

1 SUMMARY

To read a file containing a sparse matrix held in Rutherford-Boeing format and manipulate it to the desired sparse matrix format. The user may specify the storage format the matrix is returned in, and random values can be optionally generated to match the matrix pattern. Rutherford-Boeing format can be used to specify either matrix data or supplementary data, however this package only supports matrix data. To read supplementary data, the HSL routine MC56 can be used. To write data in Rutherford-Boeing format the HSL routines MC54 and MC55 can be used for matrix data and supplementary data, respectively.

For information on the Rutherford-Boeing sparse matrix format, the user should consult the report

[1] I.S. Duff, R.G. Grimes and J.G. Lewis. The Rutherford-Boeing Sparse Matrix Collection. Rutherford Appleton Laboratory Technical Report RAL-TR-97-031 Revision 1, 1999.

ATTRIBUTES — Version: 1.1.0. **Types:** Real (single, double), Integer, Complex (single, double). **Calls:** HSL_FA14, HSL_MC34, MC56, HSL_ZD11, HSL_ZD13. **Date:** April 2010. **Origin:** J. D. Hogg, Rutherford Appleton Laboratory. **Language:** Fortran 95 + TR 15581 (allocatable components).

2 HOW TO USE THE PACKAGE

Access to the package requires a USE statement such as

Single precision version

```
USE HSL_MC56_single
```

Double precision version

```
USE HSL_MC56_double
```

Integer version

```
USE HSL_MC56_integer
```

Complex version

```
USE HSL_MC56_complex
```

Double complex version

```
USE HSL_MC56_double_complex
```

The version used determines the type of the values returned. Conversion is automatically performed from the file type if it is compatible, otherwise an error is returned. File type is determined from a three-letter type code in the header of the Rutherford-Boeing file. For matrices, the first letter of this type code indicates the data type and is one of the following:

"p", "q" - the file contains only the pattern of the matrix ("q" indicates the values are in an supplementary file). This can be read by any version of HSL_MC56.

"i" - the file contains an integer matrix. This can be read by any version of HSL_MC56.

"r" - the file contains a real matrix. This can be read by the `_single`, `_double`, `_complex` and `_double_complex` versions of HSL_MC56.

"c" - the file contains a complex matrix. This can be read by the `_complex` and `_double_complex` versions of HSL_MC56.

If it is required to use more than one of these modules at the same time, the derived type `mc56_control` described in Section 2.1 and the subroutine `mc56_peek` should be used only from one of the packages. This can be done, for example, as follows:

```
use hsl_mc56_double
use hsl_mc56_double_complex, only: mc56_read
```

The following subroutines are available to the user:

- `mc56_peek` may be called to read the header information of a file. This may be used determine the file type code so that the correct version of HSL_MC56 may be used on a subsequent call to `mc56_read`.
- `mc56_read` reads a matrix held in Rutherford-Boeing format into the supplied `zd11_type` or `zd13_type` variable. Optionally, the matrix may be converted between standard sparse matrix formats and random values may be generated to match a sparsity pattern read from the file.

2.1 The derived data types

For each problem, the user must employ the derived type defined by the module to declare a scalar of type `mc56_control`. The following pseudocode illustrates this.

```
use hsl_mc56_double
...
type (zd11_type) :: matrix
type (mc56_control) :: control
```

The derived data type `zd11_type` is used to return a sparse matrix in assembled form. To read an sparse matrix stored by elements, the derived data type `zd13_type` is used instead. The components of `mc56_control` are described in Section 2.2.4. The various sparse matrix formats offered by this package are described in Section 4.

2.2 Argument lists and calling sequences

2.2.1 Optional arguments

We use square brackets [] to indicate OPTIONAL arguments, which are always at the end of the argument list. Since we reserve the right to modify the argument list and to add additional optional arguments in future releases of the code, **we strongly recommend that all optional arguments be called by keyword, not by position.**

2.2.2 To obtain information about a matrix in a Rutherford-Boeing file

To obtain information found in the header of a file, the user may call the routine

```
call mc56_peek(filename, info[, m, n, nelt, nvar, nval, type_code, title, identifier])
```

`filename` is a scalar INTENT(IN) argument of type CHARACTER(LEN=*). It specifies the filename of the file to be read. HSL_MC56 will open the file, read the header and then close the file.

