



# GALAHAD

# CLLS

## USER DOCUMENTATION

## GALAHAD Optimization Library version 5.0

### 1 SUMMARY

This package uses a primal-dual interior-point method to solve the **polyhedrally-constrained regularized linear least-squares problem**

$$\text{minimize } \frac{1}{2} \|\mathbf{A}_o \mathbf{x} - \mathbf{b}\|_W^2 + \frac{1}{2} \sigma \|\mathbf{x}\|^2 \quad (1.1)$$

subject to the general linear constraints

$$\mathbf{c}_i^l \leq \mathbf{a}_i^T \mathbf{x} \leq \mathbf{c}_i^u, \quad i = 1, \dots, m,$$

and the simple bound constraints

$$x_j^l \leq x_j \leq x_j^u, \quad j = 1, \dots, n,$$

where the norms  $\|r\|_W = \sqrt{\sum_{i=1}^o w_i r_i^2}$  and  $\|x\| = \sqrt{\sum_{i=1}^n x_i^2}$ , and the  $o$  by  $n$  matrix  $\mathbf{A}_o$ , the vectors  $\mathbf{b}$ ,  $\mathbf{a}_i$ ,  $\mathbf{c}^l$ ,  $\mathbf{c}^u$ ,  $\mathbf{x}^l$ ,  $\mathbf{x}^u$  and the weights  $w > 0$  and  $\sigma \geq 0$  are given. Any of the constraint bounds  $\mathbf{c}_i^l$ ,  $\mathbf{c}_i^u$ ,  $x_j^l$  and  $x_j^u$  may be infinite. Full advantage is taken of any zero coefficients in the matrix  $\mathbf{A}_o$  and the matrix  $\mathbf{A}$  of vectors  $\mathbf{a}_i$ .

**ATTRIBUTES — Versions:** GALAHAD\_CLLS\_single, GALAHAD\_CLLS\_double. **Uses:** GALAHAD\_CLOCK, GALAHAD\_SYMBOLS, GALAHAD\_SPACE, GALAHAD\_SPECFILE, GALAHAD\_SMT, GALAHAD\_QPT, GALAHAD\_LSP, GALAHAD\_QPD, GALAHAD\_CQP, GALAHAD\_FIT, GALAHAD\_ROOTS, GALAHAD\_NORMS, GALAHAD\_SLS, GALAHAD\_CRO, GALAHAD\_FDC. **Date:** October 2023. **Origin:** N. I. M. Gould. **Language:** Fortran 95 + TR 15581 or Fortran 2003. **Parallelism:** Some options may use OpenMP and its runtime library.

