalid value.
- 18 The call follows a call with data%JOB = 5.
- 24 Either the array data%NORDER has not been allocated or has been allocated with an incorrect size (ICNTL(9) > 0). This error is also returned if the supplied element order is found not to be a permutation for

one or more of the subdomains.

Warning messages are associated with positive values of `data%ERROR`. Warning messages are output on `data%ICNTL(2)`. Possible warnings are:

- +1 Warning issued by MC53A/AD for one or more subdomain.

### 2.5.3 Error diagnostics for `data%JOB = 3` or `23`

A negative value for `data%ERROR` is associated with a fatal error. Error messages are output on unit `data%ICNTL(1)`. Possible values are:

- 10 If `data%ICNTL(7) = 0, 1, or 2`, either `data%VALNAM` or `data%RHSNAM` is not allocated or is allocated with size less than `data%NDOM`. If `data%ICNTL(7) = 3 or 4`, either `data%VALUES` or `data%RHS` is not allocated or is allocated with incorrect size. If `data%ICNTL(7) = 5`, either `data%RVAL` or `data%RHS_VAL` is not allocated or is allocated with incorrect size.
- 11 Error in Fortran ALLOCATE statement. The `STAT` parameter is returned in `data%STAT`.
- 12 Singularity detected in the matrix during the factorization with the control component `data%ICNTL(8)` equal to zero.
- 13 `data%JOB` does not have the same value on all processes or has an invalid value.
- 14 Error in Fortran INQUIRE statement. `data%IOSTAT` holds the `IOSTAT` parameter.
- 15 Error when writing to a direct-access file.
- 16 Error when reading from a direct-access file.
- 17 Error in Fortran OPEN statement.
- 19 An error was returned on a previous call or the call follows a call with `data%JOB = 1` (no `data%JOB = 2` call) or follows a call with `data%JOB = 5`.
- 20 Failed to find a unit to which a file could be connected.
- 21 Either `data%LENBUF` has not been allocated or has been allocated with incorrect size, or `data%LENBUF(1,JDOM) ≤ 0`, or `data%LENBUF(3,JDOM) ≤ 0`, or `data%ICNTL(11) = 0` and `data%LENBUF(2,JDOM) ≤ 0` ( $1 ≤ JDOM ≤ data%NDOM+1$ ) (`data%ICNTL(13)` nonzero).
- 22 `data%NRHS < 0`.
- 23 `data%ICNTL(7) = 0` and `data%MFRELT` is less than the maximum number of variables per element. `data%MAX_NDF` holds the maximum number of variables per element.
- 25 `data%FILES1` is either not allocated or is allocated but with incorrect size (`ICNTL(14) < 0`).
- 26 `data%FILES2` is either not allocated or is allocated but with incorrect size (`ICNTL(15) < 0`).

Warning messages are associated with positive values of `data%ERROR`. Warning messages are output on `data%ICNTL(2)`. Possible warnings are:

- +2 The matrix **A** has been found to be singular and the control component `data%ICNTL(8)` was nonzero (see Section 2.4).
- +4 One or more of the user-supplied buffer sizes in `data%LENBUF` have been altered (`data%ICNTL(13)` nonzero).
- +3,+5,+6,+7 Combination of the above warnings.

### 2.5.4 Error diagnostics for `data%JOB = 4`

A negative value for `data%ERROR` is associated with a fatal error. Error messages are output on unit `data%ICNTL(1)`. Possible values are:

- 11 Error in Fortran ALLOCATE statement. The STAT parameter is returned in data%STAT.
- 13 data%JOB does not have the same value on all processes or has an invalid value.
- 16 Error when reading from a direct-access file.
- 17 Error in Fortran OPEN statement.
- 19 An error was returned on a previous call or the call was not preceded by a call with data%JOB = 3, or follows a call with data%JOB = 3 and data%ICNTL(11) nonzero, or follows a call with data%JOB = 5.
- 22 data%NRHS < 1. This error is also returned if data%B is either not allocated or is allocated but with incorrect size.

### 2.5.5 Error diagnostics for data%JOB = 5

A negative value for data%ERROR is associated with a fatal error. Error messages are output on unit data%ICNTL(1). Possible values are:

- 13 data%JOB does not have the same value on all processes or has an invalid value.

## 3 GENERAL INFORMATION

### 3.1 Summary of information.

**Use of common:** Common blocks are not used.

**Other routines called directly:** The HSL routines MA42I/ID, MA42A/AD, MA42B/BD, MA42C/CD, MA42J/JD, MA52A/AD, MA52C/CD, MA52F/FD, MC53I/ID, MC53A/AD, MC63I/ID, MC63A/AD, KB08A/AD. Subroutines private to the module are MP42B/BD, MP42C/CD, MP42L/LD, MP42M/MD, MP42N/ND, and MP42P/PD. In addition, MPI routines are called.