`info` is a scalar INTENT(OUT) argument of type INTEGER. On exit it contains a status code indicating success or failure of the subroutine, see Section 2.3 for details.

`m` is an optional scalar INTENT(OUT) argument of type INTEGER. On exit it contains the number of rows in the matrix.

`n` is an optional scalar `INTENT(OUT)` argument of type `INTEGER`. On exit it contains the number of columns in the matrix.

`nelt` is an optional scalar `INTENT(OUT)` argument of type `INTEGER`. On exit it contains the number of elements in the file, or 0 if the matrix is assembled.

`nvar` is an optional scalar `INTEGER(OUT)` argument of type `INTEGER`. On exit it contains the number of variable indices specified in the file.

`nval` is an optional scalar `INTEGER(OUT)` argument of type `INTEGER`. On exit it contains the number of values specified in the file.

`type_code` is an optional `INTENT(OUT)` argument of type `CHARACTER(LEN=3)`. On exit it contains the three-letter type code found in the Rutherford-Boeing file.

`title` is an optional `INTENT(OUT)` argument of type `CHARACTER(LEN=72)`. On exit it contains the title of the matrix read from the Rutherford-Boeing file.

`identifier` is an optional `INTENT(OUT)` argument of type `CHARACTER(LEN=8)`. On exit it contains the 8 character identifier read from the Rutherford-Boeing file.

2.2.3 To read a matrix from a Rutherford-Boeing file

To read a file, the user may call the routine

```
call mc56_read(filename, matrix, control, info, [type_code, title, identifier, seed])
```

`filename` is a scalar `INTENT(IN)` argument of type `CHARACTER(LEN=*)`. It specifies the filename of the file to be read. HSL_MC56 will open the file, read it and close it.

`matrix` is a scalar `INTENT(OUT)` argument of type `ZD11_type` if the matrix to be read is an assembled matrix, or `ZD12_type` if the matrix to be read is in element form.

`control` is a scalar `INTENT(IN)` argument of type `MC56_control` that contains parameters affecting how the file is interpreted. See Section 2.2.4 for further details.

`info` is a scalar `INTENT(OUT)` argument of type `INTEGER`. On exit it contains a status code indicating success or failure of the subroutine, see Section 2.3 for details.

`type_code` is an optional `INTENT(OUT)` argument of type `CHARACTER(LEN=3)`. On exit it contains the three letter type code found in the Rutherford-Boeing file.

`title` is an optional `INTENT(OUT)` argument of type `CHARACTER(LEN=72)`. On exit it contains the title of the matrix read from the Rutherford-Boeing file.

`identifier` is an optional `INTENT(OUT)` argument of type `CHARACTER(LEN=8)`. On exit it contains the 8 character identifier read from the Rutherford-Boeing file.

`seed` is an optional `INTENT(INOUT)` argument of type `FA14_seed`. If present and random values are to be generated (`control%values ≥ 2`), it is used as the seed for the random number generator used. If it is not present, HSL_MC56 will use its own random seed.

2.2.4 The derived data type for holding control parameters

The derived data type `MC56_control` is used to hold controlling data. The components, which are automatically given default values in the definition of the type, are:

*Components that apply to both **assembled** and **elemental** entry:*

`extra_space` is a scalar of type default REAL. When allocating array components `matrix`, the amount of space allocated will be the minimum amount required multiplied by this number. The default value is 1.0.

`lwr_upr_full` is a scalar of type INTEGER. It is only used when the matrix to be read is symmetric, skew symmetric or Hermitian, and it can take the following values:

- 1 Only lower triangular entries are returned.
- 2 Only upper triangular entries are returned.
- 3 Both lower and upper triangular entries are returned.

The default value is 1.

*Components that apply to only **assembled** entry:*

`add_diagonal` is a logical of type LOGICAL. If `.true.`, then missing diagonal entries will be added to the matrix as explicit zeros.