### 2 HOW TO USE THE PACKAGE

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_CLLS_single
```

with the obvious substitution GALAHAD\_CLLS\_double, GALAHAD\_CLLS\_single\_64 and GALAHAD\_CLLS\_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, QPT\_problem\_type, NLPT\_userdata\_type, CLLS\_time\_type, CLLS\_control\_type, CLLS\_inform\_type and CLLS\_data\_type (Section 2.4) and the subroutines CLLS\_initialize, CLLS\_solve, CLLS\_terminate, (Section 2.5) and CLLS\_read\_specfile (Section 2.7) must be renamed on one of the USE statements.

#### 2.1 Matrix storage formats

Both the objective design matrix  $\mathbf{A}_o$  and the constraint Jacobian  $\mathbf{A}$ , the matrix whose rows are the vectors  $\mathbf{a}_i^T$ ,  $i = 1, \dots, m$ , may be stored in a variety of input formats.

##### 2.1.1 Dense row-wise 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. Component  $n * (i - 1) + j$  of the storage array `A%val` will hold the value  $a_{ij}$  for  $i = 1, \dots, m$ ,  $j = 1, \dots, n$ .

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### 2.1.2 Dense column-wise storage format

The matrix  $\mathbf{A}$  is stored as a compact dense matrix by columns, that is, the values of the entries of each column in turn are stored in order within an appropriate real one-dimensional array. Component  $m * (j - 1) + i$  of the storage array `A%val` will hold the value  $a_{ij}$  for  $i = 1, \dots, m, j = 1, \dots, n$ .

### 2.1.3 Sparse co-ordinate storage format

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

### 2.1.4 Sparse row-wise storage format

Again only the nonzero entries 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  $\mathbf{A}$ , the  $i$ -th component of a integer array `A%ptr` holds the position of the first entry in this row, while `A%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  $l = \text{A\%ptr}(i), \dots, \text{A\%ptr}(i + 1) - 1$  of the integer array `A%col`, and real array `A%val`, respectively.

### 2.1.5 Sparse column-wise storage format

Once again only the nonzero entries are stored, but this time they are ordered so that those in column  $j$  appear directly before those in column  $j + 1$ . For the  $j$ -th column of  $\mathbf{A}$ , the  $j$ -th component of a integer array `A%ptr` holds the position of the first entry in this column, while `A%ptr(n + 1)` holds the total number of entries plus one. The row indices  $i$  and values  $a_{ij}$  of the entries in the  $j$ -th column are stored in components  $l = \text{A\%ptr}(j), \dots, \text{A\%ptr}(j + 1) - 1$  of the integer array `A%row`, and real array `A%val`, respectively.

For sparse matrices, the latter pair schemes almost always require less storage than the co-ordinate one.

## 2.2 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.

## 2.3 Parallel usage

OpenMP may be used by the `GALAHAD_CLLS` 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 `-mpi`). 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

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

The code may be compiled and run in serial mode.

## 2.4 The derived data types

Ten derived data types are accessible from the package.

### 2.4.1 The derived data type for holding matrices

The derived data type `SMT_TYPE` is used to hold the matrices  $\mathbf{A}_o$  and  $\mathbf{A}$ . The components of `SMT_TYPE` used here are:

- `m` is a scalar component of type `INTEGER(ip_)`, that holds the number of rows in the matrix.
- `n` is a scalar component of type `INTEGER(ip_)`, that holds the number of columns in the matrix.
- `ne` is a scalar variable of type `INTEGER(ip_)`, that holds the number of matrix entries.
- `type` is a rank-one allocatable array of type default `CHARACTER`, that is used to indicate the matrix storage scheme used. Its precise length and content depends on the type of matrix to be stored (see §2.4.2).
- `val` is a rank-one allocatable array of type `REAL(rp_)` and dimension at least `ne`, that holds the values of the entries.
- `row` is a rank-one allocatable array of type `INTEGER(ip_)`, and dimension at least `ne`, that may hold the row indices of the entries. (see §2.1.3 & 2.1.5).
- `col` is a rank-one allocatable array of type `INTEGER(ip_)`, and dimension at least `ne`, that may hold the column indices of the entries (see §2.1.3–2.1.4).
- `ptr` is a rank-one allocatable array of type `INTEGER(ip_)`, and dimension at least `m + 1`, that may hold the pointers to the first entry in each row (see §2.1.4), or dimension at least `n + 1`, that may hold the pointers to the first entry in each column (see §2.1.5),

### 2.4.2 The derived data type for holding the problem

The derived data type `QPT_problem_type` is used to hold the problem. The components of `QPT_problem_type` are:

- `n` is a scalar variable of type `INTEGER(ip_)`, that holds the number of optimization variables,  $n$ .
- `o` is a scalar variable of type `INTEGER(ip_)`, that holds the number of observations,  $o$ .
- `m` is a scalar variable of type `INTEGER(ip_)`, that holds the number of general linear constraints,  $m$ .
- `Ao` is scalar variable of type `SMT_TYPE` that holds the objective design matrix  $\mathbf{A}_o$ . The following components are used:

`Ao%type` is an allocatable array of rank one and type default `CHARACTER`, that is used to indicate the storage scheme used. If the dense row-wise storage scheme (see Section 2.1.1) is used, the first five components of `Ao%type` must contain the string `DENSE`. By contrast, if the dense column-wise storage scheme (see Section 2.1.2) is used, the first fifteen components of `Ao%type` must contain the string `DENSE_BY_COLUMNS`. For the sparse co-ordinate scheme (see Section 2.1.3), the first ten components of `Ao%type` must contain the string `COORDINATE`, while for the sparse row-wise storage scheme (see Section 2.1.4), the first fourteen components of `Ao%type` must contain the string `SPARSE_BY_ROWS`, and for the sparse column-wise

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storage scheme (see Section 2.1.5), the first seventeen components of `Ao%type` must contain the string `SPARSE_BY_COLUMNS`,

The procedure `SMT_put` may be used to allocate sufficient space and insert the required keyword into `Ao%type`. For example, if `prob` is of derived type `CLLS_problem_type` and involves an objective design matrix we wish to store using the co-ordinate storage scheme, we may simply