**Workspace:** Workspace is allocated by the code as required. The amount of workspace needed is dependent upon how the element matrices are stored, on data%LENBUF, and on the largest integer used to index a variable.

**Input/output:** The output units for the error and warning messages are data%ICNTL(1) and data%ICNTL(2) (see Section 2.3). The output unit for diagnostic printing is data%ICNTL(3).

**Restrictions:**

data%NDOM > 1,  
 data%NELT ≥ data%NDOM,  
 data%NRHS ≥ 0 (data%JOB = 3 or 23),  
 data%NRHS ≥ 1 (data%JOB = 4),  
 data%NELTSB(:) > 0,  
 0 ≤ data%INV\_LIST(:) < data%NPROC (data%ICNTL(10) nonzero),  
 data%LENBUF(:, :) ≥ 1 (data%ICNTL(13) nonzero).

**Portability:** Fortran 95 + TR 15581 (allocatable components) with MPI for message passing.

**Changes between Version 1.0.0 and Version 2.0.0:**

The addition of HSL\_MP01 to HSL has allowed the source form to be changed to free format and means that the user of no longer needs an INCLUDE line for the MPI constants. All the pointer array components have been changed to allocatable components, which should be more efficient and avoids any danger of memory leakage.

## 4 METHOD

HSL\_MP42 implements a multiple front algorithm. Details of the algorithm are given in Duff and Scott (1994) and Scott (1999).

data%JOB = 1

The control components are given default values.

data%JOB = 2

The input data is first checked for errors. The control components and scalar input components are then broadcast from the host to all processes. The host process calls MA52A/AD to generate lists of interface variables (the guard elements). Unless data%ICNTL(10) has been reset to a nonzero value, the host assigns each subdomain to a process. This division of the subdomains between the processes aims to balance the floating-point operations.

data%JOB = 3

Data for each subdomain is sent from the host to its assigned process IPROC. For each of its assigned subdomains, IPROC calls MC53 to order the elements. Process IPROC generates unit numbers for the direct-access files that will hold the matrix factors, calls the analyse and factorize phases of MA42, and uses MA52F/FD to preserve the partial factorization.

Data from MA52B/BD is sent to the host. The host reorders the subdomains using MC63 and uses MA42 to solve the interface problem. If data%NRHS > 0, the solution for the interface problem is sent to each process, and on each process MA52C/CD is called to perform the back substitution for its assigned subdomains.

data%JOB = 4

The host first performs error checks and broadcasts the number of right-hand sides to each process. For each of its assigned subdomains, process IPROC calls MA52C/CD to perform forward substitution. The partial solution vectors are sent to the host. Forward and back substitution for the interface problem is performed by the host using MA42C/CD. The solution for the interface problem is sent to each process, and on each process MA52C/CD is called to perform the back substitution on its subdomains.

data%JOB = 5

Arrays allocated by the code are deallocated, the direct-access files used to hold the matrix factors are closed and (optionally) are deleted.

MPI is used throughout for message passing.

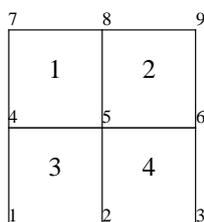
## References

Duff, I. S. and Scott, J. A. (1994). The use of multiple fronts in Gaussian elimination. Rutherford Appleton Laboratory Report RAL-94-040.

Scott, J. A. (1999). The design of a parallel frontal solver. Rutherford Appleton Laboratory Report RAL-TR-99-075.

## 5 EXAMPLE OF USE

We wish to solve the following simple finite-element problem in which the finite-element mesh comprises four 4-noded quadrilateral elements with one of degree of freedom at each node  $i$ ,  $1 \leq i \leq 6$  (the nodes 7, 8, and 9 are assumed constrained). The mesh is divided into 2 subdomains in which elements 1 and 2 comprise subdomain 1 and elements 3 and 4 comprise subdomain 2. We supply one right-hand side with the elements and then use data%JOB = 4 to solve for two further right-hand sides.



