


GALAHAD SLS

USER DOCUMENTATION GALAHAD Optimization Library version 5.0

1 SUMMARY

This package **solves dense or sparse symmetric systems of linear equations** using variants of Gaussian elimination. Given a sparse symmetric matrix $\mathbf{A} = \{a_{ij}\}_{n\times n}$, and an n-vector $\mathbf{b}$ or a matrix $\mathbf{B} = \{b_{ij}\}_{n\times r}$, this subroutine solves the system $\mathbf{Ax} = \mathbf{b}$ or the system $\mathbf{AX} = \mathbf{B}$. The matrix $\mathbf{A}$ need not be definite.

The method provides a common interface to a variety of well-known solvers from HSL and elsewhere. Currently supported solvers include `MA27/SILS`, `HSL_MA57`, `HSL_MA77` , `HSL_MA86`, `HSL_MA87` and `HSL_MA97` from HSL, `SSIDS` from SPRAL, `MUMPS` from Mumps Technologies, `PARDISO` both from the Pardiso Project and Intel's MKL, `PaStiX` from Inria, and `WSMP` from the IBM alpha Works, as well as `POTR`, `SYTR` and `SBTR` from LAPACK. Note that, with the exception of `SSIDS` and the Netlib reference LAPACK codes, **the solvers themselves do not form part of this package and must be obtained separately.** Dummy instances are provided for solvers that are unavailable. Also note that additional flexibility may be obtained by calling the solvers directly rather that via this package.

ATTRIBUTES — Versions: `GALAHAD_SLS_single`, `GALAHAD_SLS_double`. **Calls:** `GALAHAD_CLOCK`, `GALAHAD_SYMBOLS`, `GALAHAD_SORT`, `GALAHAD_SPACE`, `GALAHAD_SPECFILE`, `GALAHAD_STRING`, `GALAHAD_SMT`, `GALAHAD_SILS` and optionally `HSL_MA57`, `HSL_MA77`, `HSL_MA86`, `HSL_MA87`, `HSL_MA97`, `HSL_MC64`, `HSL_MC68`, `MC61`, `MC77`, and `METIS`. **Date:** August 2009. **Origin:** N. I. M. Gould, Rutherford Appleton Laboratory. **Language:** Fortran 95 + TR 15581 or Fortran 2003. **Parallelism:** Some solvers may use OpenMP and its runtime library.

2 HOW TO USE THE PACKAGE

2.1 Calling sequences

The package is available using both single and double precision reals, and either 32-bit or 64-bit integers. Access to the 32-bit integer, single precision version requires the `USE` statement

```
USE GALAHAD_SLS_single
```

with the obvious substitution `GALAHAD_SLS_double`, `GALAHAD_SLS_single_64` and `GALAHAD_SLS_double_64` for the other variants.

If it is required to use more than one of the modules at the same time, the derived types `SMT_type`, `SLS_control_type`, `SLS_time_type`, `SLS_data_type`, and `SLS_inform_type` (§2.6), and the subroutines `SLS_initialize`, `SLS_analyse`, `SLS_factorize`, `SLS_solve`, `SLS_terminate` (§2.7), `SLS_enquire`, `SLS_alter_d`, and `SLS_part_solve` (§2.9) must be renamed on one of the `USE` statements.

There are five principal subroutines for user calls (see §2.9 for further features):

The subroutine `SLS_initialize` must be called to specify the external solver to be used. It may also be called to set default values for solver-specific components of the control structure. If non-default values are wanted for any of the control components, the corresponding components should be altered after the call to `SLS_initialize`.

`SLS_analyse` accepts the pattern of $\mathbf{A}$ and optionally chooses pivots for Gaussian elimination using a selection criterion to preserve sparsity. It subsequently constructs subsidiary information for actual factorization by `SLS_factorize`. If the user provides the pivot sequence, only the necessary information for `SLS_factorize` will be generated.

`SLS_factorize` factorizes the matrix $\mathbf{A}$ using the information from a previous call to `SLS_analyse`. The actual pivot sequence used may differ from that of `SLS_analyse` if $\mathbf{A}$ is not definite.

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SLS_solve uses the factors generated by SLS_factorize to solve a system of equations with one ($\mathbf{Ax} = \mathbf{b}$) or several ($\mathbf{AX} = \mathbf{B}$) right-hand sides. Iterative refinement may be used to improve a given solution or set of solutions.

SLS_terminate deallocates the arrays held inside the structure for the factors. It should be called when all the systems involving its matrix have been solved or before another external solver is to be used.

2.2 Supported external solvers

In Table 2.1 we summarize key features of the external solvers supported by SLS. Further details are provided in the references cited in §4.

solver	factorization	indefinite **A**	out-of-core	parallelised
SILS/MA27	multifrontal	yes	no	no
HSL_MA57	multifrontal	yes	no	no
HSL_MA77	multifrontal	yes	yes	OpenMP core
HSL_MA86	left-looking	yes	no	OpenMP fully
HSL_MA87	left-looking	no	no	OpenMP fully
HSL_MA97	multifrontal	yes	no	OpenMP core
SSIDS	multifrontal	yes	no	CUDA core
MUMPS	multifrontal	yes	optionally	MPI
PARDISO	left-right-looking	yes	no	OpenMP fully
MKL_PARDISO	left-right-looking	yes	optionally	OpenMP fully
PaStiX	left-right-looking	yes	no	OpenMP fully
WSMP	left-right-looking	yes	no	OpenMP fully
POTR	dense	no	no	with parallel LAPACK
SYTR	dense	yes	no	with parallel LAPACK
PBTR	dense band	no	no	with parallel LAPACK

Table 2.1: External solver characteristics.

2.3 Matrix storage formats

The matrix **A** may be stored in a variety of input formats.

2.3.1 Sparse co-ordinate storage format

Only the nonzero entries of the lower-triangular part of **A** are stored. For the l-th entry of the lower-triangular portion of **A**, its row index i, column index j and value a_{ij} are stored in the l-th components of the integer arrays row, col and real array val, respectively. The order is unimportant, but the total number of entries ne is also required.

2.3.2 Sparse row-wise storage format

Again only the nonzero entries of the lower-triangular part are stored, but this time they are ordered so that those in row i appear directly before those in row $i+1$. For the i-th row of **A**, the i-th component of an integer array ptr holds the position of the first entry in this row, while ptr $(m+1)$ holds the total number of entries plus one. The column indices j and values a_{ij} of the entries in the i-th row are stored in components $l =$ ptr(i), ...,ptr $(i+1)-1$ of the integer array col, and real array val, respectively.

For sparse matrices, this scheme almost always requires less storage than its predecessor.

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2.3.3 Dense storage format

The matrix $\mathbf{A}$ is stored as a compact dense matrix by rows, that is, the values of the entries of each row in turn are stored in order within an appropriate real one-dimensional array. Since $\mathbf{A}$ is symmetric, only the lower triangular part (that is the part a_{ij} for $1 \leq j \leq i \leq n$) need be held, and this part will be stored by rows, that is component $i*(i-1)/2+j$ of the storage array `val` will hold the value a_{ij} (and, by symmetry, a_{ji}) for $1 \leq j \leq i \leq n$.

2.4 Real and integer kinds

We use the terms integer and real to refer to the fortran keywords `REAL(rp_)` and `INTEGER(ip_)`, where `rp_` and `ip_` are the relevant kind values for the real and integer types employed by the particular module in use. The former are equivalent to default `REAL` for the single precision versions and `DOUBLE PRECISION` for the double precision cases, and correspond to `rp_ = real32` and `rp_ = real64`, respectively, as supplied by the fortran `iso_fortran_env` module. The latter are default (32-bit) and long (64-bit) integers, and correspond to `ip_ = int32` and `ip_ = int64`, respectively, again from the `iso_fortran_env` module.

2.5 Parallel usage

OpenMP may be used by the `GALAHAD_SLS` package to provide parallelism for some solvers in shared memory environments. See the documentation for the GALAHAD package `SLS` for more details. To run in parallel, OpenMP must be enabled at compilation time by using the correct compiler flag (usually some variant of `-openmp`). The number of threads may be controlled at runtime by setting the environment variable `OMP_NUM_THREADS`.

MPI may also be used by the package to provide parallelism for some solvers in a distributed memory environment. To use this form of parallelism, MPI must be enabled at runtime by using the correct compiler flag (usually some variant of `-lmpi`). Although the MPI process will be started automatically when required, it should be stopped by the calling program once no further use of this form of parallelism is needed. Typically, this will be via statements of the form

```
CALL MPI_INITIALIZED( flag, ierr )
IF ( flag ) CALL MPI_FINALIZE( ierr )
```

The code may be compiled and run in serial mode.

2.6 The derived data types

Five derived data types are used by the package.

2.6.1 The derived data type for holding the matrix

The derived data type `SMT_type` is used to hold the matrix $\mathbf{A}$. The components of `SMT_type` used are:

`n` is a scalar variable of type `INTEGER(ip_)`, that holds the order n of the matrix $\mathbf{A}$. **Restriction:** `n` $\geq$ `1`.

`type` is an allocatable array of rank one and type default `CHARACTER`, that indicates the storage scheme used. If the sparse co-ordinate scheme (see §2.3.1) is used the first ten components of `type` must contain the string `COORDINATE`. For the sparse row-wise storage scheme (see §2.3.2), the first fourteen components of `type` must contain the string `SPARSE_BY_ROWS`, and for dense storage scheme (see §2.3.3) the first five components of `type` must contain the string `DENSE`.