```
CALL SMT_put( prob%Ao%type, 'COORDINATE', istat )
```

`Ao%ne` is a scalar variable of type `INTEGER(ip_)`, that holds the number of entries in  $\mathbf{A}_o$  in the sparse co-ordinate storage scheme (see Section 2.1.3). It need not be set for any of the other appropriate schemes.

`Ao%val` is a rank-one allocatable array of type `REAL(rp_)`, that holds the values of the entries of the design matrix  $\mathbf{A}_o$  in any of the appropriate storage schemes discussed in Section 2.1.

`Ao%row` is a rank-one allocatable array of type `INTEGER(ip_)`, that holds the row indices of  $\mathbf{A}_o$  in the sparse co-ordinate storage or sparse column-wise schemes (see Sections 2.1.3 and 2.1.5). It need not be allocated for any of the other schemes.

`Ao%col` is a rank-one allocatable array variable of type `INTEGER(ip_)`, that holds the column indices of  $\mathbf{A}_o$  in either the sparse co-ordinate (see Section 2.1.3), or the sparse row-wise (see Section 2.1.4) storage scheme. It need not be allocated for any of the other schemes.

`Ao%ptr` is a rank-one allocatable array of dimension `o+1` and type `INTEGER(ip_)`, that holds the starting position of each row of  $\mathbf{A}_o$ , as well as the total number of entries plus one, in the sparse row-wise storage scheme (see Section 2.1.4). By contrast, for the sparse column-wise storage scheme (see Section 2.1.5), it should be of dimension `n+1` and holds the starting position of each column of  $\mathbf{A}_o$ , as well as the total number of entries plus one. It need not be allocated when the other appropriate schemes are used.

**B** is a rank-one allocatable array type `REAL(rp_)`, that should be allocated to have length `o`, and its  $i$ -th component filled with the value  $b_i$  for  $i = 1, \dots, o$ .

**A** is scalar variable of type `SMT_TYPE` that holds the constraint Jacobian matrix  $\mathbf{A}$ . The following components are used:

`A%type` is an allocatable array of rank one and type default `CHARACTER`, that is used to indicate the storage scheme used. If the dense row-wise storage scheme (see Section 2.1.1) is used, the first five components of `A%type` must contain the string `DENSE`. By contrast, if the dense column-wise storage scheme (see Section 2.1.2) is used, the first fifteen components of `A%type` must contain the string `DENSE_BY_COLUMNS`. For the sparse co-ordinate scheme (see Section 2.1.3), the first ten components of `A%type` must contain the string `COORDINATE`, while for the sparse row-wise storage scheme (see Section 2.1.4), the first fourteen components of `A%type` must contain the string `SPARSE_BY_ROWS`, and for the sparse column-wise storage scheme (see Section 2.1.5), the first seventeen components of `A%type` must contain the string `SPARSE_BY_COLUMNS`,

The procedure `SMT_put` may be used to allocate sufficient space and insert the required keyword into `A%type`. For example, if `prob` is of derived type `CLLS_problem_type` and involves a Jacobian we wish to store using the sparse row-wise storage scheme, we may simply