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

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

where the variable indices are indicated by the integers before each matrix (columns are identified symmetrically to rows). The corresponding element right-hand side  $\mathbf{B}^{(k)}$  ( $1 \leq k \leq 4$ ) are

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

The (assembled) right-hand sides that are used in the call with `data%JOB = 4` are

$$\begin{pmatrix} 12 \\ 28 \\ 14 \\ 15 \\ 36 \\ 18 \end{pmatrix} \quad \begin{pmatrix} 6 \\ 1 \\ 2 \\ 7 \\ 4 \\ -1 \end{pmatrix}.$$

The following program is used to solve this problem.

```

! Code to run MP42 on a finite element mesh composed of
! two subdomains.

      USE HSL_MP42_DOUBLE
      IMPLICIT NONE

      TYPE (MP42_DATA) data

      INTEGER ERCODE,NE,RHSCRD,VALCRD

! Start MPI
      CALL MPI_INIT(ERCODE)

! Define a communicator for the module
      data%COMM = MPI_COMM_WORLD

! Initialize instance
      data%JOB = 1
      CALL MP42AD(data)
! No need to order the elements within each subdomain. Reset data%ICNTL(9).
      data%ICNTL(9) = -1
! We will read in all matrix values to data%VALUES and data%RHSVAL
      data%ICNTL(7) = 3

! Read in data on host
      IF (data%RANK .EQ. 0) THEN

! Number of subdomains is 2

```

```

        data%NDOM = 2
! Solve for 1 right hand side
        data%NRHS = 1

! Read in the number of elements in whole domain
        OPEN (UNIT=5,FILE='mp42ads.data')
        READ (5,FMT=*) data%NELT

! Read number of elements in each subdomain
        ALLOCATE(data%NELTSB(1:data%NDOM))

        READ (5,FMT=*) data%NELTSB(1:data%NDOM)
! Read element variable lists
        ALLOCATE(data%ELTPTR(1:data%NELT+1))
        READ (5,FMT=*) data%ELTPTR(1:data%NELT+1)

        NE = data%ELTPTR(data%NELT+1) - 1
        ALLOCATE(data%ELTVAR(1:NE))
        READ (5,FMT=*) data%ELTVAR(1:NE)

! Read in reals
        READ (5,FMT=*) VALCRD
        ALLOCATE(data%VALUES(1:VALCRD))
        READ (5,FMT=*) data%VALUES(1:VALCRD)

! Read in element right hand sides
        READ (5,FMT=*) RHSCRD
        ALLOCATE(data%RHS(1:RHSCRD))
        READ (5,FMT=*) data%RHS(1:RHSCRD)

        END IF
        CALL MPI_BARRIER(data%COMM,ERCODE)
! Analyse and factorize phases
        data%JOB = 23
        CALL MP42AD(data)
        IF (data%ERROR.LT.0) GO TO 20
        IF (data%RANK.EQ.0) THEN
            WRITE (*,FMT=9000)
            WRITE (*,FMT=9010) data%X(1:data%LARGEST_INDEX,1)
        END IF

! We want to solve for 2 further right-hand sides.
! Allocate array B to hold right assembled right-hand sides.
        IF (data%RANK.EQ.0) THEN
            WRITE (*,FMT=9020)
            data%NRHS = 2
            ALLOCATE(data%B(1:data%LARGEST_INDEX,1:data%NRHS) )
            READ (5,FMT=*) data%B(1:data%LARGEST_INDEX,1:2)
        END IF

        data%JOB = 4
        CALL MP42AD(data)
        IF (data%ERROR.LT.0) GO TO 20

        IF (data%RANK.EQ.0)
&         WRITE (*,FMT=9010) data%X(1:data%LARGEST_INDEX,1:2)

! Final call
20 data%JOB = 5
        CALL MP42AD(data)
        CALL MPI_FINALIZE(ERCODE)

```

```

9000 FORMAT (' The solution is:')
9010 FORMAT (6F12.4)
9020 FORMAT (' Now solving for assembled right-hand sides.')
      STOP
      END

```

The input data used for this problem is:

```

4
2 2
1 3 5 9 13
4 5 5 6 4 5 1 2 5 6 2 3
40
2. 1. 1. 7. 3. 2. 2. 8. 4. 3. 2. 3. 3. 1. 3.
2. 2. 3. 6. 1. 3. 2. 1. 5. 2. 1. 8. 3. 1. 3.
2. 2. 8. 2. 2. 5. 3. 2. 5. 4.
12
3. 8. 5. 10. 12. 9. 12. 11. 14. 8. 17. 14.
12. 28. 14. 15. 36. 18.
6. 1. 2. 7. 4. -1.

```

When run using 1 or 2 processes, this produces the following output:

```

The solution is:
 1.0000      1.0000      1.0000      1.0000      1.0000      1.0000

Now solving for assembled right-hand sides.
 1.0000      1.0000      1.0000      1.0000      1.0000      1.0000
 1.0000      1.0000      0.0000      1.0000     -1.0000      0.0000

```