For convenience, the procedure `SMT_put` may be used to allocate sufficient space and insert the required keyword into `type`. For example, if $\mathbf{A}$ is to be stored in the structure `A` of derived type `SMT_type` and we wish to use the co-ordinate scheme, we may simply

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```
CALL SMT_put( A%type, 'COORDINATE', istat )
```

See the documentation for the GALAHAD package SMT for further details on the use of SMT_put.

ne is a scalar variable of type INTEGER(ip_), that holds the number of entries in the **lower triangular** part of **A** in the sparse co-ordinate storage scheme (see §2.3.1). It need not be set for any of the other three schemes.

val is a rank-one allocatable array of type REAL(rp_), that holds the values of the entries of the **lower triangular** part of the matrix **A** for each of the storage schemes discussed in §2.3. Any duplicated entries that appear in the sparse co-ordinate or row-wise schemes will be summed.

row is a rank-one allocatable array of type INTEGER(ip_), that holds the row indices of the **lower triangular** part of **A** in the sparse co-ordinate storage scheme (see §2.3.1). It need not be allocated for any of the other schemes. Any entry whose row index lies out of the range [1,n] will be ignored.

col is a rank-one allocatable array variable of type INTEGER(ip_), that holds the column indices of the **lower triangular** part of **A** in either the sparse co-ordinate (see §2.3.1), or the sparse row-wise (see §2.3.2) storage scheme. It need not be allocated when the dense storage scheme is used. Any entry whose column index lies out of the range [1,n] will be ignored, while the row and column indices of any entry from the **strict upper triangle** will implicitly be swapped.

ptr is a rank-one allocatable array of size n+1 and type INTEGER(ip_), that holds the starting position of each row of the **lower triangular** part of **A**, as well as the total number of entries plus one, in the sparse row-wise storage scheme (see §2.3.2). It need not be allocated for the other schemes.

Although any of the above-mentioned matrix storage formats may be used with each supported solver, MA27/SILS and HSL_MA57 from HSL are most efficient if co-ordinate input is provided.

2.6.2 The derived data type for holding control parameters

The derived data type SLS_control_type is used to hold controlling data. Default values specifically for the desired solver may be obtained by calling SLS_initialize (see §2.7.1), while components may be changed at run time by calling SLS_read_specfile (see §2.10.1). The components of SLS_control_type are:

error is a scalar variable of type INTEGER(ip_), that holds the unit number for error messages. Printing of error messages is suppressed if error < 0. The default is error = 6.

warning is a scalar variable of type INTEGER(ip_), that holds the unit number for warning messages. Printing of warning messages is suppressed if warning < 0. The default is warning = 6.

out is a scalar variable of type INTEGER(ip_), that holds the unit number for informational messages. Printing of informational messages is suppressed if out < 0. The default is out = 6.

statistics is a scalar variable of type INTEGER(ip_), that holds the unit number for statistical output, if any. Printing of statistical messages is suppressed if statistics < 0. The default is statistics = 0.

print_level is a scalar variable of type INTEGER(ip_), that is used to control the amount of informational output that is required. No informational output will occur if print_level ≤ 0. If print_level ≥ 1 a single line of output will be produced for each step of iterative refinement performed. The default is print_level = 0.

print_level_solver is a scalar variable of type INTEGER(ip_), that is used to control the amount of informational output that is required by the exteral solver. No informational output will occur if print_level ≤ 0. If print_level ≥ 1 the amount of output produced is solver dependent. The default is print_level_solver = 0.

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bits is a scalar variable of type INTEGER(ip_), that indicates the machine architecture being used. It should be set to 32 on a 32-bit architecture and to 64 on a 64-bit architecture. The default value is 32, and this default is used if bits $\neq$ 64.

block_size_kernel is a scalar variable of type INTEGER(ip_), that gives the target block size for the kernel factorization, if any. The default value is 40, and this default is used if block_size_kernel < 1.

block_size_elimination is a scalar variable of type INTEGER(ip_), that gives the target block size for parallel factorization, if any. The default is block_size_elimination = 32, and this default is used if block_size_elimination < 1.

blas_block_size_factorize is a scalar variable of type INTEGER(ip_), that gives the block size for level-three basic linear algebra subprograms (BLAS) in the factorization phase. The default is blas_block_size_factorize = 16, and this default is used if blas_block_size_factorize < 1.

blas_block_size_solve is a scalar variable of type INTEGER(ip_), that gives the block size for level-two and -three basic linear algebra subprograms (BLAS) in the solution phase. The default is blas_block_size_solve = 16, and this default is used if blas_block_size_solve < 1.

node_amalgamation is a scalar variable of type INTEGER(ip_), that controls node amalgamation. Two neighbours in the elimination tree are merged if they both involve fewer than node_amalgamation eliminations. The default is node_amalgamation=32, and this default is used if node_amalgamation < 1.

initial_pool_size is a scalar variable of type INTEGER(ip_), that holds the initial size of the arrays that store the task pool for parallel factorization, if any. The default is initial_pool_size = 100000, and this default is used if initial_pool_size < 1.

min_real_factor_size is a scalar variable of type INTEGER(ip_), that specifies the amount of real storage that will initially be allocated for the factors and other data. The default is min_real_factor_size = 10000, and this default is used if min_real_factor_size < 1.

min_integer_factor_size is a scalar variable of type INTEGER(ip_), that specifies the amount of integer storage that will initially be allocated for the factors and other data. The default is min_integer_factor_size = 10000, and this default is used if min_integer_factor_size < 1.

max_real_factor_size is a scalar variable of type INTEGER(int64), that specifies the maximum amount of real storage that will be allocated for the factors and other data. The default is max_real_factor_size = HUGE(0).

max_integer_factor_size is a scalar variable of type INTEGER(int64), that specifies the maximum amount of integer storage that will be allocated for the factors and other data. The default is max_integer_factor_size = HUGE(0).

max_in_core_store is a scalar variable of type INTEGER(int64), that specifies the maximum amount of storage (measured in Fortran storage units) to be used if the user wants to use in-core arrays when possible in place of out-of-core direct-access files for solvers that support out-of-core factorization. If max_in_core_store = 0, factorization will occur entirely out-of-core. The default is max_in_core_store = HUGE(0)/4 (HUGE(0)/8 in GALAHAD_SLS_double) for 32-bit architectures and max_in_core_store = HUGE(0_long)/4 (HUGE(0_long)/8 in GALAHAD_SLS_double) in the 64-bit case.

array_increase_factor is a scalar variable of type REAL(rp_), that holds the factor by which arrays sizes are to be increased if they are too small. The default is array_increase_factor = 2.0.

array_decrease_factor is a scalar variable of type REAL(rp_), that holds a factor that is used to assess whether previously allocated internal workspace arrays are excessive. In particular, if current requirements are less than array_decrease_factor times the currently allocated space, the space will be re-allocated to current requirements. The default is array_decrease_factor = 2.0.

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pivot_control is a scalar variable of type INTEGER(ip_), that is used to control numerical pivoting by SLS_factorize. Possible values are:

- 1 Numerical pivoting will be performed, with relative pivot tolerance given by the component relative_pivot_tolerance.
- 2 No pivoting will be performed and an error exit will occur immediately a sign change is detected among the pivots. This is suitable for cases when **A** is thought to be definite and is likely to decrease the factorization time while still providing a stable decomposition.
- 3 No pivoting will be performed and an error exit will occur if a zero pivot is detected. This is likely to decrease the factorization time, but may be unstable if there is a sign change among the pivots or a tiny pivot is encountered.
- 4 No pivoting will be performed but the matrix will be altered to ensure that the result is "sufficiently" positive definite if a non-positive pivot is encountered.

The default is pivot_control = 1, and any value outside of [1,4] will be reset to the default.

ordering is a scalar variable of type INTEGER(ip_), that controls the initial order of the rows when performing the factorization. This will be ignored if an explicit permutation is specified (see the argument PERM for SLS_analyse). Possible values are:

- < 0 The ordering will be chosen by the specified solver with its own ordering-selection value - ordering.
- 0 The ordering will be chosen to be the default for the solver used. If the specified solver has no default, the rows will be unordered which is unlikely to be satisfactory.
- 1 The ordering will be chosen by the Approximate Minimum Degree method with provisions for "dense" rows/columns.
- 2 The ordering will be chosen by the Minimum Degree method.
- 3 The ordering will be chosen by the Nested Dissection method; this requires the user to have installed the external package METIS.
- 4 An indefinite ordering involving a combination of 1x1 and 2x2 pivots will be used.
- 5 An ordering that aims to provide a small profile or wavefront will be used.
- 6 An ordering that aims to provide a small bandwidth will be used.
- 7 The ordering will be chosen by an earlier implementation of the Approximate Minimum Degree method with no provisions for "dense" rows/columns.
- > 7 The ordering will be chosen automatically depending on matrix characteristics (not yet implemented).

Values 1 to 4 are only supported if the HSL package HSL_MC68 is available, while 5 and 6 are only possible when the HSL package MC61 is provided. The default is ordering = 0, and currently any value > 6 will be reset to this default.

full_row_threshold is a scalar variable of type INTEGER(ip_), that controls the threshold for detecting rows with a large percentage (relative to the matrix order) of nonzeros by SLS_analyse. Such rows will normally be ordered last when the factorization occurs. If full_row_threshold = 100, only fully dense rows will be detected. The default is full_row_threshold = 100, and any value outside of [0,100] will be reset to the default.

row_search_indefinite is a scalar variable of type INTEGER(ip_), that controls the maximum number of rows searched for a pivot when using the indefinite ordering (see ordering = 4 above). The default is row_search_indefinite = 10, and this default is used if row_search_indefinite < 1.

scaling is a scalar variable of type INTEGER(ip_), that may control scaling of the matrix. Possible values are:

- < 0 The scaling will be chosen by the specified solver with its own scaling-selection value - scaling.

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0 No scaling is used.

1 Scale the matrix so that the diagonal and off diagonal entries of the result are one and smaller than one, respectively, in absolute value using the package HSL_MC64.

2 Scale the matrix so that ℓ_1-norms of each column of the result are approximately one using the package MC77.

3 Scale the matrix so that ℓ_∞-norms of each column of the result are approximately one using the package MC77.

4 Use the default for the specified solver, or 0 (no scaling) if there is no default.

This option is not currently available for all solvers; -1 is only available for HSL_MA57, -2 for HSL_MA77 and -3 to -1 for HSL_MA97. The default is scaling = 0, and any value larger than 4 will be reset to the default.

scale_maxit is a scalar variable of type INTEGER(ip_), that controls the maximum number of iterations performed by MC77 when scaling is requested (see scale above). The default is scale_maxit = 10, and this default is used if scale_maxit < 1.

scale_thresh is a scalar variable of type REAL(rp_), that is used by MC77 to terminate the scaling iteration. The iteration stops as soon as the the difference between every column norm and one is smaller that scale_thresh in magnitude. The default is scale_thresh = 0.1.

relative_pivot_tolerance is a scalar variable of type REAL(rp_), that holds the relative pivot tolerance that is used to control the stability of the factorization of indefinite **A**. The default is relative_pivot_tolerance = 0.01. For problems requiring greater than average numerical care a higher value than the default would be advisable. Values greater than 0.5 are treated as 0.5 for all solvers except HSL_MA77 (where an upper bound 1.0 is enforced) and less than 0.0 as 0.0.

minimum_pivot_tolerance is a scalar variable of type REAL(rp_), that holds the minimum permitted value of the relative pivot tolerance. If, at any stage of the computation, fewer than the expected number of stable pivots have been found using the current tolerance but the largest candidate pivot would be acceptable with tolerance minimum_pivot_tolerance, the pivot is accepted, and all subsequent pivots will be assessed relative to minimum_pivot_tolerance rather than relative_pivot_tolerance. The default is minimum_pivot_tolerance=0.01. Values of minimum_pivot_tolerance greater than relative_pivot_tolerance are treated as relative_pivot_tolerance, while values less than 0 are treated as 0.

absolute_pivot_tolerance is a scalar variable of type REAL(rp_), that holds the absolute pivot tolerance that is used to control the stability of the factorization of indefinite **A**. No pivot smaller than absolute_pivot_tolerance in absolute value will be accepted. The default is absolute_pivot_tolerance = EPSILON(1.0) (EPSILON(1.0D0) in GALAHAD_SLS_double).

zero_tolerance is a scalar variable of type REAL(rp_), that controls which small entries are to be ignored during the factorization of **A**. Any entry smaller in absolute value than zero_tolerance will be treated as zero; as a consequence when zero_tolerance > 0, the factors produced will be of a perturbation of order zero_tolerance of **A**. The default is zero_tolerance = 0.0.

static_pivot_tolerance and static_level_switch are scalar variables of type REAL(rp_), that are used to set the static pivot level when the solvers HSL_MA57 or HSL_MA77 are used. If static_pivot_tolerance>0.0 and if, at any stage of the computation, relatively fewer than static_level_switch pivots can be found with relative pivot tolerance greater than minimum_pivot_tolerance, diagonal entries are accepted as pivots. If a candidate diagonal entry has absolute value at least static_pivot_tolerance, it is selected as a pivot; otherwise, the pivot is given the value that has the same sign but absolute value static_pivot_tolerance. The defaults are static_pivot_tolerance = 0.0 and static_level_switch = 0.0. If static_pivot_tolerance is larger than zero, but smaller than zero_tolerance, the value zero_tolerance will be used.

consistency_tolerance is a scalar variable of type REAL(rp_), that holds the tolerance used to access whether a singular system is consistent or not. The default is xonsistency_tolerance = EPSILON(1.0) (EPSILON(1.0D0) in GALAHAD_SLS_double).

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max_iterative_refinements is a scalar variable of type default INTEGER(ip_), that holds the maximum number of iterative refinements that may be attempted. The default is max_iterative_refinements = 0.

acceptable_residual_relative and acceptable_residual_absolute are scalar variables of type REAL(rp_), that specify an acceptable level for the residual $\mathbf{A}\mathbf{x}-\mathbf{b}$ or residuals $\mathbf{A}\mathbf{x}_i-\mathbf{b}_i$, $i=1,\ldots,r$, when there are more than one. In particular, iterative refinement will cease as soon as $\|\mathbf{A}\mathbf{x}-\mathbf{b}\|_\infty$ falls below max($\|\mathbf{b}\|_\infty$* acceptable_residual_relative, acceptable_residual_absolute); for the multiple residual case, we require that $\|\mathbf{A}\mathbf{x}_i-\mathbf{b}_i\|_\infty$ falls below max($\|\mathbf{b}_i\|_\infty$* acceptable_residual_relative, for each $i=1,\ldots,r$. The defaults are acceptable_residual_relative = acceptable_residual_absolute = $10u$, where u is EPSILON(1.0) (EPSILON(1.0D0) in GALAHAD_SLS_double).

out_of_core_directory is a scalar variable of type default CHARACTER and length 400, that identifies the full path name of the directory in which direct-access files will be written if out-of-core factorization is performed; the full path must end with a /. Exceptionally, the "empty" string "" refers to the current directory. The default is out_of_core_directory = "".

out_of_core_integer_factor_file is a scalar variable of type default CHARACTER and length 400, that identifies the base files name for direct-access files that hold integer components of the matrix factors when an out-of-core factorization is obtained. Files with names out_of_core_integer_factor_file appended with 1, 2, ... will be created as needed. There should be no other files with this base file name in the directory specified for the task. The default is out_of_core_integer_factor_file = "factor_integer_ooc".

