

PACKAGE SPECIFICATION HSL

#### 1 SUMMARY

HSL\_MC69 offers routines for converting matrices held in a number of sparse matrix formats to the compressed sparse column (CSC) format used by many HSL routines. This format requires the entries within each column of A to be ordered by increasing row index. For symmetric, skew symmetric or Hermitian matrices, only entries in the lower triangle are held. This format is the one used by many of the recent HSL packages; we shall refer to it as the standard HSL format.

Routines are offered for **converting** matrices held in lower or upper compressed sparse column format or in lower or upper compressed sparse row format or in coordinate format, and for **verification** and **correction** of matrices believed to already be in standard HSL format. The conversion routines check the user-supplied data for errors and handle duplicate entries (they are summed) and out-of-range entries (they are discarded).

**ATTRIBUTES** — **Version:** 1.4.2 (28 July 2022). **Types:** Real (single, double), Complex (single, double). **Calls:** None **Original date:** January 2011. **Origin:** J.D. Hogg, Rutherford Appleton Laboratory. **Language:** Fortran 95, plus allocatable components of derived types. **Interfaces:** Fortran, C.

## 2 HOW TO USE THE PACKAGE

## 2.1 Calling sequences

Access to the package requires a USE statement

Single precision version

USE HSL\_MC69\_single

Double precision version

USE HSL\_MC69\_double

Complex version

USE  $HSL\_MC69\_complex$ 

Double complex version

USE HSL\_MC69\_double\_complex

A verification routine for matrices in standard HSL format can be found on page 4. Routines for handling user-supplied matrices that are held in other formats may be found as specified below. **The section on each format is designed to be self contained**, thus users only need to read the section relevant to them.

Input format	matrix type	Page
Compressed sparse column	All	8
Upper compressed sparse column	Symmetric, skew symmetric, Hermitian	16
Full compressed sparse column	Symmetric, skew symmetric, Hermitian	21
Compressed sparse row	All	26
Upper compressed sparse row	Symmetric, skew symmetric, Hermitian	31
Compressed sparse row	Symmetric, skew symmetric, Hermitian	36
Coordinate	All	41

# 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 Integer, real and package types

INTEGER denotes default integer and INTEGER (long) denotes INTEGER (kind=selected\_int\_kind(18)).

REAL denotes default real if the single precision version or the complex version is being used, and double precision.

REAL denotes default real if the single precision version or the complex version is being used, and double precision real if the double precision or double precision complex version is being used.

We use the term **package type** to mean default real if the single precision version is being used, double precision real for the double precision version, default complex for the complex version and double precision complex for the double complex version.

# 2.3 Matrix type constants

The following INTEGER parameters are defined:

HSL\_MATRIX\_UNDEFINED = 0 undefined/unknown

HSL\_MATRIX\_REAL\_RECT = 1 real rectangular HSL\_MATRIX\_REAL\_UNSYM = 2 real unsymmetric

HSL\_MATRIX\_REAL\_SYM\_PSDEF = 3 real symmetric, positive definite HSL\_MATRIX\_REAL\_SYM\_INDEF = 4 real symmetric, indefinite HSL\_MATRIX\_REAL\_SKEW = 6 real skew symmetric

HSL\_MATRIX\_CPLX\_RECT = -1 complex rectangular HSL\_MATRIX\_CPLX\_UNSYMMETRIC = -2 complex unsymmetric

HSL\_MATRIX\_CPLX\_HERM\_PSDEF = -3 complex Hermitian, positive definite HSL\_MATRIX\_CPLX\_HERM\_INDEF = -4 complex Hermitian, indefinite

HSL\_MATRIX\_CPLX\_SYM = -5 complex symmetric HSL\_MATRIX\_CPLX\_SKEW = -6 complex skew symmetric

#### 2.4 Matrices held in standard HSL format

The following routines handle a matrix A held in standard HSL format (that is, CSC format with the entries within each column ordered by increasing row index). For symmetric, skew symmetric or Hermitian matrices, only the **lower triangle** is held. There is no requirement that zero entries on the diagonal be explicitly included.

A valid matrix of this form has no out-of-range or duplicate entries, and is stored as a series of compressed columns using the following data:

- m is an INTEGER scalar that holds the number of rows in A.
- n is an INTEGER scalar that holds the number of columns in A.
- ptr is a rank-one INTEGER array of size n+1. ptr(j) must hold the position in row of the first entry in column j and ptr(n+1) must be one more than the total number of entries.
- row is a rank-one INTEGER array. The first ptr(n+1)-1 entries hold the row indices of the entries of A, with the row indices for the entries in column 1 preceding those for column 2, and so on. The indices within each column **must** be in increasing order.

If the values are required in addition to the matrix pattern, the following array is used:

val is a rank-one array of package type. val (k) must hold the value of the entry in row (k).

## 2.4.1 To verify a matrix is in standard HSL format

To verify a matrix is in standard HSL format, or to identify why it is not, the user may make the following call. Note that this routine does **not** handle duplicates or out-of-range entries (they are flagged as errors). It is intended for debugging rather than for use in a performance code.

```
call mc69_verify(lp, matrix_type, m, n, ptr, row, flag, more [,val])
```

lp is an INTENT (IN) scalar of type INTEGER. If  $lp \ge 0$ , error messages are printed on unit lp.

- matrix\_type is an INTENT (IN) scalar of type INTEGER that describes the type of the matrix. It must have one of the values given in Section 2.3. If it has value 0 (HSL\_MATRIX\_UNDEFINED) requirements that depend on the matrix type will not be checked. For positive-definite matrices, the positive-definite property is not tested (except that diagonal entries must be present and positive).
- m, n, ptr and row are of INTENT (IN) and must be set by the user to hold A in standard HSL format as described in Section 2.4.
- flag is a scalar INTENT (OUT) of type INTEGER. On exit, a value of 0 indicates the matrix is in standard HSL format. Negative values are associated with an error; see Section 2.4.3 for details.
- more is a scalar INTENT (OUT) of type INTEGER. If flag has a negative value on exit, more may provide further information; see Section 2.4.3.
- val is an optional INTENT (IN) rank-one array of package type. If present, val(k) must hold the value of the entry in row(k).

## 2.4.2 To print a matrix in standard HSL format

To print a matrix in standard HSL format (or print a summary of one), the user may make the following call:

```
call mc69_print(lp, lines, matrix_type, m, n, ptr, row[, val])
```

- lp is an INTENT (IN) scalar of type INTEGER. If  $lp \ge 0$ , the matrix is printed on unit lp. There is an immediate return if lp < 0.
- lines is an INTENT (IN) scalar of type INTEGER. If lines ≥ 0, a summary of the matrix will be printed of not more than lines lines. Otherwise, the whole matrix will be printed.
- matrix\_type is an INTENT (IN) scalar of type INTEGER that describes the type of the matrix. It must have one of the values given in Section 2.3.
- m, n, ptr and row are of INTENT (IN) and must be set by the user to hold A in standard HSL format as described in Section 2.4.
- val is an optional INTENT (IN) rank-one array of package type. If present, it must be of size ptr (n+1) -1 and val (k) must hold the value of the entry in row (k).

#### 2.4.3 Return codes

Possible negative values of flag that may be returned by mc69\_verify are:

- -1 Allocation error. more will be set to the Fortran stat value from the failed allocate.
- -2 Invalid value of matrix\_type.
- -3 m < 0 or n < 0.
- -4  $|matrix\_type| > 1$  (square matrix) but m≠n.
- -5 ptr(1) < 1. more is set to ptr(1).
- -6 ptr is not monotonically increasing. more is set to the least value of i such that ptr(i) < ptr(i-1).
- -7 Entries within one or more columns are not sorted by increasing row index. more is set to the first index such that row (more) < row (more-1) and both are in the same column.
- -8 row contains one or more out-of-range entries. more holds the index of the first out-of-range entry in row.
- -9 row contains one or more duplicate entries. more is set such that row (more) and row (more+1) are the first pair of duplicate entries.
- -11 |matrix\_type| = 3 (positive-definite case) but one or more diagonal entries are missing or are not positive. more is set to the index of the first column with such a diagonal entry.
- -12 matrix\_type = -3 or -4 (Hermitian case) but one or more diagonal entries have non-zero imaginary part. more is set to the index of the first column with such a diagonal entry.
- -14 matrix is symmetric, skew-symmetric or Hermitian and an entry is present in the upper triangle or on the diagonal of a skew-symmetric matrix. more is set so that row (more) is the first such entry.

## **2.4.4** Example

Usage of the routines in this section will be demonstrated using the following matrix

$$A = \left(\begin{array}{cccc} 1.0 & 3.0 & -2.0 \\ 3.0 & 4.0 & 5.0 & \\ & 5.0 & 6.0 & 7.0 \end{array}\right).$$

The following code reads a matrix in HSL standard form, verifies the matrix is a valid using mc69\_verify, and then displays the matrix using mc69\_print.

```
program hsl mc69ds
   use hsl_mc69_double
   implicit none
   integer, parameter :: wp = kind(0d0)
   integer :: matrix_type, m, n, flag, more
   integer, dimension(:), allocatable :: ptr, row
   real(wp), dimension(:), allocatable :: val
   ! Read matrix in HSL standard form
   read(*, "(3i8)") matrix_type, m, n
   allocate(ptr(n+1)); read(*, "(6i8)") ptr(:)
   allocate(row(ptr(n+1)-1)); read(*, "(6i8)") row(:)
   allocate(val(ptr(n+1)-1)); read(*, "(4es12.4)") val(:)
   ! Verify matrix is in correct form
   call mc69_verify(6, matrix_type, m, n, ptr, row, flag, more, val=val)
   if(flag.ne.0) then
      write(*, "(a,i3,a,i5)") &
         "Error return from mc69 verify with flag = ", flag, ", more = ", more
      stop
   endif
   ! Print out pattern in no more than 10 lines
   write(*, "(a)") "Matrix pattern:"
   call mc69_print(6, 10, matrix_type, m, n, ptr, row)
   ! Print out matrix values in no more than 10 lines
   write(*, "(/a)") "Matrix values:"
   call mc69_print(6, 10, matrix_type, m, n, ptr, row, val=val)
end program hsl_mc69ds
```

If provided with the following input (matching the matrix A above),

# the code produces the following output.

```
1.0000E+00 3.0000E+00 -2.0000E+00 4.0000E+00
  5.0000E+00 6.0000E+00 7.0000E+00
Matrix pattern:
Real symmetric indefinite matrix, dimension 4x4 with 7 entries.
1: x x x
2: x x x
3: x x
4: x x x
Matrix values:
Real symmetric indefinite matrix, dimension 4x4 with 7 entries.
    1.0000E+00
                 3.0000E+00
                                          -2.0000E+00
2:
    3.0000E+00
                 4.0000E+00
                              5.0000E+00
                 5.0000E+00
                                           6.0000E+00
3:
4: -2.0000E+00
                              6.0000E+00
                                           7.0000E+00
```

## 2.5 Compressed sparse column format

The following routines handle a matrix stored in compressed sparse column format, with entries only in the lower triangle for symmetric, skew-symmetric or Hermitian matrices. Entries within each column of the user-supplied matrix do **not** need to be ordered. There is no requirement that zero entries on the diagonal be explicitly included. For a skew-symmetric matrix, no diagonal entries are held.

The input matrix is stored as a series of compressed columns using the following data:

- m is a scalar of type INTEGER that holds the number of rows of A.
- n is a scalar of type INTEGER that holds the number of columns of A.
- ptr is a rank-one array of type INTEGER. The first n values must be set such that ptr(j) holds the position in row of the first entry in column j and ptr(n+1) must be one more than the total number of entries.
- row is a rank-one array of type INTEGER. The first ptr (n+1) -1 entries hold the row indices of the entries, with the row indices for the entries in column 1 preceding those for column 2, and so on. The indices within each column may be unordered.

If the values are required in addition to the matrix pattern, the following array is used:

val is a rank-one array of package type. val (k) must hold the value of the entry in row (k).

## 2.5.1 To perform an in-place conversion from compressed sparse column format to standard HSL format

To convert a matrix held in compressed sparse column format to standard HSL format **in-place** (that is, the user's data is overwritten), the user may make a call of the following form. This routine checks the user's data and handles duplicate entries (they are summed) and out-of-range entries (they are removed). For symmetric, skew-symmetric and Hermitian matrices, entries in the upper triangle are removed. For skew-symmetric matrices only, entries on the diagonal are treated as out-of-range entries, and are removed.

```
call mc69_cscl_clean(matrix_type, m, n, ptr, row, flag[, val, lmap, map, lp, noor, ndup])
```

- matrix\_type is an INTENT(IN) scalar of type INTEGER that describes the type of matrix. It must take one of the values described in Section 2.3. If this argument has value 0 (HSL\_MATRIX\_UNDEFINED), the matrix will be treated as if it were rectangular.
- m, n are of INTENT (IN), ptr and row are of INTENT (INOUT) and must be set by the user to hold A in compressed sparse column format, as described in Section 2.5. On exit, ptr and row will have been modified to hold the matrix in standard HSL format.
- flag is an INTENT (OUT) scalar of type INTEGER. On exit, a value of 0 indicates successful conversion. Positive values indicate successful conversion but a warning was issued. Negative values are associated with an error; see Section 2.5.4 for details.
- val is an optional INTENT (INOUT) rank-one array of package type. If present, on input the first ptr(n+1)-1 entries must be set so that val(k) holds the value of the entry in row(k). On exit, it will hold the (potentially modified) values of the matrix entries corresponding to those of the array row.

lmap is an optional INTENT (OUT) scalar of type INTEGER. If lmap is present, map must also be present.

map is an optional INTENT (OUT) rank-one ALLOCATABLE array of type INTEGER. It should be present if the user wishes to change the values of the entries of A following the call to mc69\_cscl\_clean, and should be passed unaltered to any subsequent calls to mc69\_set\_values. A detailed description of the output format is given in Section 4.1. If map is present, lmap must also be present.