`format` is a scalar of type INTEGER. It determines the output sparse matrix format for assembled matrices, and can take the following values:

- 1 Compressed sparse column. `matrix%ptr` and `matrix%row` are used to store the pattern, and `matrix%val` to store the values if required.
- 2 Compressed sparse row. `matrix%ptr` and `matrix%col` are used to store the pattern, and `matrix%val` to store the values if required.
- 3 Coordinate. `matrix%row` and `matrix%col` are used to store the pattern, and `matrix%val` to store the values if required.

The default value is 1.

`values` is a scalar of type INTEGER. It determines what, if any, values are returned. It can take the values listed below. If a negative value is supplied then values from the file are ignored, if positive then values are only generated if no values are found in the file.

0 Matrix values are returned if and only if they are given in the file to be read.

1 Matrix values are not returned, only the pattern is read.

-2, 2 Values are distributed uniformly over the interval $[-1, 1]$. If the type code indicates the pattern is symmetric, skew-symmetric or Hermitian, this is reflected in the numerically values.

-3, 3 If the matrix is real symmetric or complex Hermitian, the off-diagonal values are distributed uniformly over the interval $[-1, 1]$ (real) or ball $\|x\|_\infty < 1.0$ (complex) such that the matrix has the specified property. Diagonal entries are given a real value $\max(100.0, 10k)$, where k is the number of entries in the column. This ensures the matrix is strongly diagonally dominant, and hence that a Cholesky factorization exists. Additional entries are added to the diagonal if required. If the matrix is not real symmetric or complex Hermitian, this option is equivalent to `control%values = 2`.

-4, 4 If the matrix is symmetric, skew symmetric or Hermitian, but `control%lwr_upr_full = 3`, values are distributed uniformly over the interval $[-1, 1]$ and the matrix is numerically unsymmetric. If the matrix is unsymmetric, or `control%lwr_upr_full \neq 3`, this has the same effect as `control%values = 2`.

The default value is 0.

2.3 Warning and error messages

A successful return is indicated by `info` having the value zero. A negative value is associated with an error. Possible negative values are:

- 1 Unable to find an available unit on which to open the file.
- 2 File does not exist, or insufficient permissions to read the file.
- 3 File does not appear to be in Rutherford-Boeing format.
- 4 Error on file i/o.
- 5 Attempted to read non-compatible type. Complex matrices cannot be read with the `_integer`, `_single` or `_double` versions of this package. Real matrices cannot be read with the `_integer` version of this package.
- 6 Attempted to read elemental matrix into assembled data type, or assembled matrix into elemental data type.
- 10 `control%extra_space < 1.0`.
- 11 `control%lwr_upr_full` has invalid value.
- 12 `control%format` has invalid value.
- 13 `control%values` has invalid value.
- 20 Allocation error.

Possible positive values are:

- +1 Auxiliary file exists. The first letter of `type_code` read from the file is 'q'. This indicates that there exists an auxiliary file containing matrix values, however only the pattern has been read. Values to match the pattern found have been generated if `control%values < 0` or `≥ 2`.

3 GENERAL INFORMATION

Workspace: Provided automatically by the module.

Other routines called directly: HSL_FA14, HSL_MC34, MC56, HSL_ZD11, HSL_ZD13.

Input/output: No printing or other output occurs. The specified file is opened read-only mode on a unit number chosen by HSL_MC56, is read and is then closed before returning to the user.

Restrictions: `filename` must be a valid Rutherford-Boeing file, `control%extra_space ≥ 1.0`,
`1 ≤ control%lwr_upr_full ≤ 3`, `1 ≤ control%format ≤ 3`, `control%values = -4, -3, -2, 0, 1, 2, 3, or 4`.

Portability: Fortran 95, plus allocatable components of derived types.

`matrix%starts(:)` is allocated to have size `matrix%nel+1`, and `matrix%starts(elt)` has been set to the position within `matrix%vars(:)` of the first variable in element `elt`. `matrix%starts(matrix%nel+1)` has been set to one more than the position of the last variable of the final element.

`matrix%vars(:)` is allocated to have size equal to the number of variables. For each element `elt`, the array slice `matrix%vars(matrix%starts(elt):matrix%starts(elt+1)-1)` holds the associated variable list.