```
CALL SMT_put( prob%A%type, 'SPARSE_BY_ROWS', istat )
```

`A%ne` is a scalar variable of type `INTEGER(ip_)`, that holds the number of entries in  $\mathbf{A}$  in the sparse co-ordinate storage scheme (see Section 2.1.3). It need not be set for any of the other appropriate schemes.

`A%val` is a rank-one allocatable array of type `REAL(rp_)`, that holds the values of the entries of the Jacobian matrix  $\mathbf{A}$  in any of the appropriate storage schemes discussed in Section 2.1.

`A%row` is a rank-one allocatable array of type `INTEGER(ip_)`, that holds the row indices of  $\mathbf{A}$  in the sparse co-ordinate storage or sparse column-wise schemes (see Sections 2.1.3 and 2.1.5). It need not be allocated for any of the other schemes.

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- `A%col` is a rank-one allocatable array variable of type `INTEGER(ip_)`, that holds the column indices of **A** in either the sparse co-ordinate (see Section 2.1.3), or the sparse row-wise (see Section 2.1.4) storage scheme. It need not be allocated for any of the other schemes.
- `A%ptr` is a rank-one allocatable array of dimension  $m+1$  and type `INTEGER(ip_)`, that holds the starting position of each row of **A**, as well as the total number of entries plus one, in the sparse row-wise storage scheme (see Section 2.1.4). By contrast, for the sparse column-wise storage scheme (see Section 2.1.5), it should be of dimension  $n+1$  and holds the starting position of each column of **A**, as well as the total number of entries plus one, It need not be allocated when the other appropriate schemes are used.
- `C_l` is a rank-one allocatable array of dimension  $m$  and type `REAL(rp_)`, that holds the vector of lower bounds  $\mathbf{c}^l$  on the general constraints. The  $i$ -th component of `C_l`,  $i = 1, \dots, m$ , contains  $\mathbf{c}_i^l$ . Infinite bounds are allowed by setting the corresponding components of `C_l` to any value smaller than `-infinity`, where `infinity` is a component of the control array `control` (see Section 2.4.3).
- `C_u` is a rank-one allocatable array of dimension  $m$  and type `REAL(rp_)`, that holds the vector of upper bounds  $\mathbf{c}^u$  on the general constraints. The  $i$ -th component of `C_u`,  $i = 1, \dots, m$ , contains  $\mathbf{c}_i^u$ . Infinite bounds are allowed by setting the corresponding components of `C_u` to any value larger than `infinity`, where `infinity` is a component of the control array `control` (see Section 2.4.3).
- `X_l` is a rank-one allocatable array of dimension  $n$  and type `REAL(rp_)`, that holds the vector of lower bounds  $\mathbf{x}^l$  on the variables. The  $j$ -th component of `X_l`,  $j = 1, \dots, n$ , contains  $\mathbf{x}_j^l$ . Infinite bounds are allowed by setting the corresponding components of `X_l` to any value smaller than `-infinity`, where `infinity` is a component of the control array `control` (see Section 2.4.3).
- `X_u` is a rank-one allocatable array of dimension  $n$  and type `REAL(rp_)`, that holds the vector of upper bounds  $\mathbf{x}^u$  on the variables. The  $j$ -th component of `X_u`,  $j = 1, \dots, n$ , contains  $\mathbf{x}_j^u$ . Infinite bounds are allowed by setting the corresponding components of `X_u` to any value larger than that `infinity`, where `infinity` is a component of the control array `control` (see Section 2.4.3).
- `X` is a rank-one allocatable array of dimension  $n$  and type `REAL(rp_)`, that holds the values  $\mathbf{x}$  of the optimization variables. The  $j$ -th component of `X`,  $j = 1, \dots, n$ , contains  $x_j$ .
- `R` is a rank-one allocatable array of dimension  $o$  and type default `REAL(rp_)`, that holds the values  $\mathbf{r} = \mathbf{A}_o \mathbf{x} - \mathbf{b}$  of the residuals. The  $i$ -th component of `R`,  $i = 1, \dots, o$ , contains  $\mathbf{r}_i$ .
- `C` is a rank-one allocatable array of dimension  $m$  and type default `REAL(rp_)`, that holds the values  $\mathbf{Ax}$  of the constraints. The  $i$ -th component of `C`,  $i = 1, \dots, m$ , contains  $\mathbf{a}_i^T \mathbf{x} \equiv (\mathbf{Ax})_i$ .