- lp is an optional INTENT (IN) scalar of type INTEGER. If present and  $lp \ge 0$ , error and warning messages are written to unit lp.
- noor is an optional INTENT (OUT) scalar of type INTEGER. If present, on exit it contains the number of out-of-range entries that were discarded.
- ndup is an optional INTENT (OUT) scalar of type INTEGER. If present, on exit it contains the number of duplicate entries that were summed.

## 2.5.2 To perform an out-of-place conversion from compressed sparse column format to standard HSL format

To convert a matrix held in lower compressed sparse column format to standard HSL format, the user may make a call of the following form. This routine leaves the user's data unchanged. This routine checks the user's data and handles duplicate entries (they are summed) and out-of-range entries (they are discarded). For symmetric, skew-symmetric and Hermitian matrices, entries in the upper triangle are discarded. For skew-symmetric matrices only, entries on the diagonal are treated as out-of-range entries, and are discarded.

```
call mc69_cscl_convert(matrix_type, m, n, ptr_in, row_in, ptr_out, row_out, &
    flag[, val_in, val_out, lmap, map, lp, noor, ndup])
```

- matrix\_type is an INTENT(IN) scalar of type INTEGER that describes the type of matrix. It must take one of the values described in Section 2.3. If this argument has value 0 (HSL\_MATRIX\_UNDEFINED), the matrix will be treated as if it were rectangular.
- m, n, ptr\_in and col\_in are of INTENT(IN) and must be set by the user to hold A in compressed sparse column format, as described in Section 2.5.
- ptr\_out and row\_out are INTENT (OUT) rank-one arrays of type INTEGER. ptr\_out is of size n+1 and row\_out is allocatable. On exit, they hold A in HSL standard format, as described in Section 2.4.
- flag is an INTENT (OUT) scalar of type INTEGER. On exit, a value of 0 indicates successful conversion. Positive values indicate successful conversion but a warning was issued. Negative values are associated with an error; see Section 2.5.4 for details.
- val\_in is an optional INTENT(IN) rank-one array of package type. If present, on input the first ptr\_in(n+1)-1 entries must be set so that val\_in(k) holds the value of the entry row\_in(k). If val\_in is present, val\_out must also be present.
- val\_out is an optional INTENT (OUT) rank-one allocatable array of package type. If present, on exit it will be allocated and the first ptr\_out (n+1) -1 entries will be set such that val\_out (k) holds the value of the entry row\_out (k). If val\_out is present, val\_in must also be present.
- lmap is an optional INTENT (OUT) scalar of type INTEGER. If lmap is present, map must also be present.
- map is an optional INTENT (OUT) rank-one ALLOCATABLE array of type INTEGER. It should be present if the user wishes to change the values of the entries of A following the call to mc69\_cscl\_convert, and should be passed unaltered to any subsequent calls to mc69\_set\_values. A detailed description of the output format is given in Section 4.1. If map is present, lmap must also be present.

lp is an optional INTENT (IN) scalar of type INTEGER. If present and  $lp \ge 0$ , error and warning messages are written to unit lp.

- noor is an optional INTENT (OUT) scalar of type INTEGER. If present, on exit it contains the number of out-of-range entries that were discarded.
- ndup is an optional INTENT (OUT) scalar of type INTEGER. If present, on exit it contains the number of duplicate entries that were summed.

# 2.5.3 To set values of A following a conversion

The user may want to change the values of the entries of A following a successful call to mc69\_cscl\_clean or mc69\_cscl\_convert. Alternatively, the user may want to include matrix values after a call to mc69\_cscl\_clean or mc69\_cscl\_convert with matrix values not present. This can be done by making a call of the following form, however note that no checks are made on the values of the diagonal entries.

```
call mc69_set_values(matrix_type, lmap, map, val_in, ne, val_out)
```

- matrix\_type is an INTENT (IN) scalar of type INTEGER that describes the type of matrix. It must be unchanged since the call to mc69\_cscl\_clean or mc69\_cscl\_convert that generated map.
- lmap is an INTENT(IN) scalar of type INTEGER that must be unchanged since the call to mc69\_cscl\_clean or mc69\_cscl\_convert that generated map.
- map is an INTENT (IN) rank-one array of type INTEGER that must be unchanged since the call to mc69\_cscl\_clean or mc69\_cscl\_convert that generated it.
- val\_in is an INTENT(IN) rank-one array of package type. It must have size at least the value of ptr(n+1)-1 on the call to mc69\_cscl\_clean (or ptr\_in(n+1)-1 for a call to mc69\_cscl\_convert). It must be set by the user to hold the new values of the entries of A matching the original matrix that was input to mc69\_cscl\_clean or mc69\_cscl\_convert.
- ne is an INTENT(IN) scalar argument of type INTEGER that must be set to the value of ptr(n+1)-1 on exit from mc69\_cscl\_clean or mc69\_cscl\_convert.
- val\_out is an INTENT (OUT) rank-one array of package type. It must have size at least the value of ptr(n+1)-1 on exit from  $mc69\_csc1\_clean$  (or  $ptr\_out(n+1)-1$  on exit from  $mc69\_csc1\_convert$ ). On exit, it contains the new values of A in standard HSL format, as described in Section 2.4.

#### 2.5.4 Return codes

A successful return from a call to mc69\_cscl\_clean or mc69\_cscl\_convert is indicated by flag taking the value 0. Possible negative values that are associated with an error are:

- -1 Allocation error.
- -2 Invalid value of matrix\_type.
- -3 m < 0 or n < 0.
- -4  $|matrix\_type| > 1$  (square matrix) but  $m \neq n$ .
- -5 ptr(1) < 1.

- -6 ptr(1:n+1) is not monotonic increasing.
- -10 All entries for a column are out of range.
- -11 |matrix\_type| =3 (positive-definite case) but one or more diagonal entries are not positive.
- -12 matrix\_type =-3 or -4 (Hermitian case) but one or more entries on the diagonal have non-zero imaginary part.
- -15 Only one of val\_in and val\_out is present.
- -16 Only one of 1map and map is present.

Possible positive values are:

- +1 Out-of-range indices found in row\_in.
- +2 Duplicate indices found in row\_in.
- +3 Both out-of-range and duplicate entries found.
- +4 |matrix\_type| ≠ 3, 6 and not all entries on the diagonal are present. (Note that no HSL package requires explicit zeros to be on input on the diagonal.)
- +5 |matrix\_type| ≠ 3,6 and not all entries on the diagonal are present and out-of-range and/or duplicate entries found. (Note that no HSL package requires explicit zeros to be on input on the diagonal.)

## **2.5.5** Example

Usage of the routines in this section will be demonstrated using the following matrices

$$A = \begin{pmatrix} 1.0 & 3.0 & -2.0 \\ 3.0 & 4.0 & 5.0 & \\ 5.0 & 5.0 & 6.0 \\ -2.0 & 6.0 & 7.0 + 2.0 \end{pmatrix}, \qquad B = \begin{pmatrix} 2.0 & 4.0 & -3.0 \\ 4.0 & 6.0 & 6.0 & \\ 6.0 & 7.0 & 8.0 - 1.0 \end{pmatrix}.$$

The following code reads a matrix in Compressed Sparse Column form, and then performs an *in-place* conversion to HSL standard form using mc69\_cscl\_clean.

```
program hsl_mc69ds1
  use hsl_mc69_double
  implicit none

integer, parameter :: wp = kind(0d0)

integer :: i, j, matrix_type, m, n, flag
  integer, dimension(:), allocatable :: ptr, row
  real(wp), dimension(:), allocatable :: val

! Read matrix in CSC form
  read(*, "(3i8)") matrix_type, m, n
  allocate(ptr(n+1)); read(*, "(6i8)") ptr(:)
  allocate(row(ptr(n+1)-1)); read(*, "(6i8)") row(:)
  allocate(val(ptr(n+1)-1)); read(*, "(4es12.4)") val(:)
```

```
do i = 1, n
      write(*, "(a,i2,':')",advance="no") "Column ", i
      do j = ptr(i), ptr(i+1)-1
         write(*, "(2x,i4,1x,'(',es12.2,')')", advance="no") row(j), val(j)
      end do
      write(*, "()")
   end do
   ! Convert to HSL standard form in place
   call mc69_cscl_clean(matrix_type, m, n, ptr, row, flag, val=val)
   if(flag.lt.0) then
      write(*, "(a,i3)") &
         "Error return from mc69_cscl_clean with flag = ", flag
      stop
   endif
   write(*, "(/a)") "Output:"
   do i = 1, n
      write(*, "(a,i2,':')",advance="no") "Column ", i
      do j = ptr(i), ptr(i+1)-1
         write(*, "(2x,i4,1x,'(',es12.2,')')", advance="no") row(j), val(j)
      end do
      write(*, "()")
   end do
   ! Print out matrix values in no more than 10 lines
   write(*, "()")
   call mc69_print(6, 10, matrix_type, m, n, ptr, row, val=val)
end program hsl_mc69ds1
If provided with the following input (matching the matrix A above),
       4
               4
                       4
       1
               4
                               7
                       6
       1
               4
                       2
                               2
                                        3
 1.0000E+00 -2.0000E+00 3.0000E+00 4.0000E+00
  5.0000E+00 6.0000E+00 7.0000E+00 2.0000E+00
the code produces the following output.
Input:
Column 1:
               1 (
                      1.00E+00)
                                     4 ( -2.00E+00)
                                                          2 ( 3.00E+00)
Column 2:
               2 (
                      4.00E+00)
                                            5.00E+00)
                                     3 (
Column 3:
               4 (
                      6.00E+00)
Column 4:
               4 (
                      7.00E+00)
                                     4 (
                                            2.00E+00)
Output:
Column 1:
               1 (
                      1.00E+00)
                                     2 (
                                            3.00E+00)
                                                          4 ( -2.00E+00)
Column 2:
               2 (
                      4.00E+00)
                                     3 (
                                            5.00E+00)
               4 (
Column 3:
                      6.00E+00)
```

write(\*, "(a)") "Input:"

```
Column 4:
               4 (
                      9.00E+00)
Real symmetric indefinite matrix, dimension 4x4 with 7 entries.
1:
    1.0000E+00
                  3.0000E+00
                                            -2.0000E+00
    3.0000E+00
                                5.0000E+00
2.
                  4.0000E+00
                  5.0000E+00
                                             6.0000E+00
3:
4: -2.0000E+00
                                6.0000E+00
                                             9.0000E+00
```