`matrix%values(:)` is allocated to have size equal to the number of entries if values are to be returned (otherwise it is unallocated). Elements are stored consecutively, and element `elt` has a number of values equal to either n^2 in the unsymmetric (or full symmetric) case, or $n(n+1)$ in the symmetric case, where $n=(matrix%starts(elt+1)-matrix%starts(elt))$. For each element the variables are stored as either a dense matrix in the unsymmetric case, or a packed matrix in the symmetric case, both by columns.

For example, reading the above matrix is equivalent to the following:

```
matrix%n = 6
matrix%nel = 4
allocate(matrix%starts(5), matrix%vars(12), matrix%values(40))
matrix%starts(:) = (/ 1, 3, 5, 9, 13 /)
matrix%vars(:) = (/ 4, 5, 5, 6, 4, 5, 1, 2, 5, 6, 2, 3 /)
matrix%values(1:4) = (/ 2., -1., 1., 7. /)
matrix%values(5:8) = (/ 3., 4., 2., 8. /)
matrix%values(9:24) = (/ 4., ..., 5. /)
matrix%values(25:40) = (/ 2., ..., 4. /)
```

4.2 Coordinate format

Coordinate format stores an assembled matrix as a series of non-zero entries. A list of triples (i, j, v) is stored that indicates $A_{ij} = v$. If an entry corresponding to A_{ij} does not occur in the list, then $A_{ij} = 0$. After reading a matrix in assembled format using HSL_MC56 with `control%format=3`, the following components of the derived type `zd11_type` are set:

`matrix%m` is the number of rows in the matrix

`matrix%n` is the number of columns in the matrix

`matrix%ne` is the number of entries in the matrix

`matrix%row(:)`, `matrix%col(:)` and `matrix%val(:)` are allocated to have size `matrix%ne`. The triple $(matrix%row(i), matrix%col(i), matrix%val(i))$ represents the row, column and value of the i -th entry of the matrix. They need not be in any particular order. If only the pattern is to be returned, then `matrix%val(:)` will be unallocated.

For example, reading the above matrix is equivalent to the following:

```
matrix%n = 6
matrix%m = 6
matrix%ne = 28
allocate(matrix%rows(28), matrix%cols(28), matrix%val(28))
matrix%row(:) = (/ 1, 2, 4, 5, 1, 2, 3, 4, 5, 6, ..., 6 /)
matrix%col(:) = (/ 1, 1, 1, 1, 2, 2, 2, 2, 2, 2, ..., 6 /)
matrix%val(:) = (/ 6., 1., 2., 3., 1., 7., 5., 3., 10., 2., ..., 11. /)
```

4.3 Compressed Sparse Column (CSC)

Compressed sparse column (CSC) format stores columns of the matrix consecutively as sparse vectors. That is to say that each column of the matrix is stored as a list of row indices and associated values. If row i is not present in the list for column j , then $A_{ij} = 0$. After reading a matrix in assembled format using HSL_MC56 with `control%format=1`, the following components of the derived type `zd11_type` are set:

`matrix%m` is the number of rows in the matrix

`matrix%n` is the number of columns in the matrix

`matrix%ne` is the number of entries in the matrix

`matrix%ptr(:)` is allocated to have size `matrix%n+1`, and `matrix%ptr(col)` is set to the position within `matrix%row(:)` of the first variable in column `col`. `matrix%starts(matrix%n+1)` is set to one more than the position of the last variable of the final column.

`matrix%row(:)` and `matrix%val(:)` are allocated to have size equal to the number of entries. For each column `col`, the array sections `matrix%row(matrix%ptr(col):matrix%ptr(col+1)-1)` and `matrix%val(matrix%ptr(col):matrix%ptr(col+1)-1)` hold the associated row indices and values respectively. If only the pattern is to be returned, then `matrix%val(:)` will be unallocated.