out_of_core_real_factor_file is a scalar variable of type default CHARACTER and length 400, that identifies the base files name for direct-access files that hold real components of the matrix factors when an out-of-core factorization is obtained. Files with names out_of_core_real_factor_file appended with 1, 2, ... will be created as needed. There should be no other files with this base file name in the directory specified for the task. The default is out_of_core_real_factor_file = "factor_real_ooc".

out_of_core_real_work_file is a scalar variable of type default CHARACTER and length 400, that identifies the base files name for direct-access files that hold real workspace components when an out-of-core factorization is obtained. Files with names out_of_core_real_work_file appended with 1, 2, ... will be created as needed. There should be no other files with this base file name in the directory specified for the task. The default is out_of_core_real_work_file = "work_real_ooc".

out_of_core_indefinite_file is a scalar variable of type default CHARACTER and length 400, that identifies the base files name for direct-access files that hold additional real workspace components in the indefinite case when an out-of-core factorization is obtained. Files with names out_of_core_indefinite_file appended with 1, 2, ... will be created as needed. There should be no other files with this base file name in the directory specified for the task. The default is out_of_core_indefinite_file = "work_indefinite_ooc".

prefix is a scalar variable of type default CHARACTER and length 30, that may be used to provide a user-selected character string to preface every line of printed output. Specifically, each line of output will be prefaced by the string prefix(2:LEN(TRIM(prefix))-1), thus ignoring the first and last non-null components of the supplied string. If the user does not want to preface lines by such a string, the default prefix = "" should be used.

2.6.3 The derived data type for holding timing information

The derived data type SLS_time_type is used to hold elapsed CPU and system clock times for the various parts of the calculation. The components of SLS_time_type are:

total is a scalar variable of type REAL(rp_), that gives the total CPU time (in seconds) spent in the package.

analyse is a scalar variable of type REAL(rp_), that gives the CPU time spent in the analysis phase.

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factorize is a scalar variable of type REAL(rp_), that gives the CPU time spent in the factorization phase.

solve is a scalar variable of type REAL(rp_), that gives the CPU time spent in the solve phases.

order_external is a scalar variable of type REAL(rp_), that gives the CPU time spent by the external solvers in the ordering phase.

analyse_external is a scalar variable of type REAL(rp_), that gives the CPU time spent by the external solvers in the analysis phase.

factorize_external is a scalar variable of type REAL(rp_), that gives the CPU time spent by the external solvers in the factorization phase.

solve_external is a scalar variable of type REAL(rp_), that gives the CPU time spent by the external solvers in the solve phases.

clock_total is a scalar variable of type REAL(rp_), that gives the total elapsed system clock time (in seconds) spent in the package.

clock_analyse is a scalar variable of type REAL(rp_), that gives the elapsed system clock time spent in the analysis phase.

clock_factorize is a scalar variable of type REAL(rp_), that gives the elapsed system clock time spent in the factorization phase.

clock_solve is a scalar variable of type REAL(rp_), that gives the elapsed system clock time spent in the solve phases.

clock_order_external is a scalar variable of type REAL(rp_), that gives the elapsed system clock time spent by the external solvers in the ordering phase.

clock_analyse_external is a scalar variable of type REAL(rp_), that gives the elapsed system clock time spent by the external solvers in the analysis phase.

clock_factorize_external is a scalar variable of type REAL(rp_), that gives the elapsed system clock time spent by the external solvers in the factorization phase.

clock_solve_external is a scalar variable of type REAL(rp_), that gives the elapsed system clock time spent by the external solvers in the solve phases.

2.6.4 The derived data type for holding informational parameters

The derived data type SLS_inform_type is used to hold parameters that give information about the progress and needs of the algorithm. The components of SLS_inform_type are as follows—any component that is not relevant to the solver being used will have the value -1 or -1.0 as appropriate:

status is a scalar variable of type INTEGER(ip_), that gives the exit status of the algorithm. See §2.8 for details.

alloc_status is a scalar variable of type INTEGER(ip_), that gives the status of the last attempted array allocation or deallocation.

bad_alloc is a scalar variable of type default CHARACTER and length 80, that gives the name of the last internal array for which there were allocation or deallocation errors. This will be the null string if there have been no allocation or deallocation errors.

entries is a scalar variable of type INTEGER(ip_), that is set to the total number of entries of **A** supplied.

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out_of_range is a scalar variable of type INTEGER(ip_), that is set to the number of entries of **A** supplied with one or both indices out of range.

duplicates is a scalar variable of type INTEGER(ip_), that is set to the number of duplicate off-diagonal entries of **A** supplied.

upper is a scalar variable of type INTEGER(ip_), that is set to the number of input entries from the strict upper triangle of **A**.

missing_diagonals is a scalar variable of type INTEGER(ip_), that gives the number of diagonal entries entries missing for an allegedly-definite matrix **A**.

max_depth_assembly_tree is a scalar variable of type INTEGER(ip_), that gives the maximum depth of the assembly tree.

nodes_assembly_tree is a scalar variable of type INTEGER(ip_), that holds the number of nodes in the assembly tree.

real_size_desirable is a scalar variable of type INTEGER(int64), that give the total number of real words required for a successful factorization without the need for data compression, provided no numerical pivoting is performed.

integer_size_desirable is a scalar variable of type INTEGER(int64), that give the total number of integer words required for a successful factorization without the need for data compression, provided no numerical pivoting is performed.

real_size_necessary is a scalar variable of type INTEGER(int64), that give the total number of real words required for a successful factorization allowing for data compression, provided no numerical pivoting is performed.

integer_size_necessary is a scalar variable of type INTEGER(int64), that give the total number of real words required for a successful factorization allowing for data compression, provided no numerical pivoting is performed.

real_size_factors is a scalar variable of type INTEGER(int64), that gives the predicted or actual number of real words to hold factors of **A**.

integer_size_factors is a scalar variable of type INTEGER(int64), that gives the predicted or actual number of integer words to hold factors of **A**.

entries_in_factors is a scalar variable of type INTEGER(int64), that gives the number of entries in the factors of **A**.

max_task_pool_size is a scalar variable of type INTEGER(ip_), that gives the maximum number of tasks in the parallel factorization task pool.

max_front_size is a scalar variable of type INTEGER(ip_), that gives the forecast or actual size of the largest front encountered during the factorization.

compresses_real is a scalar variable of type INTEGER(ip_), that gives the number of compresses of real data required.

compresses_integer is a scalar variable of type INTEGER(ip_), that gives the number of compresses of integer data required.

two_by_two_pivots is a scalar variable of type INTEGER(ip_), that gives the number of two-by-two pivots used in the factorization.

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semi_bandwidths is a scalar variable of type INTEGER(ip_), that gives the semi-bandwidth of the input matrix following profile or bandwidth reduction.

delayed_pivots is a scalar variable of type INTEGER(ip_), that gives the total number of delayed pivots in the factorization.

pivot_sign_changes is a scalar variable of type INTEGER(ip_), that gives the number of pivot sign changes encountered if the no pivoting option (control%pivot_control = 3) is used successfully.

static_pivots is a scalar variable of type INTEGER(ip_), that gives the number of modified pivots during static pivoting are chosen.

first_modified_pivot is a scalar variable of type INTEGER(ip_), that gives the step at which the first pivot is modified when performing static pivoting (i.e., if control%static_pivot_tolerance>0.0) or when modifying the matrix to ensure it is sufficiently positive definite (i.e., if control%pivot_control = 4).

rank is a scalar variable of type INTEGER(ip_), that gives an estimate of the rank of $\mathbf{A}$.

negative_eigenvalues is a scalar variable of type INTEGER(ip_), that gives an estimate of the number of negative eigenvalues of $\mathbf{A}$.

iterative_refinements is a scalar variable of type INTEGER(ip_), that gives the number of iterative refinements performed.

alternative is a scalar variable of type default LOGICAL, that will be set .FALSE. on exit from SLS_fredholm_alternative (see §2.9.5) if a solution $\mathbf{x}$ to $\mathbf{A}\mathbf{x} = \mathbf{b}$ has been found, and .TRUE. if instead the alternative vector $\mathbf{x}$ for which $\mathbf{A}\mathbf{x} = \mathbf{0}$ and $\mathbf{b}^T\mathbf{x} > 0$ has been determined.

flops_assembly is a scalar variable of type INTEGER(int64), that gives the anticipated or actual number of floating-point operations performed when manipulating the matrix prior to factorization.

flops_elimination is a scalar variable of type INTEGER(int64), that gives the anticipated or actual number of floating-point operations performed during the factorization.

flops_blas is a scalar variable of type INTEGER(int64), that gives the number of additional floating-point operations that result from using the basic linear algebra subprograms (BLAS) in the factorization phase.

largest_modified_pivot is a scalar variable of type REAL(rp_), that gives the value of the largest pivot modification when performing static pivoting (i.e., if control%static_pivot_tolerance>0.0) or when modifying the matrix to ensure it is sufficiently positive definite (i.e., if control%pivot_control = 4).

minimum_scaling_factor is a scalar variable of type REAL(rp_), that gives the minimum scaling factor used.

maximum_scaling_factor is a scalar variable of type REAL(rp_), that gives the maximum scaling factor used.

backward_error_1 and backward_error_2 are scalar variables of type REAL(rp_), that gives estimates of the scaled backward errors (i.e., the residuals of the equations suitably normalised by the sizes of $\mathbf{A}$ and $\mathbf{b}$/$\mathbf{B}$) for category-1 and -2 equations, respectively; category-2 equations are exceptional ones for which the residuals are nonzero but the normalising factors are large.

condition_number_1 and condition_number_2 are scalar variables of type REAL(rp_), that gives estimates of the condition numbers of the matrix for category-1 and -2 equations, respectively.

forward_error is a scalar variable of type REAL(rp_), that gives an estimate of the forward error (i.e., the error in the solution).

solver is a scalar variable of type default CHARACTER and length 20, that gives the name of the actual solver used.

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time is a scalar variable of type SLS_time_type whose components are used to hold elapsed CPU and system clock times (in seconds) for the various parts of the calculation (see Section 2.6.3).

sils_ainfo is a scalar variable of type sils_ainfo, that corresponds to the output value sils_ainfo from SILS. See the documentation for SILS for further details.

sils_finfo is a scalar variable of type sils_finfo, that corresponds to the output value sils_finfo from SILS. See the documentation for SILS for further details.

sils_sinfo is a scalar variable of type sils_sinfo, that corresponds to the output value sils_sinfo from SILS. See the documentation for SILS for further details.

ma57_ainfo is a scalar variable of type ma57_ainfo, that corresponds to the output value ma57_ainfo from HSL_MA57. See the documentation for HSL_MA57 for further details.

ma57_finfo is a scalar variable of type ma57_finfo, that corresponds to the output value ma57_finfo from HSL_MA57. See the documentation for HSL_MA57 for further details.

ma57_sinfo is a scalar variable of type ma57_sinfo, that corresponds to the output value ma57_sinfo from HSL_MA57. See the documentation for HSL_MA57 for further details.

ma77_info is a scalar variable of type ma77_info, that corresponds to the output value ma77_info from HSL_MA77. See the documentation for HSL_MA77 for further details.

ma86_info is a scalar variable of type ma86_info, that corresponds to the output value ma86_info from HSL_MA86. See the documentation for HSL_MA86 for further details.

ma87_info is a scalar variable of type ma87_info, that corresponds to the output value ma87_info from HSL_MA87. See the documentation for HSL_MA87 for further details.

ma97_info is a scalar variable of type ma97_info, that corresponds to the output value ma97_info from HSL_MA97. See the documentation for HSL_MA97 for further details.

ssids_inform is a scalar variable of type ssids_inform, that corresponds to the output value ssids_inform from SSIDS. See the documentation for SSIDS for further details.

mc64_info is a scalar variable of type mc64_info, that corresponds to the output value mc64_info from HSL_MC64. See the documentation for HSL_MC64 for further details.

mc61_info is an array of size 10 and type INTEGER(ip_), that corresponds to the output array INFO from MC61. See the HSL documentation for MC61 for further details.

mc61_rinfo is an array of size 15 and type REAL(rp_), that corresponds to the output array RINFO from MC61. See the HSL documentation for MC61 for further details.

mc68_info is a scalar variable of type mc68_info, that corresponds to the output value mc68_info from HSL_MC68. See the documentation for HSL_MC68 for further details.

mc77_info is an array of rank one, of dimension 10 and of type INTEGER(ip_), that corresponds to the output array INFO from the primary subroutine in MC77. See the documentation for MC77 for further details.

mc77_rinfo is an array of rank one, of dimension 10 and of type REAL(rp_), that corresponds to the output array RINFO from the primary subroutine in MC77. See the documentation for MC77 for further details.

MUMPS_error is a scalar variable of type INTEGER(ip_), that corresponds to the component INFOG(1) in the solver derived type from MUMPS. See the documentation for MUMPS for further details.

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MUMPS_info is an array of size 80 and type INTEGER(ip_), whose components correspond to those in the array INFOG in the solver derived type from MUMPS. See the documentation for MUMPS for further details.

MUMPS_rinfo is an array of size 40 and type REAL(rp_), whose components correspond to those in the array RINFOG in the solver derived type from MUMPS. See the documentation for MUMPS for further details.

PARDISO_error is a scalar variable of type INTEGER(ip_), that corresponds to the output value error from PARDISO. See the documentation for PARDISO for further details.

PARDISO_iparm is an array of size 64 and type INTEGER(ip_), whose components correspond to those in the output array IPARM from PARDISO. See the documentation for PARDISO for further details.

PARDISO_dparm is an array of size 64 and type REAL(rp_), whose components correspond to those in the output array DPARM from PARDISO. See the documentation for PARDISO for further details. This is only available for the Pardiso Project version of the package.

pastix_info is a scalar variable of type INTEGER(ip_), that corresponds to the output value info returned from the PaStix. See the documentation for PaStiX for further details.

WSMP_error is a scalar variable of type INTEGER(ip_), that corresponds to the output value error from WSMP. See the documentation for WSMP for further details.

WSMP_iparm is an array of size 64 and type INTEGER(ip_), whose components correspond to those in the output array IPARM from WSMP. See the documentation for WSMP for further details.

WSMP_dparm is an array of size 64 and type REAL(rp_), whose components correspond to those in the output array DPARM from WSMP. See the documentation for WSMP for further details.

lapack_error is a scalar variable of type INTEGER(ip_), that corresponds to the output value info returned from the LAPACK routines S/DPOTRF/S, S/DSYTRF/S and S/DPBTRF/S See the documentation for LAPACK for further details.

2.6.5 The derived data type for holding problem data

The derived data type SLS_data_type is used to hold all the data for a particular problem, or sequences of problems with the same structure, between calls to SLS procedures. All components are private.

2.7 Argument lists and calling sequences

We use square brackets [ ] to indicate OPTIONAL arguments.

2.7.1 The initialization subroutine

The initialization subroutine must be called for each solver used to initialize data and solver-specific control parameters.