For an *out-of-place* conversion, the following code calling mc69\_csc1\_convert may be used instead. In addition to the initial conversion, a second set of values matching the same pattern is read. These values are then converted to HSL standard form using mc69\_set\_values.

```
program hsl mc69ds2
  use hsl mc69 double
   implicit none
   integer, parameter :: wp = kind(0d0)
  integer :: i, j, matrix_type, m, n, flag, lmap
   integer, dimension(:), allocatable :: ptr, row, ptr_out, row_out, map
   real(wp), dimension(:), allocatable :: val, val_out
   ! Read matrix in CSC form
   read(*, "(3i8)") matrix_type, m, n
  allocate(ptr(n+1)); read(*, "(6i8)") ptr(:)
  allocate(row(ptr(n+1)-1)); read(*, "(6i8)") row(:)
  allocate(val(ptr(n+1)-1)); read(*, "(4es12.4)") val(:)
  write(*, "(a)") "Input:"
  do i = 1, n
      write(*, "(a,i2,':')",advance="no") "Column ", i
      do j = ptr(i), ptr(i+1)-1
        write(*, "(2x,i4,1x,'(',es12.2,')')", advance="no") row(j), val(j)
      end do
      write(*, "()")
   end do
   ! Convert to HSL standard form out of place
  allocate(ptr_out(n+1))
  call mc69_cscl_convert(matrix_type, m, n, ptr, row, ptr_out, row_out, flag, &
      val_in=val, val_out=val_out, lmap=lmap, map=map)
   if(flag.lt.0) then
      write(*, "(a,i3)") &
         "Error return from mc69_cscl_convert with flag = ", flag
      stop
  endif
  write(*, "(/a)") "Output:"
  do i = 1, n
      write(*, "(a,i2,':')",advance="no") "Column ", i
```

do  $j = ptr_out(i)$ ,  $ptr_out(i+1)-1$ 

```
write(*, "(2x,i4,1x,'(',es12.2,')')", advance="no") &
            row_out(j), val_out(j)
      end do
      write(*, "()")
   end do
   ! Print out matrix
   write(*, "()")
   call mc69_print(6, 0, matrix_type, m, n, ptr_out, row_out, val=val_out)
   ! Read and apply new values
   read(*, "(4es12.4)") val(:)
   call mc69_set_values(matrix_type, lmap, map, val, ptr_out(n+1)-1, val_out)
   write(*, "(/a)") "After applying new values:"
   call mc69_print(6, 0, matrix_type, m, n, ptr_out, row_out, val=val_out)
end program hsl_mc69ds2
If provided with the following input (matching the matrices A and B above),
                       4
       1
               4
                       6
                               7
                                       3
       1
               4
                       2
                               2
                                                4
       4
               4
 1.0000E+00 -2.0000E+00 3.0000E+00 4.0000E+00
 5.0000E+00 6.0000E+00 7.0000E+00 2.0000E+00
  2.0000E+00 -3.0000E+00 4.0000E+00 6.0000E+00
  6.0000E+00 7.0000E+00 8.0000E+00 -1.0000E+00
the code produces the following output.
Input:
Column 1:
               1 (
                     1.00E+00)
                                        -2.00E+00)
                                                          2 ( 3.00E+00)
                                    4 (
Column 2:
               2 (
                      4.00E+00)
                                    3 (
                                           5.00E+00)
Column 3:
               4 (
                      6.00E+00)
Column 4:
               4 (
                      7.00E+00)
                                    4 (
                                           2.00E+00)
Output:
                                    2 (
                                                          4 ( -2.00E+00)
Column 1:
               1 (
                      1.00E+00)
                                           3.00E+00)
Column 2:
               2 (
                      4.00E+00)
                                    3 (
                                           5.00E+00)
Column 3:
               4 (
                      6.00E+00)
Column 4:
               4 (
                      9.00E+00)
Real symmetric indefinite matrix, dimension 4x4 with 7 entries.
1: 1.0000E+00
                  3.0000E+00
                                            -2.0000E+00
2:
    3.0000E+00
                  4.0000E+00
                               5.0000E+00
                  5.0000E+00
                                             6.0000E+00
3:
4: -2.0000E+00
                               6.0000E+00
                                             9.0000E+00
After applying new values:
Real symmetric indefinite matrix, dimension 4x4 with 7 entries.
     2.0000E+00
                  4.0000E+00
                                           -3.0000E+00
```

2: 4.0000E+00 6.0000E+00 6.0000E+00

3: 6.0000E+00 7.0000E+00 4: -3.0000E+00 7.0000E+00

## 2.6 Symmetric, skew symmetric and Hermitian matrices in upper compressed sparse column format

The following routines handle a symmetric, skew-symmetric or Hermitian matrix stored in upper compressed sparse column format (only entries in the upper triangle are stored). Entries within each column of the user-supplied matrix do **not** need to be ordered. There is no requirement that zero entries on the diagonal be explicitly included.

The input matrix is stored as a series of compressed columns using the following data:

- n is a scalar of type INTEGER that holds the order of A.
- ptr is a rank-one array of type INTEGER. The first n values must be set such that ptr(j) holds the position in row of the first entry in column j and ptr(n+1) must be one more than the total number of entries.
- row is a rank-one array of type INTEGER. The first ptr(n+1)-1 entries hold the row indices of the entries in the **upper triangle** of A, with the row indices for the entries in column 1 preceding those for column 2, and so on. The indices within each column may be unordered.

If the values are required in addition to the matrix pattern, the following array is used:

val is a rank-one array of package type. val(k) must hold the value of the entry in row(k).

## 2.6.1 To perform a conversion from upper compressed sparse column format to standard HSL format

To convert a symmetric, skew-symmetric or Hermitian matrix held in upper compressed sparse column format to standard HSL format, the user may make a call of the following form. This routine checks the user's data and handles duplicate entries (they are summed) and out-of-range entries (they are discarded). Entries in the lower triangle are discarded. For skew-symmetric matrices only, entries on the diagonal are treated as out-of-range entries, and are discarded.

```
call mc69_cscu_convert(matrix_type, n, ptr_in, row_in, ptr_out, row_out, &
    flag[, val_in, val_out, lmap, map, lp, noor, ndup])
```

- matrix\_type is an INTENT(IN) scalar of type INTEGER that describes the type of matrix. It must take one of the values described in Section 2.3 for a symmetric, skew-symmetric or Hermitian matrix.
- n, ptr\_in and row\_in are of INTENT(IN) and must be set by the user to hold A in upper compressed sparse row format, as described in Section 2.6.
- ptr\_out and row\_out are INTENT(OUT) rank-one arrays of type INTEGER. ptr\_out is of size n+1 and row\_out is allocatable. On exit, they hold A in HSL standard format, as described in Section 2.4.
- flag is an INTENT (OUT) scalar of type INTEGER. On exit, a value of 0 indicates successful conversion. Positive values indicate successful conversion but a warning was issued. Negative values are associated with an error; see Section 2.6.3 for details.
- val\_in is an optional INTENT(IN) rank-one array of package type. If present, on input the first ptr\_in(n+1)-1 entries must be set so that val\_in(k) holds the value of the entry row\_in(k). If val\_in is present, val\_out must also be present.
- val\_out is an optional INTENT (OUT) rank-one allocatable array of package type. If present, on exit it will be allocated and the first ptr\_out (n+1) -1 entries will be set such that val\_out (k) holds the value of the entry row\_out (k). If val\_out is present, val\_in must also be present.

lmap is an optional INTENT (OUT) scalar of type INTEGER. If lmap is present, map must also be present.

map is an optional INTENT (OUT) rank-one ALLOCATABLE array of type INTEGER. It should be present if the user wishes to change the values of the entries of A following the call to mc69\_cscu\_convert, and should be passed unaltered to any subsequent calls to mc69\_set\_values. A detailed description of the output format is given in Section 4.1. If map is present, lmap must also be present.

- lp is an optional INTENT (IN) scalar of type INTEGER. If present and  $lp \ge 0$ , error and warning messages are written to unit lp.
- noor is an optional INTENT (OUT) scalar of type INTEGER. If present, on exit it contains the number of out-of-range entries that were discarded.
- ndup is an optional INTENT (OUT) scalar of type INTEGER. If present, on exit it contains the number of duplicate entries that were summed.

## **2.6.2** To set values of A following a conversion

The user may want to change the values of the entries of A following a successful call to mc69\_cscu\_convert. Alternatively, the user may want to include matrix values after a call to mc69\_cscu\_convert with matrix values not present. This can be done by making a call of the following form, however note that no checks are made on the values of the diagonal entries.

```
call mc69_set_values(matrix_type, lmap, map, val_in, ne, val_out)
```

- matrix\_type is an INTENT(IN) scalar of type INTEGER that describes the type of matrix. It must be unchanged since the call to mc69\_cscu\_convert that generated map.
- lmap is an INTENT(IN) scalar of type INTEGER that must be unchanged since the call to mc69\_cscu\_convert that generated map.
- map is an INTENT (IN) rank-one array of type INTEGER that must be unchanged since the call to mc69\_cscu\_convert that generated it.
- val\_in is an INTENT(IN) rank-one array of package type. It must have size at least the value of ptr\_in(n+1)-1 on the call to mc69\_cscu\_convert. It must be set by the user to hold the new values of the entries of A matching the original matrix that was input to mc69\_cscu\_convert.
- ne is an INTENT(IN) scalar argument of type INTEGER that must be set to the value of ptr\_out(n+1)-1 on exit from mc69\_cscu\_convert.
- val\_out is an INTENT (OUT) rank-one array of package type. It must have size at least the value of ptr\_out (n+1) -1 on exit from mc69\_cscu\_convert. On exit, it contains the new values of A in standard HSL format, as described in Section 2.4.

# 2.6.3 Return codes

A successful return from a call to mc69\_cscu\_convert is indicated by flag taking the value 0. Possible negative values that are associated with an error are:

- -1 Allocation error.
- -2 Invalid value of matrix\_type.
- -3 n < 0.

- -5 ptr(1) < 1.
- -6 ptr(1:n+1) is not monotonic increasing.
- -10 All entries for a column are out of range.
- -11 |matrix\_type| =3 (positive-definite case) but one or more diagonal entries are not positive.
- -12 matrix\_type =-3 or -4 (Hermitian case) but one or more entries on the diagonal have non-zero imaginary part.
- -15 Only one of val\_in and val\_out is present.
- -16 Only one of 1map and map is present.

Possible positive values are:

- +1 Out-of-range indices found in row\_in.
- +2 Duplicate indices found in row\_in.
- +3 Both out-of-range and duplicate entries found.
- +4 |matrix\_type| ≠ 3, 6 and not all entries on the diagonal are present. (Note that no HSL package requires explicit zeros to be on input on the diagonal.)
- +5 |matrix\_type| ≠ 3, 6 and not all entries on the diagonal are present and out-of-range and/or duplicate entries found. (Note that no HSL package requires explicit zeros to be on input on the diagonal.)

## **2.6.4** Example

Usage of the routines in this section will be demonstrated using the following matrices

$$A = \begin{pmatrix} 1.0 & 3.0 & -2.0 \\ 3.0 & 4.0 & 5.0 & \\ & 5.0 & 6.0 \\ -2.0 & 6.0 & 7.0 + 2.0 \end{pmatrix}, \qquad B = \begin{pmatrix} 2.0 & 4.0 & -3.0 \\ 4.0 & 6.0 & 6.0 & \\ & 6.0 & 7.0 \\ -3.0 & 7.0 & 8.0 - 1.0 \end{pmatrix}.$$

The following code reads a matrix in upper Compressed Sparse Column form, and then converts it to HSL standard format using mc69\_cscu\_convert. In addition to the initial conversion, a second set of values matching the same pattern is read. These values are then converted to HSL standard form using mc69\_set\_values.

```
program hsl_mc69ds3
  use hsl_mc69_double
  implicit none

integer, parameter :: wp = kind(0d0)

integer :: i, j, matrix_type, n, flag, lmap
  integer, dimension(:), allocatable :: ptr, row, ptr_out, row_out, map
  real(wp), dimension(:), allocatable :: val, val_out

! Read symmetric matrix in upper CSC form
  read(*, "(2i8)") matrix_type, n
  allocate(ptr(n+1)); read(*, "(6i8)") ptr(:)
```

```
allocate(row(ptr(n+1)-1)); read(*, "(6i8)") row(:)
   allocate(val(ptr(n+1)-1)); read(*, "(4es12.4)") val(:)
   write(*, "(a)") "Input:"
   do i = 1, n
      write(*, "(a,i2,':')",advance="no") "Column ", i
      do j = ptr(i), ptr(i+1)-1
         write(*, "(2x,i4,1x,'(',es12.2,')')", advance="no") row(j), val(j)
      end do
      write(*, "()")
   end do
   ! Convert to HSL standard form out of place
   allocate(ptr_out(n+1))
   call mc69_cscu_convert(matrix_type, n, ptr, row, ptr_out, row_out, flag, &
      val_in=val, val_out=val_out, lmap=lmap, map=map)
   if(flag.lt.0) then
      write(*, "(a,i3)") &
         "Error return from mc69_cscl_convert with flag = ", flag
      stop
   endif
   write(*, "(/a)") "Output:"
   do i = 1, n
      write(*, "(a,i2,':')",advance="no") "Column ", i
      do j = ptr_out(i), ptr_out(i+1)-1
         write(*, "(2x,i4,1x,'(',es12.2,')')", advance="no") &
            row_out(j), val_out(j)
      end do
      write(*, "()")
   end do
   ! Print out matrix
   write(*, "()")
   call mc69_print(6, 0, matrix_type, n, n, ptr_out, row_out, val=val_out)
   ! Read and apply new values
   read(*, "(4es12.4)") val(:)
   call mc69_set_values(matrix_type, lmap, map, val, ptr_out(n+1)-1, val_out)
   write(*, "(/a)") "After applying new values:"
   call mc69_print(6, 0, matrix_type, n, n, ptr_out, row_out, val=val_out)
end program hsl_mc69ds3
If provided with the following input (matching the matrices A and B above),
       4
               4
       1
               2
                                5
                                        9
                       4
               1
                       2
                                2
                                        3
                                                1
```

1.0000E+00 3.0000E+00 4.0000E+00 5.0000E+00

```
6.0000E+00 -2.0000E+00 7.0000E+00 2.0000E+00
 2.0000E+00 4.0000E+00 6.0000E+00 6.0000E+00
 7.0000E+00 -3.0000E+00 8.0000E+00 -1.0000E+00
the code produces the following output.
Input:
Column 1:
               1 (
                      1.00E+00)
Column 2:
               1 (
                      3.00E+00)
                                     2 (
                                            4.00E+00)
Column 3:
               2 (
                      5.00E+00)
Column 4:
               3 (
                      6.00E+00)
                                     1 (
                                          -2.00E+00)
                                                          4 (
                                                                 7.00E+00)
                                                                                4 (
                                                                                       2.00E+00)
Output:
Column 1:
                                            3.00E+00)
                                                                -2.00E+00)
               1 (
                      1.00E+00)
                                     2 (
                                                          4 (
Column 2:
                                            5.00E+00)
               2 (
                      4.00E+00)
                                     3 (
Column 3:
               4 (
                      6.00E+00)
Column 4:
               4 (
                      9.00E+00)
Real symmetric indefinite matrix, dimension 4x4 with 7 entries.
     1.0000E+00
                  3.0000E+00
                                            -2.0000E+00
     3.0000E+00
2:
                  4.0000E+00
                                5.0000E+00
3:
                  5.0000E+00
                                             6.0000E+00
4: -2.0000E+00
                                6.0000E+00
                                             9.0000E+00
After applying new values:
Real symmetric indefinite matrix, dimension 4x4 with 7 entries.
1:
     2.0000E+00
                  4.0000E+00
                                            -3.0000E+00
```

7.0000E+00

7.0000E+00

2:

3:

4.0000E+00

4: -3.0000E+00

6.0000E+00

6.0000E+00

6.0000E+00

7.0000E+00

## 2.7 Symmetric, skew symmetric and Hermitian matrices in full compressed sparse column format

The following routines handle a symmetric, skew symmetric or Hermitian matrix stored in full compressed sparse column format (entries in both the lower and upper triangles are supplied by the user). Entries within each column of the user-supplied matrix do **not** need to be ordered. There is no requirement that zero entries on the diagonal be explicitly included.