- `Y` is a rank-one allocatable array of dimension  $m$  and type `REAL(rp_)`, that holds the values  $\mathbf{y}$  of estimates of the Lagrange multipliers corresponding to the general linear constraints (see Section 4). The  $i$ -th component of `Y`,  $i = 1, \dots, m$ , contains  $y_i$ .
- `Z` is a rank-one allocatable array of dimension  $n$  and type default `REAL(rp_)`, that holds the values  $\mathbf{z}$  of estimates of the dual variables corresponding to the simple bound constraints (see Section 4). The  $j$ -th component of `Z`,  $j = 1, \dots, n$ , contains  $z_j$ .
- `C_status` is a rank-one allocatable array argument of dimension  $m$  and type `INTEGER(ip_)`, that indicates which of the general linear constraints are in the optimal active set. Possible values for `C_status(i)`,  $i = 1, \dots, m$ , and their meanings are
- `<0` the  $i$ -th general constraint is in the active set, on its lower bound,
  - `>0` the  $i$ -th general constraint is in the active set, on its upper bound, and
  - `0` the  $i$ -th general constraint is not in the active set.

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When `control%crossover` is `.TRUE.`, more specific values are

- 1 the  $i$ -th general constraint is both independent and active on its lower bound,
- 2 the  $i$ -th general constraint is on its lower bound but linearly dependent on others,
- 1 the  $i$ -th general constraint is both independent and active on its upper bound,
- 2 the  $i$ -th general constraint is on its upper bound but linearly dependent on others, and
- 0 the  $i$ -th general constraint is not in the active set.

`X_status` is a rank-one allocatable array argument of dimension  $n$  and type `INTEGER(ip_)`, that indicates which of the simple bound constraints are in the current active set. Possible values for `X_status(j)`,  $j = 1, \dots, n$ , and their meanings are

- <0 the  $j$ -th simple bound constraint is in the active set, on its lower bound,
- >0 the  $j$ -th simple bound constraint is in the active set, on its upper bound, and
- 0 the  $j$ -th simple bound constraint is not in the active set.

When `control%crossover` is `.TRUE.`, more specific values are

- 1 the  $j$ -th simple bound constraint is both independent and active on its lower bound,
- 2 the  $j$ -th simple bound constraint is on its lower bound but linearly dependent on others,
- 1 the  $j$ -th simple bound constraint is both independent and active on its upper bound,
- 2 the  $j$ -th simple bound constraint is on its upper bound but linearly dependent on others, and
- 0 the  $j$ -th simple bound constraint is not in the active set.

### 2.4.3 The derived data type for holding control parameters

The derived data type `CLLS_control_type` is used to hold controlling data. Default values may be obtained by calling `CLLS_initialize` (see Section 2.5.1), while components may also be changed by calling `CLLS_read_specfile` (see Section 2.7.1). The components of `CLLS_control_type` are:

`error` is a scalar variable of type `INTEGER(ip_)`, that holds the stream number for error messages. Printing of error messages in `CLLS_solve` and `CLLS_terminate` is suppressed if `error`  $\leq 0$ . The default is `error` = 6.

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

`print_level` is a scalar variable of type `INTEGER(ip_)`, that is used to control the amount of informational output which is required. No informational output will occur if `print_level`  $\leq 0$ . If `print_level` = 1, a single line of output will be produced for each iteration of the process. If `print_level`  $\geq 2$ , this output will be increased to provide significant detail of each iteration. The default is `print_level` = 0.

`maxit` is a scalar variable of type `INTEGER(ip_)`, that holds the maximum number of iterations which will be allowed in `CLLS_solve`. The default is `maxit` = 1000.