For example, reading the above matrix is equivalent to the following:

```
matrix%n = 6
matrix%m = 6
matrix%ne = 28
allocate(matrix%ptr(7), matrix%row(28), matrix%val(28))
matrix%ptr(:) = (/ 1, 5, 11, 15, 19, 25, 29 /)
matrix%row(:) = (/ 1, 2, 4, 5, 1, 2, 3, 4, 5, 6, ..., 6 /)
matrix%val(:) = (/ 6., 1., 2., 3., 1., 7., 5., 3., 10., 2., ..., 11. /)
```

4.4 Compressed Sparse Row (CSR)

Compressed sparse row (CSR) is similar to CSC, except the matrix is stored by rows rather than columns. After reading a matrix in assembled format using HSL_MC56 with `control%format=2`, the following components of the derived type `zd11_type` are set:

`matrix%m` is the number of rows in the matrix

`matrix%n` is the number of columns in the matrix

`matrix%ne` is the number of entries in the matrix

`matrix%ptr(:)` is allocated to have size `matrix%n+1`, and `matrix%ptr(row)` is set to the position within `matrix%col(:)` of the first variable in column `row`. `matrix%starts(matrix%n+1)` is set to one more than the position of the last variable of the final row.

`matrix%col(:)` and `matrix%val(:)` are allocated to have size equal to the number of entries. For each row `row`, the array slices `matrix%col(matrix%ptr(row):matrix%ptr(row+1)-1)` and `matrix%val(matrix%ptr(row):matrix%ptr(row+1)-1)` hold the associated column indices and values respectively. If only the pattern is to be returned, then `matrix%val(:)` will be unallocated.

For example, reading the above matrix is equivalent to the following:

```

matrix%n = 6
matrix%m = 6
matrix%ne = 28
allocate(matrix%ptr(7), matrix%col(28), matrix%val(28))
matrix%ptr(:) = (/ 1, 5, 11, 15, 19, 25, 29 /)
matrix%col(:) = (/ 1, 2, 4, 5, 1, 2, 3, 4, 5, 6, ..., 6 /)
matrix%val(:) = (/ 6., 1., 2., 3., 1., 7., 5., 3., 10., 2., ..., 11. /)

```

5 EXAMPLE OF USE

The following program demonstrates the use of HSL_MC56 to read an unsymmetric matrix:

```

program hsl_mc56ds
  use hsl_mc56_double
  use hsl_zd11_double
  use hsl_zd13_double
  implicit none

  type(zd11_type) :: assembled_matrix ! Type for reading assembled matrices
  type(zd13_type) :: elemental_matrix ! Type for reading elemental matrices
  type(mc56_control) :: control ! Type for hsl_mc56 control parameters
  integer :: info ! Return flag for hsl_mc56 subroutines
  character(len=3) :: type_code ! String used to hold file data type
  character(len=72) :: title ! String used to hold matrix title
  integer :: i, j, k ! Temporary variables
  integer :: vptr ! Pointer into elemental_matrix%values

  ! Determine if this is an assembled or elemental matrix
  call mc56_peek("hsl_mc56ds.data", info, type_code=type_code)

  ! Read into correct data type
  if(type_code(3:3).eq."a") then
    ! Assembled matrix
    call mc56_read("hsl_mc56ds.data", assembled_matrix, control, info, &
      title=title)
    write(*, "(a)") title
    write(*, "(a,3(i4,a))") "Assembled matrix of size ", assembled_matrix%m, &
      "x", assembled_matrix%n, " (ne = ", assembled_matrix%ne, ")"
    do i = 1, assembled_matrix%n
      j = assembled_matrix%ptr(i)
      k = assembled_matrix%ptr(i+1)-1
      write(*,"(a,i4,a)",advance="no") "Col ", i, " row : "
      write(*,"(10i6)") assembled_matrix%row(j:k)
      write(*,"(8x,a)",advance="no") " val : "
      write(*,"(10f6.2)") assembled_matrix%val(j:k)
    end do
  else ! type_code(3:3) = "e"
    ! Elemental matrix
    call mc56_read("hsl_mc56ds.data", elemental_matrix, control, info, &