The input matrix is stored as a series of compressed columns using the following data:

- n is a scalar of type INTEGER that holds the order of A.
- ptr is a rank-one array of type INTEGER. The first n values must be set such that ptr(j) holds the position in row of the first entry in column j and ptr(n+1) must be one more than the total number of entries.
- row is a rank-one array of type INTEGER. The first ptr (n+1)-1 entries hold the row indices of the entries of A, with the row indices for the entries in column 1 preceding those for column 2, and so on. If a non-diagonal entry (i, j) is present, its counterpart (j, i) must also be present. The indices within each column may be unordered.

If the values are required in addition to the matrix pattern, the following array is used:

val is a rank-one array of package type. val (k) must hold the value of the entry in row (k).

## 2.7.1 To convert from full compressed sparse column format to standard HSL format

To convert a symmetric, skew-symmetric or Hermitian matrix held in full compressed sparse column format to standard HSL format the user may make a call of the following form. This routine checks the user's data and handles duplicate entries (they are summed) and out-of-range entries (they are discarded). Entries in the lower triangle are ignored, except to check that there are the same number of entries in both the lower and upper triangles. For skew-symmetric matrices only, entries on the diagonal are treated as out-of-range and are discarded.

```
call mc69_csclu_convert(matrix_type, n, ptr_in, row_in, ptr_out, row_out, flag[, &
   val in, val out, lmap, map, lp, noor, ndup])
```

- matrix\_type is an INTENT (IN) scalar of type INTEGER that describes the type of matrix. It must take one of the values described in Section 2.3 for a symmetric, skew-symmetric or Hermitian matrix.
- n, ptr\_in and row\_in are of INTENT(IN) and must be set by the user to hold A in full compressed sparse column format, as described in Section 2.7.
- ptr\_out and row\_out are INTENT (OUT) rank-one arrays of type INTEGER. ptr\_out is of size n+1 and row\_out is allocatable. On exit, they hold A in HSL standard format, as described in Section 2.4.
- flag is an INTENT (OUT) scalar of type INTEGER. On exit, a value of 0 indicates successful conversion. Positive values indicate successful conversion but a warning was issued. Negative values are associated with an error; see Section 2.7.3 for details.
- val\_in is an optional INTENT (IN) rank-one array of package type. If present, the first ptr\_in(n+1)-1 entries must be set so that val\_in(k) holds the value of the entry row\_in(k). If val\_in is present, val\_out must also be present.
- val\_out is an optional INTENT (OUT) rank-one ALLOCATABLE array of package type. On exit, it is allocated to have size equal to that of row\_out and val\_out (k) holds the value of the entry row\_out (k). If val\_out is present, val\_in must also be present.

- 1map is an optional INTENT (OUT) scalar of type INTEGER. If 1map is present, map must also be present.
- map is an optional INTENT (OUT) rank-one ALLOCATABLE array of type INTEGER. It should be present if the user wishes to change the values of the entries of A following the call to mc69\_csclu\_convert, and should be passed unaltered to any subsequent calls to mc69\_set\_values. A detailed description of the output format is given in Section 4.1. If map is present, lmap must also be present.
- lp is an optional INTENT (IN) scalar of type INTEGER. If present and  $lp \ge 0$ , error and warning messages are written to unit lp.
- noor is an optional INTENT (OUT) scalar of type INTEGER. If present, on exit it contains the number of out-of-range entries that were discarded.
- ndup is an optional INTENT (OUT) scalar of type INTEGER. If present, on exit it contains the number of duplicate entries that were summed.

## 2.7.2 To set values of A following a conversion

The user may want to change the values of the entries of A following a successful call to mc69\_csclu\_convert. Alternatively, the user may want to include matrix values after a call to mc69\_csclu\_convert with matrix values not present. This can be done by making a call of the following form, however note that no checks are made on the values of the diagonal entries.

```
call mc69_set_values(matrix_type, lmap, map, val_in, ne, val_out)
```

- matrix\_type is an INTENT(IN) scalar of type INTEGER that describes the type of matrix. It must be unchanged since the call to mc69\_csclu\_convert that generated map.
- lmap is an INTENT(IN) scalar of type INTEGER that must be unchanged since the call to mc69\_csclu\_convert that
   generated map.
- map is an INTENT(IN) rank-one array of type INTEGER that must be unchanged since the call to mc69\_csclu\_convert that generated it.
- val\_in is an INTENT (IN) rank-one array of package type. It must have size at least the value of ptr\_in (n+1) -1 on the call to mc69\_csclu\_convert. It must be set by the user to hold the new values of the entries of A matching the original matrix that was input to mc69\_csclu\_convert.
- ne is an INTENT (IN) scalar argument of type INTEGER that must be set to the value of ptr\_out (n+1) -1 on exit from mc69\_csclu\_convert.
- val\_out is an INTENT (OUT) rank-one array of package type. It must have size at least the value of ptr\_out (n+1) -1 on exit from mc69\_csclu\_convert. On exit, it contains the new values of A in standard HSL format, as described in Section 2.4.

# 2.7.3 Return codes

A successful return from a call to mc69\_csclu\_convert is indicated by flag taking the value 0. Possible negative values that are associated with an error are:

- -1 Allocation error.
- -2 Invalid value of matrix\_type.

- -3 n < 0.
- -5 ptr(1) < 1.
- -6 ptr(1:n+1) is not monotonic increasing.
- -10 All entries for a column are out of range.
- -13 Number of in-range entries in lower and upper triangles do not match.
- -11 |matrix\_type| =3 (positive-definite case) but one or more diagonal entries are not positive.
- -12 matrix\_type =-3 or -4 (Hermitian case) but one or more entries on the diagonal have non-zero imaginary part.
- -15 Only one of val\_in and val\_out is present.
- -16 Only one of 1map and map is present.

Possible positive values are:

- +1 Out-of-range indices found in row\_in.
- +2 Duplicate indices found in row\_in.
- +3 Both out-of-range and duplicate entries found.
- +4 |matrix\_type| ≠ 3, 6 and not all entries on the diagonal are present. (Note that no HSL package requires explicit zeros to be on input on the diagonal.)
- +5 |matrix\_type| ≠ 3, 6 and not all entries on the diagonal are present and out-of-range and/or duplicate entries found. (Note that no HSL package requires explicit zeros to be on input on the diagonal.)

#### **2.7.4** Example

Usage of the routines in this section will be demonstrated using the following matrices

$$A = \begin{pmatrix} 1.0 & 3.0 & -2.0 \\ 3.0 & 4.0 & 5.0 & \\ 5.0 & 6.0 & -2.0 & 6.0 & 7.0 + 2.0 \end{pmatrix}, \qquad B = \begin{pmatrix} 2.0 & 4.0 & -3.0 \\ 4.0 & 6.0 & 6.0 & \\ 6.0 & 7.0 & 0.0 & -1.0 \\ -3.0 & 7.0 & 8.0 - 1.0 \end{pmatrix}.$$

The following code reads a matrix in full Compressed Sparse Column form, and then converts it to HSL standard format using mc69\_csclu\_convert. In addition to the initial conversion, a second set of values matching the same pattern is read. These values are then converted to HSL standard form using mc69\_set\_values.

```
program hsl_mc69ds4
  use hsl_mc69_double
  implicit none

integer, parameter :: wp = kind(0d0)

integer :: i, j, matrix_type, n, flag, lmap
  integer, dimension(:), allocatable :: ptr, row, ptr_out, row_out, map
  real(wp), dimension(:), allocatable :: val, val_out
```

```
! Read matrix in full CSC form
   read(*, "(2i8)") matrix_type, n
   allocate(ptr(n+1)); read(*, "(6i8)") ptr(:)
   allocate(row(ptr(n+1)-1)); read(*, "(6i8)") row(:)
   allocate(val(ptr(n+1)-1)); read(*, "(4es12.4)") val(:)
   write(*, "(a)") "Input:"
   do i = 1, n
      write(*, "(a,i2,':')",advance="no") "Column ", i
      do j = ptr(i), ptr(i+1)-1
         write(*, "(1x,i4,1x,'(',es9.2,')')", advance="no") row(j), val(j)
      end do
      write(*, "()")
   end do
   ! Convert to HSL standard form out of place
   allocate(ptr_out(n+1))
   call mc69_csclu_convert(matrix_type, n, ptr, row, ptr_out, row_out, flag, &
      val_in=val, val_out=val_out, lmap=lmap, map=map)
   if(flag.lt.0) then
      write(*, "(a,i3)") &
         "Error return from mc69 csclu convert with flag = ", flag
      stop
   endif
   write(*, "(/a)") "Output:"
   do i = 1, n
      write(*, "(a,i2,':')",advance="no") "Column ", i
      do j = ptr_out(i), ptr_out(i+1)-1
         write(*, "(1x,i4,1x,'(',es9.2,')')", advance="no") &
            row_out(j), val_out(j)
      end do
      write(*, "()")
   end do
   ! Print out matrix
   write(*, "()")
   call mc69_print(6, 0, matrix_type, n, n, ptr_out, row_out, val=val_out)
   ! Read and apply new values
   read(*, "(4es12.4)") val(:)
   call mc69_set_values(matrix_type, lmap, map, val, ptr_out(n+1)-1, val_out)
   write(*, "(/a)") "After applying new values:"
   call mc69_print(6, 0, matrix_type, n, n, ptr_out, row_out, val=val_out)
end program hsl_mc69ds4
```

If provided with the following input (matching the matrices A and B above),

```
4 4
1 4 7 9 13
```

```
1
               4
                       2
                               1
                                       2
                                                3
       2
               4
                               3
                                       4
                       1
                                                4
  1.0000E+00 -2.0000E+00
                          3.0000E+00 3.0000E+00
  4.0000E+00 5.0000E+00
                          5.0000E+00
                                      6.0000E+00
 -2.0000E+00 7.0000E+00
                          7.0000E+00
                                      2.0000E+00
  2.0000E+00 -3.0000E+00
                          4.0000E+00
                                      4.0000E+00
  6.0000E+00 6.0000E+00
                          6.0000E+00 7.0000E+00
 -3.0000E+00 7.0000E+00 8.0000E+00 -1.0000E+00
the code produces the following output.
Input:
Column 1:
              1 (1.00E+00)
                               4 (-2.00E+00)
                                                2 (3.00E+00)
                               2 ( 4.00E+00)
Column 2:
              1 (3.00E+00)
                                                3 (5.00E+00)
Column 3:
              2 (5.00E+00)
                               4 (6.00E+00)
Column 4:
              1 (-2.00E+00)
                               3 (7.00E+00)
                                                 4 (7.00E+00)
                                                                  4 (2.00E+00)
Output:
Column 1:
              1 (1.00E+00)
                               2 ( 3.00E+00)
                                                 4 (-2.00E+00)
Column 2:
              2 (4.00E+00)
                               3 (5.00E+00)
Column 3:
              4 (7.00E+00)
Column 4:
              4 (9.00E+00)
Real symmetric indefinite matrix, dimension 4x4 with 7 entries.
1:
     1.0000E+00
                  3.0000E+00
                                            -2.0000E+00
     3.0000E+00
                               5.0000E+00
2:
                  4.0000E+00
                                            7.0000E+00
                  5.0000E+00
3:
4: -2.0000E+00
                               7.0000E+00
                                             9.0000E+00
After applying new values:
Real symmetric indefinite matrix, dimension 4x4 with 7 entries.
     2.0000E+00
                  4.0000E+00
                                            -3.0000E+00
2:
     4.0000E+00
                  6.0000E+00
                               6.0000E+00
```

7.0000E+00

6.0000E+00

3:

4: -3.0000E+00

7.0000E+00

7.0000E+00

## 2.8 Matrices in compressed sparse row format

The following routines handle a matrix stored in compressed sparse row format, with entries only in the lower triangle for symmetric, skew-symmetric or Hermitian matrices. Entries within each row of the user-supplied matrix do **not** need to be ordered. There is no requirement that zero entries on the diagonal be explicitly included.