```
CALL SLS_initialize( solver, data, control, inform[, check] )
```

solver is scalar, of INTENT(IN), of type CHARACTER, and of variable length that specifies which solver to use. Possible values are

- sils if the GALAHAD solver SILS is desired.
- ma27 is an alias for sils that reflects the fact that the GALAHAD solver SILS is a Fortran-90 encapsulation of the Fortran-77 package MA27 from HSL.

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ma57 if the HSL solver HSL_MA57 is desired. This is a more advanced version of SILS/MA27.

ma77 if the HSL solver HSL_MA77 is desired. This is particularly appropriate when the matrix factors are too large to fit in main memory, and offers the option of parallel execution of core computations.

ma86 if the HSL solver HSL_MA86 is desired. This option offers the opportunity for general parallel solution, but may be less efficient than ma87 below when **A** is positive definite.

ma87 if the HSL solver HSL_MA87 is desired. This option should only be selected when **A** is positive definite, but offers the opportunity for general parallel solution.

ma97 if the HSL solver HSL_MA97 is desired. This option offers the functionality of HSL_MA57 but offers the option of parallel execution of core computations.

ssids if the HSL solver HSL_SSIDS is desired. This option offers the functionality of HSL_MA97 but additionally performs core computations on a GPU if available. N.B., SSIDS is only supported for compilers that are OMP 4.0 compliant, and only available in double precision.

mumps if the Mumps Technologies solver MUMPS (version 5.5.1 or above) is desired. Distributed parallel solution is offered with this choice.

pardiso if the Pardiso Project solver PARDISO (version 4.0.0 or above) is desired. Again parallel solution is offered with this choice.

mkl_pardiso if the Intel MKL solver PARDISO that forked from the Pardiso Project version in 2006, and supports parallel solution.

pastix if the Inria solver PaStiX (version 6.2.1 or above) is desired. The solver supports parallel solution.

wsmp if the IBM alpha Works solver WSMP (version 10.9 or above) is desired. Parallel solution is also offered with this choice.

potr if the LAPACK dense Cholesky factorization package (S/D)POTR(F/S) is desired.

sytr if the LAPACK dense symmetric indefinite factorization package S/DSYTRF/S is desired.

pbtr if the LAPACK banded Cholesky factorization package S/DPBTRF/S is desired.

Other solvers may be added in the future.

data is a scalar INTENT(OUT) argument of type SLS_data_type (see §2.6.5). It is used to hold data about the problem being solved.

control is a scalar INTENT(OUT) argument of type SLS_control_type (see §2.6.2). On exit, control contains solver-specific default values for the components as described in §2.6.2. These values should only be changed after calling SLS_initialize.

inform is a scalar INTENT(OUT) argument of type SLS_inform_type (see §2.6.4). A successful call is indicated when the component status has the value 0. For other return values of status, see §2.8.

check is an OPTIONAL scalar LOGICAL INTENT(IN) argument that if PRESENT and set .TRUE. will check to see if the requested solver is available, and if not will replace this by a suitable equivalent; the equivalent will be recorded in control%solver. In addition, the output default values of control%ordering and control%scaling may be adjusted to ensure that these options are available. No checks will be performed if check is not PRESENT or if it is set to .FALSE. .

2.7.2 The sparsity pattern analysis subroutine

The sparsity pattern of **A** may be analysed as follows:

```
CALL SLS_analyse( matrix, data, control, inform[, PERM] )
```

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matrix is scalar INTENT(IN) argument of type SMT_type that is used to specify **A**. The user must set all of the relevant components of matrix according to the storage scheme desired (see §2.6.1) except matrix%val. Incorrectly-set components will result in errors flagged in inform%status, see §2.8.

data is a scalar INTENT(INOUT) argument of type SLS_data_type (see §2.6.5). It is used to hold the factors and other data about the problem being solved. It must have been initialized by a call to SLS_initialize.

control is scalar INTENT(IN) argument of type SLS_control_type. Its components control the action of the analysis phase, as explained in §2.6.2.

inform is a scalar INTENT(INOUT) argument of type SLS_inform_type (see §2.6.4). A successful call is indicated when the component status has the value 0. For other return values of status, see §2.8.

PERM is an OPTIONAL INTENT(IN) rank-one INTEGER(ip_) argument of length matrix%n that may be used to provide a permutation/pivot order. If present, PERM(i), i $= 1, \ldots,$ matrix%n, should be set to the desired position of the input row i in the permuted matrix.

2.7.3 The numerical factorization subroutine

Once it has been analysed, the matrix **A** may be factorized as follows:

```
CALL SLS_factorize(matrix, data, control, inform )
```

matrix is scalar INTENT(IN) argument of type SMT_type that is used to specify **A**. The user must set all of the relevant components of matrix according to the storage scheme desired (see §2.6.1). Those components set for SLS_analyse must not have been altered in the interim.

data is a scalar INTENT(INOUT) argument of type SLS_data_type (see §2.6.5). It is used to hold the factors and other data about the problem being solved. It must have been initialized by a call to SLS_initialize and not altered by the user in the interim.

control is scalar INTENT(IN) argument of type SLS_control_type. Its components control the action of the factorization phase, as explained in §2.6.2.

inform is a scalar INTENT(INOUT) argument of type SLS_inform_type (see §2.6.4). A successful call is indicated when the component status has the value 0. For other return values of status, see §2.8.

2.7.4 The solution subroutine

Given the factorization, a set of equations may be solved as follows:

```
CALL SLS_solve( matrix, X, data, control, inform )
```

matrix is scalar INTENT(IN) argument of type SMT_type that is used to specify **A**. The user must set all of the relevant components of matrix according to the storage scheme desired (see §2.6.1). Those components set for SLS_factorize must not have been altered in the interim.

X is an INTENT(INOUT) assumed-shape array argument of rank 1 or 2 and of type REAL(rp_). On entry, X must be set to the vector **b** or the matrix **B** and on successful return it holds the solution **x** or **X**. For the single right-hand side case, the i-th component of **b** and the resulting i-th component of the solution **x** occupy the i-th component of X. When there are multiple right-hand sides, the i-th component of the j-th right-hand side $\mathbf{b}_j$ and the resulting solution $\mathbf{x}_j$ occupy the i, j-th component of X.

data is a scalar INTENT(INOUT) argument of type SLS_data_type (see §2.6.5). It is used to hold the factors and other data about the problem being solved. It must have been initialized by a call to SLS_initialize and not altered by the user in the interim.

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control is scalar INTENT(IN) argument of type SLS_control_type. Its components control the action of the solve phase, as explained in §2.6.2.

inform is a scalar INTENT(INOUT) argument of type SLS_inform_type (see §2.6.4). A successful call is indicated when the component status has the value 0. For other return values of status, see §2.8.

2.7.5 The termination subroutine

All previously allocated internal arrays are deallocated and OpenMP locks destroyed as follows:

```
CALL SLS_terminate( data, control, inform )
```

data is a scalar INTENT(INOUT) argument of type SLS_data_type (see §2.6.5). It is used to hold the factors and other data about the problem being solved. It must have been initialized by a call to SLS_initialize and not altered by the user in the interim. On exit, its allocatable array components will have been deallocated.

control is scalar INTENT(IN) argument of type SLS_control_type. Its components control the action of the termination phase, as explained in §2.6.2.

inform is a scalar INTENT(INOUT) argument of type SLS_inform_type (see §2.6.4). A successful call is indicated when the component status has the value 0. For other return values of status, see §2.8.

2.8 Warning and error messages

A negative value of inform%status on exit from the subroutines indicates that an error has occurred. No further calls should be made until the error has been corrected. Possible values are:

-1 An allocation error occurred. A message indicating the offending array is written on unit control%error, and the returned allocation status and a string containing the name of the offending array are held in inform%alloc_status and inform%bad_alloc respectively.

-2 A deallocation error occurred. A message indicating the offending array is written on unit control%error and the returned allocation status and a string containing the name of the offending array are held in inform%alloc_status and inform%bad_alloc respectively.

-3 One of the restrictions matrix%n > 0 or matrix%ne < 0, for co-ordinate entry, or requirements that matrix%type contain its relevant string 'COORDINATE', 'SPARSE_BY_ROWS' or 'DENSE' has been violated.

-20 The matrix is not positive definite while the solver used expected it to be.

-26 The requested solver is not available.

-29 This option is not available with this solver.

-32 More than control%max_integer_factor_size words of internal integer storage are required for in-core factorization.

-34 The package PARDISO failed; check the solver-specific information components inform%pardiso_iparm and inform%pardiso_dparm along with PARDISO's documentation for more details.

-35 The package WSMP failed; check the solver-specific information components inform%wsmp_iparm and inform%wsmp_dparm along with WSMP's documentation for more details.

-36 The scaling package HSL_MC64 failed; check the solver-specific information component inform%mc64_info along with HSL_MC64's documentation for more details.

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-37 The scaling package MC77 failed; check the solver-specific information components inform%mc77_info and inform%mc77_rinfo along with MC77's documentation for more details.

-39 The input permutation/pivot order is not a permutation or is faulty in some other way.

-40 It is not possible to alter the block diagonal factors for this solver.

-41 There is no information about the permutation used or the values of the pivots used for this solver (see §2.9.1).

-42 There is no information about the values of diagonal perturbations made for this solver (see §2.9.1).

-43 A direct-access file error occurred. See the value of inform%ma77_info%flag for more details.

-50 A solver-specific error occurred; check the solver-specific information component of inform along with the solver's documentation for more details.

2.9 Further features

In this section, we describe features for enquiring about and manipulating the parts of the factorization constructed. These features will not be needed by a user who wants simply to solve systems of equations with matrix $\mathbf{A}$.

The solvers used each produce an $\mathbf{LDL}^T$ factorization of $\mathbf{A}$ or a perturbation thereof, where $\mathbf{L}$ is a permuted lower triangular matrix and $\mathbf{D}$ is a block diagonal matrix with blocks of order 1 and 2. It is convenient to write this factorization in the form

$$\mathbf{A}+\mathbf{E}=\mathbf{PLDL}^T\mathbf{P}^T,$$

where $\mathbf{P}$ is a permutation matrix and $\mathbf{E}$ is any diagonal perturbation introduced. The following subroutines are provided:

SLS_enquire returns any of $\mathbf{P}$, $\mathbf{D}$, $\mathbf{E}$, or the pivot permutations implicit in $\mathbf{D}$.

SLS_alter_d alters $\mathbf{D}$. Note that this means that we no longer have a factorization of the given matrix $\mathbf{A}$.

SLS_part_solve solves one of the systems of equations $\mathbf{PLx}=\mathbf{b}$, $\mathbf{Dx}=\mathbf{b}$, $\mathbf{L}^T\mathbf{P}^T\mathbf{x}=\mathbf{b}$, or when $\mathbf{A}$ is positive definite, $\mathbf{PL}\sqrt{\mathbf{D}}\mathbf{x}=\mathbf{b}$, for one or more right-hand sides.

SLS_sparse_forward_solve solves $\mathbf{PLx}=\mathbf{b}$ when $\mathbf{b}$ is sparse and aims to return a sparse $\mathbf{x}$.

SLS_fredholm_alternative computes the Fredholm alternative for the data $(\mathbf{A},\mathbf{b})$, i.e., returns either $\mathbf{x}$ satisfying $\mathbf{Ax}=\mathbf{b}$ or $\mathbf{x}$ satisfying $\mathbf{Ax}=\mathbf{0}$ and $\mathbf{b}^T\mathbf{x}>0$.

Support for these features from the solvers available with SLS is summarised in Table 2.2.

2.9.1 To return P or D or both

```
CALL SLS_enquire( data, inform[, PERM][, PIVOTS][, D][, PERTURBATION] )
```

data is a scalar INTENT(INOUT) argument of type SLS_data_type (see §2.6.5). It is used to hold the factors and other data about the problem being solved. It must have been initialized by a call to SLS_initialize and not altered by the user in the interim.

inform is a scalar INTENT(INOUT) argument of type SLS_inform_type (see §2.6.4). A successful call is indicated when the component status has the value 0. For other return values of status, see §2.8.

PERM is an OPTIONAL rank-one INTEGER(ip_) array argument of INTENT(OUT) and length n. If present, PERM will be set to the pivot permutation selected by SLS_analyse.

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solver	SLS_enquire				SLS_alter_d	SLS_part_solve	SLS_sparse-_forward_solve	SLS_fredholm-_alterantive
	P	pivots	**D**	**E**				
SILS/MA27	√	√	√	√	√	√	$\times^1$	×
HSL_MA57	√	√	√	√	√	√	√	√
HSL_MA77	√	×	√	×	√	√	$\times^1$	√
HSL_MA86	√	×	√	√	×	√	$\times^1$	×
HSL_MA87	√	×	√	√	×	√	√	×
HSL_MA97	√	√	√	√	√	√	√	√
SSIDS	√	√	√	√	√	√	$\times^1$	×
MUMPS	√	×	×	×	×	×	×	×
PARDISO	×	×	×	×	×	√	$\times^1$	×
MKL_PARDISO	×	×	×	×	×	√	$\times^1$	×
PaStiX	√	×	×	×	×	×	×	×
WSMP	×	×	×	×	×	√	$\times^1$	×
POTR	×	×	√	×	√	√	$\times^1$	×
SYTR	×	√	√	×	√	√	$\times^1$	×
PBTR	×	×	√	×	√	√	$\times^1$	×

Table 2.2: Options supported. $\times^1$ indicates a feature that is not available directly from the solver, but for which an (inefficient) simulation is provided.

PIVOTS is an OPTIONAL rank-one INTEGER(ip_) array argument of INTENT(OUT) and length n. If present, the index of pivot i will be placed in PIVOTS (i), $i = 1,\ldots,n$, with its sign negative if it is the index of a 2 x 2 block.

D is an OPTIONAL rank-two REAL(rp_) array argument of INTENT(OUT) and shape (2, n). If present, the diagonal entries of $\mathbf{D}^{-1}$ will be placed in D(1, i), $i = 1,\ldots n$ and the off-diagonal entries of $\mathbf{D}^{-1}$ will be placed in D(2, i), $i = 1,\ldots n-1$.

PERTURBATION is an OPTIONAL rank-one REAL(rp_) array argument of INTENT(OUT) and length n. If present, PERTURBATION will be set to a vector of diagonal perturbations chosen by SLS_factorize. This array can only be nonzero if SLS_factorize was last called with control%pivoting = 4 or if the solver chose its own pivot sequence (control%pivoting ≤ 0).

2.9.2 To alter D

```
CALL SLS_alter_d( data, D, inform )
```

data is a scalar INTENT(INOUT) argument of type SLS_data_type (see §2.6.5). It is used to hold the factors and other data about the problem being solved. It must have been initialized by a call to SLS_initialize and not altered by the user in the interim.

D is an INTENT(INOUT) REAL(rp_) array argument of shape (2, n). The diagonal entries of $\mathbf{D}^{-1}$ will be altered to D(1, i), $i = 1,\ldots n$ and the off-diagonal entries of $\mathbf{D}^{-1}$ will be altered to D(2, i), $i = 1,\ldots n-1$.

inform is a scalar INTENT(INOUT) argument of type SLS_inform_type (see §2.6.4). A successful call is indicated when the component status has the value 0. For other return values of status, see §2.8.

2.9.3 To perform a partial solution