```

```

        title=title)
write(*, "(a)") title
write(*, "(a,3(i4,a))") "Elemental matrix of size ", elemental_matrix%n, &
  "x", elemental_matrix%n, ", ", elemental_matrix%nelt, " elements"
vptr = 1
do i = 1, elemental_matrix%nelt
  j = elemental_matrix%starts(i)
  k = elemental_matrix%starts(i+1)-1
  write(*, "(a,i4,a)", advance="no") "Element ", i, " vars : "
  write(*, "(10i6)") elemental_matrix%vars(j:k)
  write(*, "(8x,a)", advance="no") " values : "
  write(*, "(10f6.2)") elemental_matrix%values(vptr:vpvtr+(k-j+1)**2-1)
  vptr = vptr + (k-j+1)**2
end do
endif
end program hsl_mc56ds

```

If we consider the example used in the previous section, and place the following data in the file `hsl_mc56ds.data`:

```

HSL_MC56DS assembled test example                                     MC56DS
      6          1          1          4
rua          6          6          28          0
      (20i3)      (30i2)      (8es9.1)
  1  5 11 15 19 25 29
1 2 4 5 1 2 3 4 5 6 2 3 5 6 1 2 4 5 1 2 3 4 5 6 2 3 5 6
6.0E+00 1.0E+00 2.0E+00 3.0E+00 1.0E+00 7.0E+00 5.0E+00 3.0E+00
1.0E+01 2.0E+00 5.0E+00 4.0E+00 3.0E+00 2.0E+00 2.0E+00 3.0E+00
6.0E+00 -2.0E+00 3.0E+00 1.0E+01 3.0E+00 4.0E+00 1.3E+01 5.0E+00
2.0E+00 2.0E+00 3.0E+00 1.1E+01

```

then running the program will produce the following output:

```

HSL_MC56DS assembled test example
Assembled matrix of size 6x 6 (ne = 28)
Col 1 row : 1 2 4 5
      val : 6.00 1.00 2.00 3.00
Col 2 row : 1 2 3 4 5 6
      val : 1.00 7.00 5.00 3.00 10.00 2.00
Col 3 row : 2 3 5 6
      val : 5.00 4.00 3.00 2.00
Col 4 row : 1 2 4 5
      val : 2.00 3.00 6.00 -2.00
Col 5 row : 1 2 3 4 5 6
      val : 3.00 10.00 3.00 4.00 13.00 5.00
Col 6 row : 2 3 5 6
      val : 2.00 2.00 3.00 11.00

```

However, if we instead place the following data in the file `hsl_mc56ds.data`:

```

HSL_MC56DS elemental test matrix                                     MC56DS1
      7          1          1          5

```

```

rue          6          4          12          40
(26I3)      (40I2)      (8es9.1)
  1  3  5  9 13
  4  5  5  6  4  5  1  2  5  6  2  3
  2.0E+00 -1.0E+00  1.0E+00  7.0E+00  3.0E+00  4.0E+00  2.0E+00  8.0E+00
  4.0E+00 -1.0E+00  2.0E+00  3.0E+00  3.0E+00  1.0E+00  3.0E+00  2.0E+00
  2.0E+00  3.0E+00  6.0E+00  1.0E+00  3.0E+00  2.0E+00  1.0E+00  5.0E+00
  2.0E+00  1.0E+00  8.0E+00  3.0E+00  1.0E+00  3.0E+00  2.0E+00  2.0E+00
  8.0E+00  2.0E+00  2.0E+00  5.0E+00  3.0E+00  2.0E+00  5.0E+00  4.0E+00

```

then we get the following output:

```

HSL_MC56DS elemental test matrix
Elemental matrix of size 6x 6, 4 elements
Element 1 vars : 4 5
  values : 2.00 -1.00 1.00 7.00
Element 2 vars : 5 6
  values : 3.00 4.00 2.00 8.00
Element 3 vars : 4 5 1 2
  values : 4.00 -1.00 2.00 3.00 3.00 1.00 3.00 2.00 2.00 3.00
  6.00 1.00 3.00 2.00 1.00 5.00
Element 4 vars : 5 6 2 3
  values : 2.00 1.00 8.00 3.00 1.00 3.00 2.00 2.00 8.00 2.00
  2.00 5.00 3.00 2.00 5.00 4.00

```