The input matrix is stored as a series of compressed rows using the following data:

- m is a scalar of type INTEGER that holds the number of rows of A.
- n is a scalar of type INTEGER that holds the number of columns of A.
- ptr is a rank-one array of type INTEGER. The first m values must be set such that ptr(j) holds the position in col of the first entry in row j and ptr(m+1) must be one more than the total number of entries.
- col is a rank-one array of type INTEGER. The first ptr (m+1) -1 entries hold the column indices of the entries in A, with the column indices for the entries in row 1 preceding those for row 2, and so on. For symmetric, skew symmetric and Hermitian matrices only entries in the lower triangle should be stored. The indices within each row may be unordered.

If the values are required in addition to the matrix pattern, the following array is used:

val is a rank-one array of package type. val (k) must hold the value of the entry in col (k).

## 2.8.1 To perform a conversion from compressed sparse row format to standard HSL format

To convert a matrix held in compressed sparse row format to standard HSL format, the user may make a call of the following form. This routine checks the user's data and handles duplicate entries (they are summed) and out-of-range entries (they are discarded). For symmetric, skew-symmetric and Hermitian matrices, entries in the upper triangle are discarded as out-of-range. For skew-symmetric matrices only, entries on the diagonal are treated as out-of-range entries, and are discarded.

```
call mc69_csrl_convert(matrix_type, m, n, ptr_in, col_in, ptr_out, row_out, &
    flag[, val_in, val_out, lmap, map, lp, noor, ndup])
```

- matrix\_type is an INTENT(IN) scalar of type INTEGER that describes the type of matrix. It must take one of the values described in Section 2.3. If this argument has value 0 (HSL\_MATRIX\_UNDEFINED), the matrix will be treated as if it were rectangular.
- m, n, ptr\_in and col\_in are of INTENT (IN) and must be set by the user to hold A in compressed sparse row format, as described in Section 2.8.
- ptr\_out and row\_out are INTENT(OUT) rank-one arrays of type INTEGER. ptr\_out is of size n+1 and row\_out is allocatable. On exit, they hold A in HSL standard format, as described in Section 2.4.
- flag is an INTENT (OUT) scalar of type INTEGER. On exit, a value of 0 indicates successful conversion. Positive values indicate successful conversion but a warning was issued. Negative values are associated with an error; see Section 2.8.3 for details.
- val\_in is an optional INTENT(IN) rank-one array of package type. If present, on input the first ptr\_in(m+1)-1 entries must be set so that val\_in(k) holds the value of the entry col\_in(k). If val\_in is present, val\_out must also be present.

val\_out is an optional INTENT (OUT) rank-one allocatable array of package type. If present, on exit it will be allocated and the first ptr\_out (n+1) -1 entries will be set such that val\_out (k) holds the value of the entry row\_out (k). If val\_out is present, val\_in must also be present.

- lmap is an optional INTENT (OUT) scalar of type INTEGER. If lmap is present, map must also be present.
- map is an optional INTENT (OUT) rank-one ALLOCATABLE array of type INTEGER. It should be present if the user wishes to change the values of the entries of A following the call to mc69\_csrl\_convert, and should be passed unaltered to any subsequent calls to mc69\_set\_values. A detailed description of the output format is given in Section 4.1. If map is present, lmap must also be present.
- lp is an optional INTENT (IN) scalar of type INTEGER. If present and  $lp \ge 0$ , error and warning messages are written to unit lp.
- noor is an optional INTENT (OUT) scalar of type INTEGER. If present, on exit it contains the number of out-of-range entries that were discarded.
- ndup is an optional INTENT (OUT) scalar of type INTEGER. If present, on exit it contains the number of duplicate entries that were summed.

## **2.8.2** To set values of *A* following a conversion

The user may want to change the values of the entries of A following a successful call to mc69\_csrl\_convert. Alternatively, the user may want to include matrix values after a call to mc69\_csrl\_convert with matrix values not present. This can be done by making a call of the following form, however note that no checks are made on the values of the diagonal entries.

```
call mc69_set_values(matrix_type, lmap, map, val_in, ne, val_out)
```

- matrix\_type is an INTENT(IN) scalar of type INTEGER that describes the type of matrix. It must be unchanged since the call to mc69\_csrl\_convert that generated map.
- lmap is an INTENT(IN) scalar of type INTEGER that must be unchanged since the call to mc69\_csrl\_convert that
   generated map.
- map is an INTENT (IN) rank-one array of type INTEGER that must be unchanged since the call to mc69\_csrl\_convert that generated it.
- val\_in is an INTENT(IN) rank-one array of package type. It must have size at least the value of ptr\_in(m+1)-1 on the call to mc69\_csrl\_convert. It must be set by the user to hold the new values of the entries of A matching the original matrix that was input to mc69\_csrl\_convert.
- ne is an INTENT(IN) scalar argument of type INTEGER that must be set to the value of ptr\_out(n+1)-1 on exit from mc69\_csrl\_convert.
- val\_out is an INTENT (OUT) rank-one array of package type. It must have size at least the value of ptr\_out (n+1) -1 on exit from mc69\_csrl\_convert. On exit, it contains the new values of A in standard HSL format, as described in Section 2.4.

## 2.8.3 Return codes

A successful return from a call to mc69\_csrl\_convert is indicated by flag taking the value 0. Possible negative values that are associated with an error are:

- -1 Allocation error.
- -2 Invalid value of matrix\_type.
- -3 m < 0 or n < 0.
- -4  $|matrix_type|$  > 1 (square matrix) but m≠n.
- -5 ptr(1) < 1.
- -6 ptr(1:n+1) is not monotonic increasing.
- -10 All entries for a row are out of range.
- -11 |matrix\_type| =3 (positive-definite case) but one or more diagonal entries are not positive.
- -12 matrix\_type = -3 or -4 (Hermitian case) but one or more entries on the diagonal have non-zero imaginary part.
- -15 Only one of val\_in and val\_out is present.
- -16 Only one of 1map and map is present.

Possible positive values are:

- +1 Out-of-range indices found in row\_in.
- +2 Duplicate indices found in row\_in.
- +3 Both out-of-range and duplicate entries found.
- +4 |matrix\_type| ≠ 3, 6 and not all entries on the diagonal are present. (Note that no HSL package requires explicit zeros to be on input on the diagonal.)
- +5 |matrix\_type| ≠ 3, 6 and not all entries on the diagonal are present and out-of-range and/or duplicate entries found. (Note that no HSL package requires explicit zeros to be on input on the diagonal.)

#### **2.8.4** Example

Usage of the routines in this section will be demonstrated using the following matrices

$$A = \begin{pmatrix} 1.0 & 3.0 & -2.0 \\ 3.0 & 4.0 & 5.0 & \\ 5.0 & 5.0 & 6.0 \\ -2.0 & 6.0 & 7.0 + 2.0 \end{pmatrix}, \qquad B = \begin{pmatrix} 2.0 & 4.0 & -3.0 \\ 4.0 & 6.0 & 6.0 & \\ 6.0 & 7.0 & \\ -3.0 & 7.0 & 8.0 - 1.0 \end{pmatrix}.$$

The following code reads a matrix in Compressed Sparse Row form, and then converts it to HSL standard format using mc69\_csrl\_convert. In addition to the initial conversion, a second set of values matching the same pattern is read. These values are then converted to HSL standard form using mc69\_set\_values.

```
program hsl_mc69ds5
   use hsl_mc69_double
   implicit none
   integer, parameter :: wp = kind(0d0)
   integer :: i, j, matrix_type, m, n, flag, lmap
   integer, dimension(:), allocatable :: ptr, row, ptr_out, row_out, map
   real(wp), dimension(:), allocatable :: val, val_out
   ! Read matrix in CSR form
   read(*, "(3i8)") matrix_type, m, n
   allocate(ptr(n+1)); read(*, "(6i8)") ptr(:)
   allocate(row(ptr(n+1)-1)); read(*, "(6i8)") row(:)
   allocate(val(ptr(n+1)-1)); read(*, "(4es12.4)") val(:)
   write(*, "(a)") "Input:"
   do i = 1, m
      write(*, "(a,i2,':')",advance="no") "Row ", i
      do j = ptr(i), ptr(i+1)-1
         write(*, "(2x,i4,1x,'(',es12.2,')')", advance="no") row(j), val(j)
      end do
      write(*, "()")
   end do
   ! Convert to HSL standard form out of place
   allocate(ptr_out(n+1))
   call mc69_csrl_convert(matrix_type, m, n, ptr, row, ptr_out, row_out, flag, &
      val_in=val, val_out=val_out, lmap=lmap, map=map)
   if(flag.lt.0) then
      write(*, "(a,i3)") &
         "Error return from mc69_csrl_convert with flag = ", flag
      stop
   endif
   write(*, "(/a)") "Output:"
   do i = 1, n
      write(*, "(a,i2,':')",advance="no") "Column ", i
      do j = ptr_out(i), ptr_out(i+1)-1
         write(*, "(2x,i4,1x,'(',es12.2,')')", advance="no") &
            row_out(j), val_out(j)
      end do
      write(*, "()")
   end do
   ! Print out matrix
   write(*, "()")
   call mc69_print(6, 0, matrix_type, m, n, ptr_out, row_out, val=val_out)
```

```
! Read and apply new values read(*, "(4es12.4)") val(:) call mc69_set_values(matrix_type, lmap, map, val, ptr_out(n+1)-1, val_out) write(*, "(/a)") "After applying new values:" call mc69_print(6, 0, matrix_type, m, n, ptr_out, row_out, val=val_out) end program hsl_mc69ds5

If provided with the following input (matching the matrices A and B above),
```

```
4
                     4
     1
             2
                     4
                             5
                                     9
     1
             1
                     2
                             2
                                     3
                                             1
     4
1.0000E+00 3.0000E+00 4.0000E+00 5.0000E+00
6.0000E+00 -2.0000E+00 7.0000E+00 2.0000E+00
2.0000E+00 4.0000E+00 6.0000E+00 6.0000E+00
7.0000E+00 -3.0000E+00 8.0000E+00 -1.0000E+00
```

## the code produces the following output.

```
Input:
Row 1:
            1 (
                   1.00E+00)
Row
    2:
            1 (
                   3.00E+00)
                                 2 (
                                        4.00E+00)
Row 3:
            2 (
                   5.00E+00)
Row 4:
            3 (
                   6.00E+00)
                                 1 (-2.00E+00)
                                                       4 (
                                                              7.00E+00)
                                                                            4 (
                                                                                   2.00E+00)
Output:
Column 1:
               1 (
                      1.00E+00)
                                    2 (
                                            3.00E+00)
                                                                -2.00E+00)
                                                          4 (
Column
       2:
               2 (
                      4.00E+00)
                                    3 (
                                            5.00E+00)
Column 3:
                      6.00E+00)
               4 (
Column 4:
                      9.00E+00)
               4 (
Real symmetric indefinite matrix, dimension 4x4 with 7 entries.
                                            -2.0000E+00
    1.0000E+00
                  3.0000E+00
    3.0000E+00
                  4.0000E+00
                               5.0000E+00
2:
3:
                  5.0000E+00
                                             6.0000E+00
4: -2.0000E+00
                                6.0000E+00
                                             9.0000E+00
After applying new values:
Real symmetric indefinite matrix, dimension 4x4 with 7 entries.
    2.0000E+00
                  4.0000E+00
                                            -3.0000E+00
2: 4.0000E+00
                  6.0000E+00
                                6.0000E+00
3:
                  6.0000E+00
                                             7.0000E+00
4: -3.0000E+00
                               7.0000E+00
                                            7.0000E+00
```

## 2.9 Symmetric, skew symmetric and Hermitian matrices in upper compressed sparse row format

The following routines handle symmetric, skew-symmetric of Hermitian matrices stored in upper compressed sparse row format (with entries only in the upper triangle). Entries within each row of the user-supplied matrix do **not** need to be ordered. There is no requirement that zero entries on the diagonal be explicitly included.

The input matrix is stored as a series of compressed rows using the following data:

- n is a scalar of type INTEGER that holds the order of A.
- ptr is a rank-one array of type INTEGER. The first n values must be set such that ptr(j) holds the position in col of the first entry in row j and ptr(n+1) must be one more than the total number of entries.
- col is a rank-one array of type INTEGER. The first ptr(n+1)-1 entries hold the column indices of the entries in A, with the column indices for the entries in row 1 preceding those for row 2, and so on. For symmetric, skew symmetric and Hermitian matrices only entries in the upper triangle should be stored. The indices within each row may be unordered.