`start_print` is a scalar variable of type `INTEGER(ip_)`, that specifies the first iteration for which printing will occur in `CLLS_solve`. If `start_print` is negative, printing will occur from the outset. The default is `start_print` = -1.

`stop_print` is a scalar variable of type `INTEGER(ip_)`, that specifies the last iteration for which printing will occur in `CLLS_solve`. If `stop_print` is negative, printing will occur once it has been started by `start_print`. The default is `stop_print` = -1.

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`infeas_max` is a scalar variable of type `INTEGER(ip_)`, that specifies the number of iterations for which the overall infeasibility of the problem is not reduced by at least a factor `reduce_infeas` before the problem is flagged as infeasible (see `reduce_infeas`). The default is `infeas_max = 200`.

`muzero_fixed` is a scalar variable of type `INTEGER(ip_)`, that specifies the number of iterations before the initial barrier parameter (see `muzero`) may be altered. The default is `muzero_fixed = 1`.

`restore_problem` is a scalar variable of type `INTEGER(ip_)`, that specifies how much of the input problem is to be restored on output. Possible values are:

- 0 nothing is restored.
- 1 the vector data  $\mathbf{w}$ ,  $\mathbf{b}$ ,  $\mathbf{x}^l$ , and  $\mathbf{x}^u$  will be restored to their input values.
- 2 the entire problem, that is the above vector data along with the matrices  $\mathbf{A}_o$  and  $\mathbf{A}$ , will be restored.

The default is `restore_problem = 2`.

`indicator_type` is a scalar variable of type `INTEGER(ip_)`, that specifies the type of indicator used to assess when a variable bound or constraint is active. Possible values are:

- 1 a variable bound/constraint is active if and only if the distance to its nearest bound is no larger than `indicator_tol_p` (see below).
- 2 a variable bound/constraint is active if and only if the distance to its nearest bound is no larger than `indicator_tol_pd` (see below) times the magnitude of its corresponding dual variable.
- 3 a variable bound/constraint is active if and only if the distance to its nearest bound is no larger than `indicator_tol_tapia` (see below) times the distance to the same bound at the previous iteration.

The default is `indicator_type = 3`.

`arc` is a scalar variable of type `INTEGER(ip_)`, that specifies the type of residual trajectory used to define the path to the solution. Possible values are:

- 1 the residual trajectory proposed by Zhang will be used.
- 2 the residual trajectory proposed by Zhao and Sun will be used; note this trajectory does not necessarily ensure convergence, so should be used with caution.
- 3 a combination in which Zhang's trajectory is used until the method determines that Zhou and Sun's will be better.
- 4 a mixed linear-quadratic variant of Zhang's proposal will be used.

The default is `arc = 1`.

`series_order` is a scalar variable of type `INTEGER(ip_)`, that specifies the order of (Puiseux or Taylor) series to approximate the residual trajectory. The default is `series_order = 2`.

`infinity` is a scalar variable of type `REAL(rp_)`, that is used to specify which constraint bounds are infinite. Any bound larger than `infinity` in modulus will be regarded as infinite. The default is `infinity = 1019`.

`stop_abs_p` and `stop_rel_p` are scalar variables of type `REAL(rp_)`, that hold the required absolute and relative accuracy for the primal infeasibility (see Section 4). The absolute value of each component of the primal infeasibility on exit is required to be smaller than the larger of `stop_abs_p` and `stop_rel_p` times a "typical value" for this component. The defaults are `stop_abs_p = stop_rel_p =  $u^{1/3}$` , where  $u$  is `EPSILON(1.0)` (`EPSILON(1.0D0)` in GALAHAD-CLLS-double).