```
CALL SLS_part_solve( part, X, data, control, inform )
```

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part is scalar, of INTENT(IN) and of type CHARACTER. It must have one of the values

- L for solving $\mathbf{PLx} = \mathbf{b}$ or $\mathbf{PLX} = \mathbf{B}$,
- D for solving $\mathbf{Dx} = \mathbf{b}$ or $\mathbf{DX} = \mathbf{B}$, or
- U for solving $\mathbf{L}^T\mathbf{P}^T\mathbf{x} = \mathbf{b}$ or $\mathbf{L}^T\mathbf{P}^T\mathbf{X} = \mathbf{B}$.
- S for solving $\mathbf{PL}\sqrt{\mathbf{D}}\mathbf{x} = \mathbf{b}$ or $\mathbf{PL}\sqrt{\mathbf{D}}\mathbf{X} = \mathbf{B}$ where $\sqrt{\mathbf{D}}$ is the diagonal matrix whose entries are the square roots of those of $\mathbf{D}$ when $\mathbf{A}$ is positive definite.

data is a scalar INTENT(INOUT) argument of type SLS_data_type (see §2.6.5). It is used to hold the factors and other data about the problem being solved. It must have been initialized by a call to SLS_initialize and not altered by the user in the interim.

X is an INTENT(INOUT) REAL(rp_) assumed-shape array argument of rank 1 or 2. On entry, X must be set to the vector $\mathbf{b}$ or the matrix $\mathbf{B}$ and on successful return it holds the solution $\mathbf{x}$ or $\mathbf{X}$. For the single right-hand side case, the i-th component of $\mathbf{b}$ and the resulting i-th component of the solution $\mathbf{x}$ occupy the i-th component of X. When there are multiple right-hand sides, the i-th component of the j-th right-hand side $\mathbf{b}_j$ and the resulting solution $\mathbf{x}_j$ occupy the i,j-th component of X.

control is scalar INTENT(IN) argument of type SLS_control_type. Its components control the action of the solve phase, as explained in §2.6.2.

inform is a scalar INTENT(INOUT) argument of type SLS_inform_type (see §2.6.4). A successful call is indicated when the component status has the value 0. For other return values of status, see §2.8.

2.9.4 To solve PLx = b for sparse b

```
CALL SLS_sparse_forward_solve( nnz_b, INDEX_b, B, nnz_x, INDEX_x, X, data,   &
                               control, inform )
```

nnz_b is an INTENT(IN) scalar of type INTEGER that must hold the number of nonzero entries in the right-hand side. **Restriction:** $1 \leq$ nnz_b $\leq n$.

INDEX_b is an INTENT(IN) rank-1 array of type INTEGER. The first nnz_b entries must hold the indices of the nonzero entries in the right-hand side.

B is an INTENT(IN) rank-one assumed-shape array argument of length at least n and of type REAL(rp_). If INDEX_b(i)=k, B(k) must hold the i-th nonzero component of the right-hand side; other entries of B are not accessed.

nnz_x is an INTENT(OUT) scalar of type INTEGER. On exit, nnz_x holds the number of nonzero entries in the solution.

INDEX_x is an INTENT(OUT) rank-1 array of type INTEGER and size nnz_x (that is at most n). On exit, the first nnz_x entries hold the indices of the nonzero entries in the solution.

X is an INTENT(INOUT) rank-one assumed-shape array argument of length at least n and of type REAL(rp_). On entry, its first n entries must be set by the user to zero. On exit, if INDEX_x(i)=k, X(k) holds the i-th nonzero component of the solution; all other entries of X are zero.

data, control and inform: see Section 2.7.4.

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2.9.5 To find the Fredholm alternative for the data $(\mathbf{A}, \mathbf{b})$

```
CALL SLS_fredholm_alternative( matrix, X, data, control, inform )
```

`matrix`, `data`, `control` and `inform`: see Section 2.7.4.

`X` is an `INTENT(INOUT)` rank-one assumed-shape array argument of length at least n and of type `REAL(rp_)`. On entry, its first n entries must be set by the user to the vector $\mathbf{b}$. On exit, `X` will contain a solution $\mathbf{x}$ to $\mathbf{A}\mathbf{x} = \mathbf{b}$ if `inform%alternative` is `.FALSE.` or a vector $\mathbf{x}$ for which $\mathbf{A}\mathbf{x} = \mathbf{0}$ and $\mathbf{b}^T\mathbf{x} > 0$ if `inform%alternative` is `.TRUE.`.

2.10 Setting control parameters

In this section, we describe an alternative means of setting control parameters, that is components of the variable `control` of type `SLS_control_type` (see §2.6.2), by reading an appropriate data specification file using the subroutine `SLS_read_specfile`. This facility is useful as it allows a user to change `SLS` control parameters without editing and recompiling programs that call `SLS`.

A specification file, or specfile, is a data file containing a number of "specification commands". Each command occurs on a separate line, and comprises a "keyword", that is a string (in a close-to-natural language) used to identify a control parameter, and an (optional) "value", which defines the value to be assigned to the given control parameter. All keywords and values are case insensitive, keywords may be preceded by one or more blanks but values must not contain blanks, and each value must be separated from its keyword by at least one blank. Values must not contain more than 30 characters, and each line of the specification file is limited to 80 characters, including the blanks separating keyword and value.

The portion of the specification file used by `SLS_read_specfile` must start with a "`BEGIN SLS`" command and end with an "`END`" command. The syntax of the specfile is thus defined as follows:

```
( .. lines ignored by SLS_read_specfile .. )
  BEGIN SLS
     keyword    value
     .......    .....
     keyword    value
  END
( .. lines ignored by SLS_read_specfile .. )
```

where keyword and value are two strings separated by (at least) one blank. The "`BEGIN SLS`" and "`END`" delimiter command lines may contain additional (trailing) strings so long as such strings are separated by one or more blanks, so that lines such as

```
BEGIN SLS SPECIFICATION
```

and

```
END SLS SPECIFICATION
```

are acceptable. Furthermore, between the "`BEGIN SLS`" and "`END`" delimiters, specification commands may occur in any order. Blank lines and lines whose first non-blank character is `!` or `*` are ignored. The content of a line after a `!` or `*` character is also ignored (as is the `!` or `*` character itself). This provides an easy way to "comment out" some specification commands, or to comment specific values of certain control parameters.

The value of a control parameter may be of three different types, namely integer, character or real. Integer and real values may be expressed in any relevant Fortran integer and floating-point formats (respectively).

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The specification file must be open for input when SLS_read_specfile is called, and the associated unit number passed to the routine in device (see below). Note that the corresponding file is rewound, which makes it possible to combine the specifications for more than one program/routine. For the same reason, the file is not closed by SLS_read_specfile.

2.10.1 To read control parameters from a specification file

Control parameters may be read from a file as follows:

```
CALL SLS_read_specfile( control, device )
```

control is a scalar INTENT(INOUT) argument of type SLS_control_type (see §2.6.2). Default values should have already been set, perhaps by calling SLS_initialize. On exit, individual components of control may have been changed according to the commands found in the specfile. Specfile commands and the component (see §2.6.2) of control that each affects are given in Table 2.3.

device is a scalar INTENT(IN) argument of type INTEGER(ip_), that must be set to the unit number on which the specification file has been opened. If device is not open, control will not be altered and execution will continue, but an error message will be printed on unit control%error.

3 GENERAL INFORMATION

Workspace: Provided automatically by the module.

Other modules used directly: GALAHAD_CLOCK, GALAHAD_SYMBOLS, GALAHAD_SORT_single/double, GALAHAD_SPACE_single/double, GALAHAD_SPECFILE_single/double, GALAHAD_STRING_single/double, GALAHAD_SMT_single/double, GALAHAD_SILS_single/double and optionally HSL_MA57_single/double, HSL_MA77_single/double, HSL_MA86_single/double, HSL_MA87_single/double, HSL_MA97_single/double, HSL_MC64_single/double and HSL_MC68_single/double.

Other routines called directly: Optionally MC61, MC77 and METIS.

Input/output: Output is under control of the arguments control%error, control%warning, control%out, control%statistics and control%print_level.

Restrictions: matrix%n ≥ 1, matrix%ne ≥ 0 if matrix%type = 'COORDINATE', matrix%type one of 'COORDINATE', 'SPARSE_BY_ROWS' or 'DENSE'.

Portability: ISO Fortran 95 + TR 15581 or Fortran 2003 and optionally OpenMP. The package is thread-safe.

4 METHOD

Variants of sparse Gaussian elimination are used.

The solver SILS is available as part of GALAHAD and relies on the HSL Archive package MA27. To obtain HSL Archive packages, see

http://hsl.rl.ac.uk/archive/ .

The solvers HSL_MA57, HSL_MA77, HSL_MA86, HSL_MA87 and HSL_MA97, the ordering packages MC61 and HSL_MC68, and the scaling packages HSL_MC64 and MC77 are all part of HSL 2011. To obtain HSL 2011 packages, see

http://hsl.rl.ac.uk .

The solver SSIDS is from the SPRAL sparse-matrix collection, and is available as part of GALAHAD.

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command	component of control	value type
error-printout-device	%error	integer
warning-printout-device	%warning	integer
printout-device	%out	integer
statistics-printout-device	%statistics	integer
print-level	%print_level	integer
print-level-solver	%print_level_solver	integer
architecture-bits	%bits	integer
block-size-for-kernel	%block_size_kernel	integer
block-size-for--elimination	%block_size_elimination	integer
blas-block-for-size-factorize	%blas_block_size_factorize	integer
blas-block-size-for-solve	%blas_block_size_solve	integer
node-amalgamation-tolerance	%node_amalgamation	integer
initial-pool-size	%initial_pool_size	integer
minimum-real-factor-size	%min_real_factor_size	integer
minimum-integer-factor-size	%min_integer_factor_size	integer
maximum-real-factor-size	%max_real_factor_size	integer(long)
maximum-integer-factor-size	%max_integer_factor_size	integer(long)
maximum-in-core-store	%max_in_core_store	integer(long)
pivot-control	%pivot_control	integer
ordering	%ordering	integer
full-row-threshold	%full_row_threshold	integer
pivot-row-search-when-indefinite	%row_search_indefinite	integer
scaling	%scaling	integer
scale-maxit	%scale_maxit	integer
scale-thresh	%scale_thresh	real
max-iterative-refinements	%max_iterative_refinements	integer
array-increase-factor	%array_increase_factor	real
array-decrease-factor	%array_decrease_factor	real
relative-pivot-tolerance	%relative_pivot_tolerance	real
absolute-pivot-tolerance	%absolute_pivot_tolerance	real
zero-tolerance	%zero_tolerance	real
static-pivot-tolerance	%static_pivot_tolerance	real
static-level-switch	%static_level_switch	real
consistency-tolerance	%consistency_tolerance	real
acceptable-residual-relative	%acceptable_residual_relative	real
acceptable-residual-absolute	%acceptable_residual_absolute	real
out-of-core-directory	%out_of_core_directory	character
out-of-core-integer-factor-file	%out_of_core_integer_factor_file	character
out-of-core-real-factor-file	%out_of_core_real_factor_file	character
out-of-core-real-work-file	%out_of_core_real_work_file	character
out-of-core-indefinite-file	%out_of_core_indefinite_file	character
output-line-prefix	%prefix	character

Table 2.3: Specfile commands and associated components of control.

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The solver MUMPS is available from Mumps Technologies in France, and version 5.5.1 or above is sufficient. To obtain MUMPS, see

https://mumps-solver.org .

The solver PARDISO is available from the Pardiso Project; version 4.0.0 or above is required. To obtain PARDISO, see

http://www.pardiso-project.org/ .

The solver MKL PARDISO is available as part of Intel's oneAPI Math Kernel Library (oneMKL). To obtain this version of PARDISO, see

https://software.intel.com/content/www/us/en/develop/tools/oneapi.html .

The solver PaStix is available from Inria in France, and version 6.2 or above is sufficient. To obtain PaStiX, see

https://solverstack.gitlabpages.inria.fr/pastix .

The solver WSMP is available from the IBM alpha Works; version 10.9 or above is required. To obtain WSMP, see

http://www.alphaworks.ibm.com/tech/wsmp .

The solvers POTR, SYTR and PBTR, are available as S/DPOTRF/S, S/DSYTRF/S and S/DPBTRF/S as part of LAPACK. Reference versions are provided by GALAHAD, but for good performance machined-tuned versions should be used.

Explicit sparsity re-orderings are obtained by calling the HSL package HSL_MC68. Both this, HSL_MA57 and PARDISO rely optionally on the ordering package METIS from the Karypis Lab. To obtain METIS, see

http://glaros.dtc.umn.edu/gkhome/views/metis/ .

Bandwidth, Profile and wavefront reduction is supported by calling HSL's MC61.

References:

The methods used are described in the user-documentation for

HSL 2011, A collection of Fortran codes for large-scale scientific computation (2011).
http://www.hsl.rl.ac.uk

and papers

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P. R. Amestoy, I. S. Duff, J. Koster and J.-Y. L'Excellent. A fully asynchronous multifrontal solver using distributed dynamic scheduling, SIAM Journal on Matrix Analysis and Applications **23(1)** (2001) 15-41.

A. Gupta, "WSMP: Watson Sparse Matrix Package Part I - direct solution of symmetric sparse systems". IBM Research Report RC 21886, IBM T. J. Watson Research Center. NY 10598, USA (2010),

J.D. Hogg, E. Ovtchinnikov and J.A. Scott. A sparse symmetric indefinite direct solver for GPU architectures. ACM Transactions on Mathematical Software **42(1)** (2014), Article 1,

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O. Schenk and K. Gärtner, "Solving Unsymmetric Sparse Systems of Linear Equations with PARDISO". Journal of Future Generation Computer Systems, **20(3)** (2004) 475–487, and

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5 EXAMPLE OF USE

We illustrate the use of the package on the solution of the single set of equations

$$\begin{pmatrix} 2 & 3 & & & \\ 3 & & 4 & & 6 \\ & 4 & 1 & 5 & \\ & & 5 & & \\ & 6 & & & 1 \end{pmatrix} \mathbf{x} = \begin{pmatrix} 8 \\ 45 \\ 31 \\ 15 \\ 17 \end{pmatrix}$$

(Note that this example does not illustrate all the facilities). Then, choosing the solver `SILS`, we may use the following code:

```
   PROGRAM SLS_EXAMPLE   !  GALAHAD 4.1 - 2022-11-27 AT 15:15 GMT.
   USE GALAHAD_SLS_double
   IMPLICIT NONE
   INTEGER, PARAMETER :: wp = KIND( 1.0D+0 )
   TYPE ( SMT_type ) :: matrix
   TYPE ( SLS_data_type ) :: data
   TYPE ( SLS_control_type ) control
   TYPE ( SLS_inform_type ) :: inform
   INTEGER, PARAMETER :: n = 5
   INTEGER, PARAMETER :: ne = 7
   REAL ( KIND = wp ) :: B( n ), X( n )
   INTEGER :: s
! allocate and set lower triangle of matrix in co-ordinate form
   CALL SMT_put( matrix%type, 'COORDINATE', s )
   matrix%n = n ; matrix%ne = ne
   ALLOCATE( matrix%val( ne ), matrix%row( ne ), matrix%col( ne ) )
   matrix%row( : ne ) = (/ 1, 2, 3, 3, 4, 5, 5 /)
   matrix%col( : ne ) = (/ 1, 1, 2, 3, 3, 2, 5 /)
   matrix%val( : ne ) = (/ 2.0_wp, 3.0_wp, 4.0_wp, 1.0_wp, 5.0_wp,             &
                           6.0_wp, 1.0_wp /)
! problem setup complete
! set right-hand side
   B( : n ) = (/ 8.0_wp, 45.0_wp, 31.0_wp, 15.0_wp, 17.0_wp /)
! specify the solver (in this case ssids)
   CALL SLS_initialize( 'ssids', data, control, inform, check = .TRUE. )
   WRITE( 6, "( ' solver ', A, ' used' )" ) TRIM( inform%solver )
! analyse
   CALL SLS_analyse( matrix, data, control, inform )
   IF ( inform%status < 0 ) THEN
     WRITE( 6, '( A, I0 )' )                                                  &
          ' Failure of SLS_analyse with status = ', inform%status
     STOP
   END IF
! factorize
   CALL SLS_factorize( matrix, data, control, inform )
   IF ( inform%status < 0 ) THEN
     WRITE( 6, '( A, I0 )' )                                                  &
          ' Failure of SLS_factorize with status = ', inform%status
     STOP
   END IF
! solve using iterative refinement and ask for high relative accuracy
   X = B
```

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```
   control%max_iterative_refinements = 1
   control%acceptable_residual_relative = 0.0_wp
   CALL SLS_solve( matrix, X, data, control, inform )
   IF ( inform%status == 0 ) WRITE( 6, '( A, ( 5F5.2 ) )' )                    &
     ' Solution is', X
! clean up
   CALL SLS_terminate( data, control, inform )
   DEALLOCATE( matrix%type, matrix%val, matrix%row, matrix%col )
   STOP
   END PROGRAM SLS_EXAMPLE
```

This produces the following output:

```
 solver ssids used
 Solution is 1.00 2.00 3.00 4.00 5.00
```

The same problem may be solved holding the data in a sparse row-wise storage format by replacing the lines

```
! allocate and set lower triangle of matrix in co-ordinate form
...
! problem setup complete
```

by

```
! allocate and set lower triangle of matrix in spares row form
     CALL SMT_put( matrix%type, 'SPARSE_BY_ROWS', s )
     matrix%n = n
     ALLOCATE( matrix%val( ne ), matrix%col( ne ), matrix%ptr( n + 1 ) )
     matrix%ptr = (/ 1, 2, 3, 5, 6, 8 /)
     matrix%col = (/ 1, 1, 2, 3, 3, 2, 5 /)
     matrix%val = (/ 2.0_wp, 3.0_wp, 4.0_wp, 1.0_wp, 5.0_wp, 6.0_wp, 1.0_wp /)
! problem setup complete
```

or using a dense storage format with the replacement lines

```
! allocate and set lower triangle of matrix in dense form
     CALL SMT_put( matrix%type, 'DENSE', s )
     matrix%n = n
     ALLOCATE( matrix%val( n * ( n + 1 ) / 2 ) )
     matrix%val = (/ 2.0_wp, 3.0_wp, 0.0_wp, 0.0_wp, 4.0_wp, 1.0_wp,           &
                     0.0_wp, 0.0_wp, 5.0_wp, 0.0_wp, 0.0_wp, 6.0_wp,           &
                     0.0_wp, 0.0_wp, 1.0_wp /)
! problem setup complete
```

respectively.

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