If the values are required in addition to the matrix pattern, the following array is used:

val is a rank-one array of package type. val (k) must hold the value of the entry in col (k).

## 2.9.1 To perform a conversion from upper compressed sparse row format to standard HSL format

To convert a matrix held in upper compressed sparse row format to standard HSL format, the user may make a call of the following form. This routine checks the user's data and handles duplicate entries (they are summed) and out-of-range entries (they are discarded). Entries in the lower triangle are discarded. For skew-symmetric matrices only, entries on the diagonal are treated as out-of-range entries, and are discarded.

```
call mc69_csru_convert(matrix_type, n, ptr_in, col_in, ptr_out, row_out, &
    flag[, val_in, val_out, lmap, map, lp, noor, ndup])
```

- matrix\_type is an INTENT(IN) scalar of type INTEGER that describes the type of matrix. It must take one of the values described in Section 2.3 for symmetric, skew-symmetric or Hermitian matrices.
- n, ptr\_in and col\_in are of INTENT(IN) and must be set by the user to hold A in upper compressed sparse row format, as described in Section 2.9.
- ptr\_out and row\_out are INTENT (OUT) rank-one arrays of type INTEGER. ptr\_out is of size n+1 and row\_out is allocatable. On exit, they hold A in HSL standard format, as described in Section 2.4.
- flag is an INTENT (OUT) scalar of type INTEGER. On exit, a value of 0 indicates successful conversion. Positive values indicate successful conversion but a warning was issued. Negative values are associated with an error; see Section 2.9.3 for details.
- val\_in is an optional INTENT(IN) rank-one array of package type. If present, on input the first ptr\_in(n+1)-1 entries must be set so that val\_in(k) holds the value of the entry col\_in(k). If val\_in is present, val\_out must also be present.
- val\_out is an optional INTENT (OUT) rank-one allocatable array of package type. If present, on exit it will be allocated and the first ptr\_out (n+1) -1 entries will be set such that val\_out (k) holds the value of the entry row\_out (k). If val\_out is present, val\_in must also be present.

lmap is an optional INTENT (OUT) scalar of type INTEGER. If lmap is present, map must also be present.

map is an optional INTENT (OUT) rank-one ALLOCATABLE array of type INTEGER. It should be present if the user wishes to change the values of the entries of A following the call to mc69\_csru\_convert, and should be passed unaltered to any subsequent calls to mc69\_set\_values. A detailed description of the output format is given in Section 4.1. If map is present, lmap must also be present.

- lp is an optional INTENT (IN) scalar of type INTEGER. If present and  $lp \ge 0$ , error and warning messages are written to unit lp.
- noor is an optional INTENT (OUT) scalar of type INTEGER. If present, on exit it contains the number of out-of-range entries that were discarded.
- ndup is an optional INTENT (OUT) scalar of type INTEGER. If present, on exit it contains the number of duplicate entries that were summed.

## 2.9.2 To set values of A following a conversion

The user may want to change the values of the entries of A following a successful call to mc69\_csru\_convert. Alternatively, the user may want to include matrix values after a call to mc69\_csru\_convert with matrix values not present. This can be done by making a call of the following form, however note that no checks are made on the values of the diagonal entries.

```
call mc69_set_values(matrix_type, lmap, map, val_in, ne, val_out)
```

- matrix\_type is an INTENT(IN) scalar of type INTEGER that describes the type of matrix. It must be unchanged since the call to mc69\_csru\_convert that generated map.
- lmap is an INTENT(IN) scalar of type INTEGER that must be unchanged since the call to mc69\_csru\_convert that
   generated map.
- map is an INTENT (IN) rank-one array of type INTEGER that must be unchanged since the call to mc69\_csru\_convert that generated it.
- val\_in is an INTENT(IN) rank-one array of package type. It must have size at least the value of ptr\_in(n+1)-1 on the call to mc69\_csru\_convert. It must be set by the user to hold the new values of the entries of A matching the original matrix that was input to mc69\_csru\_convert.
- ne is an INTENT(IN) scalar argument of type INTEGER that must be set to the value of ptr\_out(n+1)-1 on exit from mc69\_csru\_convert.
- val\_out is an INTENT (OUT) rank-one array of package type. It must have size at least the value of ptr\_out (n+1) -1 on exit from mc69\_csru\_convert. On exit, it contains the new values of A in standard HSL format, as described in Section 2.4.

# 2.9.3 Return codes

A successful return from a call to mc69\_csru\_convert is indicated by flag taking the value 0. Possible negative values that are associated with an error are:

- -1 Allocation error.
- -2 Invalid value of matrix\_type.
- -3 n < 0.

- -5 ptr(1) < 1.
- -6 ptr(1:n+1) is not monotonic increasing.
- -10 All entries for a row are out of range.
- -11 |matrix\_type| =3 (positive-definite case) but one or more diagonal entries are not positive.
- -12 matrix\_type =-3 or -4 (Hermitian case) but one or more entries on the diagonal have non-zero imaginary part.
- -15 Only one of val\_in and val\_out is present.
- -16 Only one of 1map and map is present.

Possible positive values are:

- +1 Out-of-range indices found in row\_in.
- +2 Duplicate indices found in row\_in.
- +3 Both out-of-range and duplicate entries found.
- +4 |matrix\_type| ≠ 3, 6 and not all entries on the diagonal are present. (Note that no HSL package requires explicit zeros to be on input on the diagonal.)
- +5 |matrix\_type| ≠ 3, 6 and not all entries on the diagonal are present and out-of-range and/or duplicate entries found. (Note that no HSL package requires explicit zeros to be on input on the diagonal.)

# **2.9.4** Example

Usage of the routines in this section will be demonstrated using the following matrices

$$A = \begin{pmatrix} 1.0 & 3.0 & -2.0 \\ 3.0 & 4.0 & 5.0 & \\ 5.0 & 5.0 & 6.0 \\ -2.0 & 6.0 & 7.0 + 2.0 \end{pmatrix}, \qquad B = \begin{pmatrix} 2.0 & 4.0 & -3.0 \\ 4.0 & 6.0 & 6.0 & \\ 6.0 & 7.0 & \\ -3.0 & 7.0 & 8.0 - 1.0 \end{pmatrix}.$$

The following code reads a matrix in upper Compressed Sparse Row form, and then converts it to HSL standard format using mc69\_csru\_convert. In addition to the initial conversion, a second set of values matching the same pattern is read. These values are then converted to HSL standard form using mc69\_set\_values.

```
program hsl_mc69ds6
  use hsl_mc69_double
  implicit none

integer, parameter :: wp = kind(0d0)

integer :: i, j, matrix_type, n, flag, lmap
  integer, dimension(:), allocatable :: ptr, row, ptr_out, row_out, map
  real(wp), dimension(:), allocatable :: val, val_out

! Read symmetric matrix in upper CSR form
  read(*, "(2i8)") matrix_type, n
  allocate(ptr(n+1)); read(*, "(6i8)") ptr(:)
```

```
allocate(row(ptr(n+1)-1)); read(*, "(6i8)") row(:)
   allocate(val(ptr(n+1)-1)); read(*, "(4es12.4)") val(:)
   write(*, "(a)") "Input:"
   do i = 1, n
      write(*, "(a,i2,':')",advance="no") "Row ", i
      do j = ptr(i), ptr(i+1)-1
         write(*, "(2x,i4,1x,'(',es12.2,')')", advance="no") row(j), val(j)
      end do
      write(*, "()")
   end do
   ! Convert to HSL standard form out of place
   allocate(ptr_out(n+1))
   call mc69_csru_convert(matrix_type, n, ptr, row, ptr_out, row_out, flag, &
      val_in=val, val_out=val_out, lmap=lmap, map=map)
   if(flag.lt.0) then
      write(*, "(a,i3)") &
         "Error return from mc69_csrl_convert with flag = ", flag
      stop
   endif
   write(*, "(/a)") "Output:"
   do i = 1, n
      write(*, "(a,i2,':')",advance="no") "Column ", i
      do j = ptr_out(i), ptr_out(i+1)-1
         write(*, "(2x,i4,1x,'(',es12.2,')')", advance="no") &
            row_out(j), val_out(j)
      end do
      write(*, "()")
   end do
   ! Print out matrix
   write(*, "()")
   call mc69_print(6, 0, matrix_type, n, n, ptr_out, row_out, val=val_out)
   ! Read and apply new values
   read(*, "(4es12.4)") val(:)
   call mc69_set_values(matrix_type, lmap, map, val, ptr_out(n+1)-1, val_out)
   write(*, "(/a)") "After applying new values:"
   call mc69_print(6, 0, matrix_type, n, n, ptr_out, row_out, val=val_out)
end program hsl_mc69ds6
```

If provided with the following input (matching the matrices A and B above),

Documentation date: May 30, 2023

34

```
5.0000E+00 6.0000E+00 7.0000E+00 2.0000E+00
  2.0000E+00 -3.0000E+00 4.0000E+00 6.0000E+00
  6.0000E+00 7.0000E+00 8.0000E+00 -1.0000E+00
the code produces the following output.
Input:
            1 (
                   1.00E+00)
                                       -2.00E+00)
                                                       2 (
                                                              3.00E+00)
Row 1:
                                 4 (
Row
     2:
            2 (
                   4.00E+00)
                                 3 (
                                        5.00E+00)
            4 (
Row 3:
                   6.00E+00)
            4 (
Row 4:
                   7.00E+00)
                                 4 (
                                        2.00E+00)
Output:
Column 1:
                                    2 (
                                           3.00E+00)
                                                          4 ( -2.00E+00)
               1 (
                      1.00E+00)
Column 2:
               2 (
                      4.00E+00)
                                    3 (
                                            5.00E+00)
Column 3:
               4 (
                      6.00E+00)
Column 4:
               4 (
                      9.00E+00)
Real symmetric indefinite matrix, dimension 4x4 with 7 entries.
    1.0000E+00
                  3.0000E+00
                                            -2.0000E+00
2:
     3.0000E+00
                  4.0000E+00
                               5.0000E+00
                  5.0000E+00
3:
                                             6.0000E+00
4: -2.0000E+00
                               6.0000E+00
                                            9.0000E+00
After applying new values:
Real symmetric indefinite matrix, dimension 4x4 with 7 entries.
1:
     2.0000E+00
                  4.0000E+00
                                            -3.0000E+00
```

6.0000E+00

7.0000E+00

7.0000E+00

7.0000E+00

2:

3:

4.0000E+00

4: -3.0000E+00

6.0000E+00

6.0000E+00

## 2.10 Symmetric, skew symmetric and Hermitian matrices in full compressed sparse row format

The following routines handle a symmetric, skew symmetric or Hermitian matrix stored in full compressed sparse row format (entries in both the lower and upper triangles are supplied by the user). Entries within each row of the user-supplied matrix do **not** need to be ordered. There is no requirement that zero entries on the diagonal be explicitly included.

The input matrix is stored as a series of compressed rows using the following data:

- n is a scalar of type INTEGER that holds the order of A.
- ptr is a rank-one array of type INTEGER. The first n values must be set such that ptr(j) holds the position in col of the first entry in row j and ptr(n+1) must be one more than the total number of entries.
- col is a rank-one array of type INTEGER. The first ptr (n+1)-1 entries hold the column indices of the entries of A, with the column indices for the entries in row 1 preceding those for row 2, and so on. If a non-diagonal entry (i, j) is present, its counterpart (j, i) must also be present. The indices within each row may be unordered,

If the values are required in addition to the matrix pattern, the following array is used:

val is a rank-one array of package type. val (k) must hold the value of the entry in col (k).

## 2.10.1 To convert from full compressed sparse row format to standard HSL format

To convert a symmetric, skew-symmetric or Hermitian matrix held in full compressed sparse row format to standard HSL format the user may make a call of the following form. This routine checks the user's data and handles duplicate entries (they are summed) and out-of-range entries (they are discarded). Entries in the upper triangle are ignored, except to check that there are the same number of entries in both the lower and upper triangles. For skew-symmetric matrices only, entries on the diagonal are treated as out-of-range and are discarded.

```
call mc69_csrlu_convert(matrix_type, n, ptr_in, col_in, ptr_out, row_out, flag[, val_in, &
    val out, lmap, map, lp, noor, ndup])
```

- matrix\_type is an INTENT(IN) scalar of type INTEGER that describes the type of matrix. It must take one of the values described in Section 2.3 for symmetric, skew-symmetric or Hermitian matrices.
- n, ptr\_in and col\_in are of INTENT(IN) and must be set by the user to hold A in full compressed sparse column format, as described in Section 2.10.
- ptr\_out and row\_out are INTENT(OUT) rank-one arrays of type INTEGER. ptr\_out is of size n+1 and row\_out is allocatable. On exit, they hold A in HSL standard format, as described in Section 2.4.
- flag is an INTENT (OUT) scalar of type INTEGER. On exit, a value of 0 indicates successful conversion. Positive values indicate successful conversion but a warning was issued. Negative values are associated with an error; see Section 2.10.3 for details.
- val\_in is an optional INTENT (IN) rank-one array of package type. If present, the first ptr\_in(n+1)-1 entries must be set so that val\_in(k) holds the value of the entry row\_in(k). If val\_in is present, val\_out must also be present.
- val\_out is an optional INTENT(OUT) rank-one ALLOCATABLE array of package type. On exit, it is allocated to have size equal to that of row\_out and val\_out(k) holds the value of the entry row\_out(k). If val\_out is present, val\_in must also be present.

lmap is an optional INTENT (OUT) scalar of type INTEGER. If lmap is present, map must also be present.

- map is an optional INTENT (OUT) rank-one ALLOCATABLE array of type INTEGER. It should be present if the user wishes to change the values of the entries of A following the call to mc69\_csrlu\_convert, and should be passed unaltered to any subsequent calls to mc69\_set\_values. A detailed description of the output format is given in Section 4.1. If map is present, lmap must also be present.
- lp is an optional INTENT (IN) scalar of type INTEGER. If present and  $lp \ge 0$ , error and warning messages are written to unit lp.
- noor is an optional INTENT (OUT) scalar of type INTEGER. If present, on exit it contains the number of out-of-range entries that were discarded.
- ndup is an optional INTENT (OUT) scalar of type INTEGER. If present, on exit it contains the number of duplicate entries that were summed.

## 2.10.2 To set values of A following a conversion

The user may want to change the values of the entries of A following a successful call to mc69\_csrlu\_convert. Alternatively, the user may want to include matrix values after a call to mc69\_csrlu\_convert with matrix values not present. This can be done by making a call of the following form, however note that no checks are made on the values of the diagonal entries.

```
call mc69_set_values(matrix_type, lmap, map, val_in, ne, val_out)
```

- matrix\_type is an INTENT(IN) scalar of type INTEGER that describes the type of matrix. It must be unchanged since the call to mc69\_csrlu\_convert that generated map.
- lmap is an INTENT(IN) scalar of type INTEGER that must be unchanged since the call to mc69\_csrlu\_convert that
   generated map.
- map is an INTENT (IN) rank-one array of type INTEGER that must be unchanged since the call to mc69\_csrlu\_convert that generated it.
- val\_in is an INTENT(IN) rank-one array of package type. It must have size at least the value of ptr\_in(n+1)-1 on the call to mc69\_csrlu\_convert. It must be set by the user to hold the new values of the entries of A matching the original matrix that was input to mc69\_csrlu\_convert.
- ne is an INTENT(IN) scalar argument of type INTEGER that must be set to the value of ptr\_out(n+1)-1 on exit from mc69\_csrlu\_convert.
- val\_out is an INTENT (OUT) rank-one array of package type. It must have size at least the value of ptr\_out (n+1) -1 on exit from mc69\_csrlu\_convert. On exit, it contains the new values of A in standard HSL format, as described in Section 2.4.

## 2.10.3 Return codes

A successful return from a call to mc69\_csrlu\_convert is indicated by flag taking the value 0. Possible negative values that are associated with an error are:

- -1 Allocation error.
- -2 Invalid value of matrix\_type.

- -3 n < 0.
- -5 ptr(1) < 1.
- -6 ptr(1:n+1) is not monotonic increasing.
- -10 All entries for a row are out of range.
- -13 Number of in-range entries in lower and upper triangles do not match.
- -11 |matrix\_type| =3 (positive-definite case) but one or more diagonal entries are not positive.
- -12 matrix\_type =-3 or -4 (Hermitian case) but one or more entries on the diagonal have non-zero imaginary part.
- -15 Only one of val\_in and val\_out is present.
- -16 Only one of 1map and map is present.

Possible positive values are:

- +1 Out-of-range indices found in row\_in.
- +2 Duplicate indices found in row\_in.
- +3 Both out-of-range and duplicate entries found.
- +4 |matrix\_type| ≠ 3, 6 and not all entries on the diagonal are present. (Note that no HSL package requires explicit zeros to be on input on the diagonal.)
- +5 |matrix\_type| ≠ 3,6 and not all entries on the diagonal are present and out-of-range and/or duplicate entries found. (Note that no HSL package requires explicit zeros to be on input on the diagonal.)

#### **2.10.4** Example

Usage of the routines in this section will be demonstrated using the following matrices

$$A = \begin{pmatrix} 1.0 & 3.0 & -2.0 \\ 3.0 & 4.0 & 5.0 & \\ 5.0 & 6.0 & 7.0 + 2.0 \end{pmatrix}, \qquad B = \begin{pmatrix} 2.0 & 4.0 & -3.0 \\ 4.0 & 6.0 & 6.0 & \\ 6.0 & 7.0 & 8.0 - 1.0 \end{pmatrix}.$$

The following code reads a matrix in full Compressed Sparse Row form, and then converts it to HSL standard format using mc69\_csrlu\_convert. In addition to the initial conversion, a second set of values matching the same pattern is read. These values are then converted to HSL standard form using mc69\_set\_values.

```
program hsl_mc69ds7
  use hsl_mc69_double
  implicit none

integer, parameter :: wp = kind(0d0)

integer :: i, j, matrix_type, n, flag, lmap
  integer, dimension(:), allocatable :: ptr, row, ptr_out, row_out, map
  real(wp), dimension(:), allocatable :: val, val_out
```

```
! Read matrix in full CSR form
   read(*, "(2i8)") matrix_type, n
  allocate(ptr(n+1)); read(*, "(6i8)") ptr(:)
  allocate(row(ptr(n+1)-1)); read(*, "(6i8)") row(:)
  allocate(val(ptr(n+1)-1)); read(*, "(4es12.4)") val(:)
  write(*, "(a)") "Input:"
  do i = 1, n
     write(*, "(a,i2,':')",advance="no") "Row ", i
      do j = ptr(i), ptr(i+1)-1
        write(*, "(1x,i4,1x,'(',es9.2,')')", advance="no") row(j), val(j)
      end do
      write(*, "()")
  end do
   ! Convert to HSL standard form out of place
  allocate(ptr_out(n+1))
   call mc69_csrlu_convert(matrix_type, n, ptr, row, ptr_out, row_out, flag, &
      val_in=val, val_out=val_out, lmap=lmap, map=map)
  if(flag.lt.0) then
      write(*, "(a,i3)") &
         "Error return from mc69 csrlu convert with flag = ", flag
      stop
  endif
  write(*, "(/a)") "Output:"
  do i = 1, n
     write(*, "(a,i2,':')",advance="no") "Column ", i
      do j = ptr_out(i), ptr_out(i+1)-1
        write(*, "(1x,i4,1x,'(',es9.2,')')", advance="no") &
           row_out(j), val_out(j)
      end do
     write(*, "()")
   end do
   ! Print out matrix
  write(*, "()")
  call mc69_print(6, 0, matrix_type, n, n, ptr_out, row_out, val=val_out)
   ! Read and apply new values
   read(*, "(4es12.4)") val(:)
  call mc69_set_values(matrix_type, lmap, map, val, ptr_out(n+1)-1, val_out)
  write(*, "(/a)") "After applying new values:"
  call mc69_print(6, 0, matrix_type, n, n, ptr_out, row_out, val=val_out)
end program hsl_mc69ds7
```

If provided with the following input (matching the matrices A and B above),

4 4 1 4 7 9 13

```
1
               4
                       2
                               1
                                        2
                                                3
       2
               4
                               3
                       1
                                        4
                                                4
 1.0000E+00 -2.0000E+00
                          3.0000E+00 3.0000E+00
 4.0000E+00 5.0000E+00
                          5.0000E+00
                                      6.0000E+00
 -2.0000E+00 7.0000E+00
                          7.0000E+00 2.0000E+00
  2.0000E+00 -3.0000E+00
                          4.0000E+00 4.0000E+00
 6.0000E+00 6.0000E+00
                          6.0000E+00 7.0000E+00
 -3.0000E+00 7.0000E+00 8.0000E+00 -1.0000E+00
the code produces the following output.
Input:
Row 1:
           1 (1.00E+00)
                            4 (-2.00E+00)
                            2 ( 4.00E+00)
```

```
2 (3.00E+00)
          1 (3.00E+00)
Row 2:
                                            3 (5.00E+00)
Row 3:
          2 (5.00E+00)
                           4 (6.00E+00)
Row 4:
          1 (-2.00E+00)
                           3 (7.00E+00)
                                           4 (7.00E+00)
                                                            4 (2.00E+00)
Output:
```

```
Column 1:
             1 (1.00E+00)
                              2 ( 3.00E+00)
                                               4(-2.00E+00)
Column 2:
             2 (4.00E+00)
                              3 (5.00E+00)
             4 (7.00E+00)
Column 3:
Column 4:
             4 (9.00E+00)
```

Real symmetric indefinite matrix, dimension 4x4 with 7 entries.

```
-2.0000E+00
1:
     1.0000E+00
                  3.0000E+00
     3.0000E+00
                                5.0000E+00
2:
                  4.0000E+00
                  5.0000E+00
                                              7.0000E+00
3:
4: -2.0000E+00
                                7.0000E+00
                                              9.0000E+00
```

## After applying new values:

2.0000E+00

Real symmetric indefinite matrix, dimension 4x4 with 7 entries.

```
2:
    4.0000E+00
                  6.0000E+00
                               6.0000E+00
3:
                  6.0000E+00
                                             7.0000E+00
4: -3.0000E+00
                               7.0000E+00
                                            7.0000E+00
```

4.0000E+00

-3.0000E+00

#### 2.11 Coordinate format

The following routines handle a user-supplied matrix stored in coordinate format. Each non-zero entry in the input matrix is held as a pair (row index, column index) or as a triplet (row index, column index, value). For symmetric, skew symmetric and Hermitian matrices each non-zero entry may be stored as either (i,j) or (j,i) (with appropriate sign or conjugacy). If both entries are input, or if duplicates are input, the values are summed by the routines described in this section.

The triplets are stored using the following data:

- m is a scalar of type INTEGER that holds the number of rows of A.
- n is a scalar of type INTEGER that holds the number of columns of A.
- ne is a scalar of type INTEGER that holds the number of entries of A.
- row is a rank-one array of type INTEGER. The first ne values row(j) must hold the row index for the j-th entry of A.
- col is a rank-one array of type INTEGER. The first ne values col (j) must hold the column index for the j-th entry of A.

If the values are required in addition to the matrix pattern, the following array is used:

val is a rank-one array of package type. The first ne values val(j) must hold the value for the j-th entry of A.

## 2.11.1 To convert from coordinate format to standard HSL format

To convert a matrix held in coordinate format to standard HSL format, the user may make a call of the following form. This routine checks the user's data and handles duplicate entries (they are summed) and out-of-range entries (they are discarded). For skew-symmetric matrices, diagonal entries are treated as out-of-range entries.

```
call mc69_coord_convert(matrix_type, m, n, ne, row, col, ptr_out, row_out, flag[, &
   val_in, val_out, lmap, map, lp, noor, ndup])
```

- matrix\_type is an INTENT(IN) scalar of type INTEGER that describes the type of matrix. It must take one of the values described in Section 2.3. If this argument has value 0 (HSL\_MATRIX\_UNDEFINED), the matrix will be treated as if it were rectangular.
- m, n, ne, row\_in and col\_in are of INTENT(IN) and must be set by the user to hold A in coordinate format, as described in Section 2.11.
- ptr\_out and row\_out are INTENT (OUT) rank-one arrays of type INTEGER. ptr\_out is of size n+1 and row\_out is allocatable. On exit, they hold A in HSL standard format, as described in Section 2.4.
- flag is an INTENT (OUT) scalar of type INTEGER. On exit, a value of 0 indicates successful conversion. Positive values indicate successful conversion but a warning was issued. Negative values are associated with an error; see Section 2.11.3 for details.
- val\_in is an optional INTENT(IN) rank-one array of package type. If present, the first ne entries must be set so that val\_in(k) holds the value of the k-th entry of A. If val\_in is present, val\_out must also be present.
- val\_out is an optional INTENT(OUT) rank-one ALLOCATABLE array of package type. On exit, it is allocated to have size equal to that of row\_out and val\_out(k) holds the value of the entry row\_out(k). If val\_out is present, val\_in must also be present.

- 1map is an optional INTENT (OUT) scalar of type INTEGER. If 1map is present, map must also be present.
- map is an optional INTENT (OUT) rank-one ALLOCATABLE array of type INTEGER. It should be present if the user wishes to change the values of the entries of A following the call to mc69\_coord\_convert, and should be passed unaltered to any subsequent calls to mc69\_set\_values. A detailed description of the output format is given in Section 4.1. If map is present, lmap must also be present.
- lp is an optional INTENT (IN) scalar of type INTEGER. If present and  $lp \ge 0$ , error and warning messages are written to unit lp.
- noor is an optional INTENT (OUT) scalar of type INTEGER. If present, on exit it contains the number of out-of-range entries that were discarded.
- ndup is an optional INTENT (OUT) scalar of type INTEGER. If present, on exit it contains the number of duplicate entries that were summed.

## **2.11.2** To set values of *A* following a conversion

The user may want to change the values of the entries of A following a successful call to mc69\_coord\_convert. Alternatively, the user may want to include matrix values after a call to mc69\_coord\_convert with matrix values not present. This can be done by making a call of the following form, however note that no checks are made on the values of the diagonal entries.

```
call mc69_set_values(matrix_type, lmap, map, val_in, ne, val_out)
```

- matrix\_type is an INTENT(IN) scalar of type INTEGER that describes the type of matrix. It must be unchanged since the call to mc69\_coord\_convert that generated map.
- lmap is an INTENT (IN) scalar of type INTEGER that must be unchanged since the call to mc69\_coord\_convert that generated map.
- map is an INTENT(IN) rank-one array of type INTEGER that must be unchanged since the call to mc69\_coord\_convert that generated it.
- val\_in is an INTENT(IN) rank-one array of package type. It must have size at least the value of ne on the call to mc69\_coord\_convert. It must be set by the user to hold the new values of the entries of A matching the original matrix that was input to mc69\_coord\_convert.
- ne is an INTENT (IN) scalar argument of type INTEGER that must be set to the value of ptr\_out (n+1) -1 on exit from mc69\_coord\_convert.
- val\_out is an INTENT (OUT) rank-one array of package type. It must have size at least the value of ptr\_out (n+1) -1 on exit from mc69\_coord\_convert. On exit, it contains the new values of A in standard HSL format, as described in Section 2.4.

# 2.11.3 Return codes

A successful return from a call to mc69\_coord\_convert is indicated by flag taking the value 0. Possible negative values that are associated with an error are:

- -1 Allocation error.
- -2 Invalid value of matrix\_type.

- -3 m < 0 or n < 0.
- -4  $|matrix_type|$  > 1 (square matrix) but m≠n.
- -10 All entries are out of range.
- -11 |matrix\_type| =3 (positive-definite case) but one or more diagonal entries are not positive.
- -12 matrix\_type =-3 or -4 (Hermitian case) but one or more entries on the diagonal have non-zero imaginary part.
- -15 Only one of val\_in and val\_out is present.
- -16 Only one of 1map and map is present.

Possible positive values are:

- +1 Out-of-range indices found in row\_in.
- +2 Duplicate indices found in row\_in.
- +3 Both out-of-range and duplicate entries found.
- +4 |matrix\_type| ≠ 3, 6 and not all entries on the diagonal are present. (Note that no HSL package requires explicit zeros to be on input on the diagonal.)
- +5 |matrix\_type| ≠ 3, 6 and not all entries on the diagonal are present and out-of-range and/or duplicate entries found. (Note that no HSL package requires explicit zeros to be on input on the diagonal.)

# **2.11.4** Example

Usage of the routines in this section will be demonstrated using the following matrices

$$A = \begin{pmatrix} 1.0 & 3.0 & -2.0 \\ 3.0 & 4.0 & 5.0 & \\ 5.0 & 5.0 & 6.0 \\ -2.0 & 6.0 & 7.0 + 2.0 \end{pmatrix}, \qquad B = \begin{pmatrix} 2.0 & 4.0 & -3.0 \\ 4.0 & 6.0 & 6.0 & \\ 6.0 & 7.0 & \\ -3.0 & 7.0 & 8.0 - 1.0 \end{pmatrix}.$$

The following code reads a matrix in Coordinate form, and then converts it to HSL standard format using mc69\_coord\_convert. In addition to the initial conversion, a second set of values matching the same pattern is read. These values are then converted to HSL standard form using mc69\_set\_values.

```
program hsl_mc69ds8
  use hsl_mc69_double
  implicit none

integer, parameter :: wp = kind(0d0)

integer :: i, j, matrix_type, m, n, ne, flag, lmap
  integer, dimension(:), allocatable :: row, col, ptr_out, row_out, map
  real(wp), dimension(:), allocatable :: val, val_out

! Read matrix in coordinate form
  read(*, "(4i8)") matrix_type, m, n, ne
  allocate(row(ne)); read(*, "(6i8)") row(:)
```

```
allocate(col(ne)); read(*, "(6i8)") col(:)
   allocate(val(ne)); read(*, "(4es12.4)") val(:)
   write(*, "(a)") "Input:"
   do i = 1, ne
      write(*, "(a,2i4,es12.2)") "row, col, val = ", row(i), col(i), val(i)
   ! Convert to HSL standard form out of place
   allocate(ptr_out(n+1))
   call mc69_coord_convert(matrix_type, m, n, ne, row, col, ptr_out, row_out, &
      flag, val_in=val, val_out=val_out, lmap=lmap, map=map)
   if(flag.lt.0) then
      write(*, "(a,i3)") &
         "Error return from mc69 coord convert with flag = ", flag
      stop
   endif
   write(*, "(/a)") "Output:"
   do i = 1, n
      write(*, "(a,i2,':')",advance="no") "Column ", i
      do j = ptr out(i), ptr out(i+1)-1
         write(*, "(2x,i4,1x,'(',es12.2,')')", advance="no") &
            row_out(j), val_out(j)
      end do
      write(*, "()")
   end do
   ! Print out matrix
   write(*, "()")
   call mc69_print(6, 0, matrix_type, m, n, ptr_out, row_out, val=val_out)
   ! Read and apply new values
   read(*, "(4es12.4)") val(:)
   call mc69_set_values(matrix_type, lmap, map, val, ptr_out(n+1)-1, val_out)
   write(*, "(/a)") "After applying new values:"
   call mc69_print(6, 0, matrix_type, m, n, ptr_out, row_out, val=val_out)
end program hsl_mc69ds8
```

If provided with the following input (matching the matrices A and B above),

```
4
             4
                     4
                             8
     1
                             2
                                     2
                                             4
             1
                     1
     4
             4
     4
1.0000E+00 -2.0000E+00 3.0000E+00 4.0000E+00
5.0000E+00 6.0000E+00 7.0000E+00 2.0000E+00
2.0000E+00 -3.0000E+00 4.0000E+00 6.0000E+00
6.0000E+00 7.0000E+00 8.0000E+00 -1.0000E+00
```

the code produces the following output.

```
Input:
row, col, val =
                   1
                       1
                            1.00E+00
row, col, val =
                   1
                       4
                           -2.00E+00
row, col, val =
                   1
                       2
                            3.00E+00
row, col, val =
                   2
                       2
                            4.00E+00
row, col, val =
                   2
                       3
                            5.00E+00
                       3
row, col, val =
                   4
                            6.00E+00
row, col, val =
                   4
                      4
                            7.00E+00
row, col, val =
                   4
                       4
                            2.00E+00
Output:
Column 1:
               1 (
                      1.00E+00)
                                    2 (
                                            3.00E+00)
                                                          4 ( -2.00E+00)
Column 2:
               2 (
                      4.00E+00)
                                    3 (
                                            5.00E+00)
Column 3:
                      6.00E+00)
               4 (
Column 4:
               4 (
                      9.00E+00)
Real symmetric indefinite matrix, dimension 4x4 with 7 entries.
     1.0000E+00
                  3.0000E+00
                                            -2.0000E+00
     3.0000E+00
2:
                  4.0000E+00
                               5.0000E+00
3:
                  5.0000E+00
                                             6.0000E+00
4: -2.0000E+00
                               6.0000E+00
                                            9.0000E+00
After applying new values:
Real symmetric indefinite matrix, dimension 4x4 with 7 entries.
     2.0000E+00
                  4.0000E+00
1:
                                            -3.0000E+00
                               6.0000E+00
2:
     4.0000E+00
                  6.0000E+00
3:
                  6.0000E+00
                                             7.0000E+00
4: -3.0000E+00
                               7.0000E+00
                                            7.0000E+00
```

#### 3 GENERAL INFORMATION

**Workspace:** HSL\_MC69 handles its own memory allocations.

Other routines called directly: None.

**Input/output:** Error, warning and requested printing only, under control of argument 1p in each subroutine call.

**Restrictions:** m, n, ne  $\geq 0$ ; ptr monotonic, ptr(1)=1; matrix\_type  $\in [-6,4] \cup \{6\}$ .

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

## 4 METHOD

## 4.1 The format of the map output array

The data stored in map is designed to be easy to apply. It consists of two parts:

• The first ptr\_out (n+1) -1 entries specify source locations for each entry of val\_out. If map(k) is positive, val\_out(k) = val\_in(map(k)), k = 1,...n. Otherwise, if map(k) is negative, the assignment depends on the type of the matrix:

```
Skew symmetric val_out(k) = -val_in(-map(k));
Hermitian val_out(k) = conjg(val_in(-map(k)));
Otherwise val_out(k) = val_in(-map(k)).
```

• The second part, map (ptr (n+1):lmap), may be empty. Otherwise entries occur in pairs. Each pair (i,j) = (map(k), map(k+1)), k = ptr(n+1), ptr(n+1)+2, ... lmap - 1, represents a duplicate that was found. If j is positive then val\_out(i) = val\_out(i) + val\_in(j). If j is negative and the matrix is Hermitian or skew symmetric, the conjugate or negative value of the val\_in(-j) is used.

Thus, for the simple case where no entries of map(:) are negative, the following code could be used to perform the work of mc69\_set\_values:

```
do k = 1, ptr(n+1)-1
    val_out(k) = val_in(map(k))
end do
do k = ptr(n+1), lmap, 2
    val_out(map(k)) = val_out(map(k)) + val_in(map(k+1))
end do
```

## 4.2 The routine mc69\_cscl\_clean

Because the size of the array map depends on the number of duplicates, we make a preliminary pass to count them. To find duplicates quickly, we use a temporary integer array temp that is allocated to have size m and is initialized to zero. When scanning column j, if we find an entry in row i that is within range, we check temp(i); if it does not have the value j, it is the first occurrence in the column and we then set temp(i) to the value j; otherwise, we have a duplicate.

We take the opportunity in this preliminary scan to count the number of out-of-range entries. To make the sorting in the main scan (slightly) easier, we set row(k) to the artificial value m+1 for each out-of-range entry row(k).

The main pass processes the columns one by one. A heap sort is used to order the entries of each column. This leaves the duplicates next to each other and the out-of-range entries at the end, so a simple scan of the revised column moves all the wanted entries forward so that they are adjacent.

If val is present, its entries are permuted during the heap sort and its wanted entries are moved forward and duplicates accumulated during the scan of the column.

If map is present, it is allocated before the pass and initialized to represent the identity permutation of the entries by setting map(k) = k, k = 1, ptr(n+1)-1. It is revised with each data movement made within the sort and the subsequent pass that handles duplicates and out-of-range entries. For each duplicate accumulation, a pair of integers is added at the end of map.

Finally, if the matrix is symmetric or Hermitian, the diagonal entries are checked for the relevant properties.

#### 4.3 The routines mc69\_cscl\_convert and mc69\_csru\_convert

Both these routines already have the data in an appropriate format, and merely require the removal of out-of-range and duplicate entries. In the upper CSR case, we exploit the fact that we are only concerned with symmetric, skew-symmetric and Hermitian matrices. In these cases, the pattern of the upper triangle held by rows is identical to the pattern of the lower triangle held by columns, and a simple transform can be applied to obtain the values.

A single pass is made. For each column, first duplicates and out-of-range entries are dropped. Next, entries are sorted into ascending order using a heap sort. Finally, duplicates are identified and removed.

#### 4.4 The routines mc69\_cscu\_convert and mc69\_csrl\_convert

In both these routines we have the transpose of the desired pattern. We proceed in three passes:

- 1. The first pass (of row\_in) counts the number of entries in each column of the output matrix. Out-of-range entries are ignored, but duplicates are counted (we cannot detect them at this stage).
- 2. The second pass (of row\_in) drops entries into destination locations so that ptr\_out and row\_out hold the final output matrix but with duplicates included. By construction, the entries are ordered within each column.
- 3. The third and final pass (of row\_out) identifies and sums duplicates to produce the desired matrix.

## 4.5 The routines mc69\_csclu\_convert and mc69\_csrlu\_convert

Both these routines proceed as mc69\_cscu\_convert, exploiting the availability of the upper triangle to avoid the heap sort required if the lower triangle is used. Entries in the lower triangle are thus ignored (but not counted as out of range). If the number of entries in the lower and upper triangles do not match (after discarding out-of-range entries) an error is issued.

## 4.6 The routine mc69\_coord\_convert

In this routine, we start with the matrix in coordinate format. We proceed in four passes:

- 1. The first pass (of row\_in) counts the number of entries in each column of the output matrix. Out-of-range entries are ignored, but duplicates are counted (we cannot detect them at this stage).
- 2. The second pass (of row\_in) drops entries into destination locations so that ptr\_out and row\_out hold the final output matrix but with duplicates included. At this stage, the entries in each column are unordered.
- 3. The third pass (of row\_out) uses a heap sort to order the entries in each column by increasing row index.
- 4. The final pass (of row\_out) identifies and sums duplicates to produce the desired matrix.