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`stop_abs_d` and `stop_rel_d` are scalar variables of type `REAL(rp_)`, that hold the required absolute and relative accuracy for the dual infeasibility (see Section 4). The absolute value of each component of the dual infeasibility on exit is required to be smaller than the larger of `stop_abs_p` and `stop_rel_p` times a “typical value” for this component. The defaults are `stop_abs_d = stop_rel_d =  $u^{1/3}$` , where  $u$  is `EPSILON(1.0)` (`EPSILON(1.0D0)` in `GALAHAD_CLLS_double`).

`stop_abs_c` and `stop_rel_c` are scalar variables of type `REAL(rp_)`, that hold the required absolute and relative accuracy for the violation of complementary slackness (see Section 4). The absolute value of each component of the complementary slackness on exit is required to be smaller than the larger of `stop_abs_p` and `stop_rel_p` times a “typical value” for this component. The defaults are `stop_abs_c = stop_rel_c =  $u^{1/3}$` , where  $u$  is `EPSILON(1.0)` (`EPSILON(1.0D0)` in `GALAHAD_CLLS_double`).

`prfeas` is a scalar variable of type `REAL(rp_)`, that aims to specify the closest that any initial variable may be to infeasibility. Any variable closer to infeasibility than `prfeas` will be moved to `prfeas` from the offending bound. However, if a variable is range bounded, and its bounds are closer than `prfeas` apart, it will be moved to the mid-point of the two bounds. The default is `prfeas =  $10^4$` .

`dufeas` is a scalar variable of type `REAL(rp_)`, that aims to specify the closest that any initial dual variable or Lagrange multiplier may be to infeasibility. Any variable closer to infeasibility than `prfeas` will be moved to `dufeas` from the offending bound. However, if a dual variable is range bounded, and its bounds are closer than `dufeas` apart, it will be moved to the mid-point of the two bounds. The default is `dufeas =  $10^4$` .

`muzero` is a scalar variable of type `REAL(rp_)`, that holds the initial value of the barrier parameter. If `muzero` is not positive, it will be reset automatically to an appropriate value. The default is `muzero = -1.0`.

`tau` is a scalar variable of type `REAL(rp_)`, that holds the weight attached to primal-dual infeasibility compared to complementarity when assessing step acceptance. The default is `tau = 1.0`.

`gamma_c` is a scalar variable of type `REAL(rp_)`, that holds the smallest value that individual complementarity pairs are allowed to be relative to the average as the iteration proceeds. The default is `gamma_c =  $10^{-5}$` .

`gamma_f` is a scalar variable of type `REAL(rp_)`, that holds the smallest value the average complementarity is allowed to be relative to the primal-dual infeasibility as the iteration proceeds. The default is `gamma_c =  $10^{-5}$` .

`reduce_infeas` is a scalar variable of type `REAL(rp_)`, that specifies the least factor by which the overall infeasibility of the problem must be reduced, over `infeas_max` consecutive iterations, for it not be declared infeasible (see `infeas_max`). The default is `reduce_infeas = 0.99`.

`identical_bounds_tol` is a scalar variable of type `REAL(rp_)`. Every pair of constraint bounds  $(c_i^l, c_i^u)$  or  $(x_j^l, x_j^u)$  that is closer than `identical_bounds_tol` will be reset to the average of their values,  $\frac{1}{2}(c_i^l + c_i^u)$  or  $\frac{1}{2}(x_j^l + x_j^u)$  respectively. The default is `identical_bounds_tol =  $u$` , where  $u$  is `EPSILON(1.0)` (`EPSILON(1.0D0)` in `GALAHAD_CLLS_double`).

`mu_pounce` is a scalar variable of type `REAL(rp_)` that specifies the value of the barrier parameter that must be attained before an extrapolating “pounce” may be attempted. The default is `mu_pounce =  $10^{-5}$` .

`indicator_tol_p` is a scalar variable of type `REAL(rp_)` that provides the indicator tolerance associated with the test `indicator_type = 1`. The default is `indicator_tol_p =  $u^{1/3}$` , where  $u$  is `EPSILON(1.0)` (`EPSILON(1.0D0)` in `GALAHAD_CLLS_double`).

`indicator_tol_pd` is a scalar variable of type `REAL(rp_)` that provides the indicator tolerance associated with the test `indicator_type = 2`. The default is `indicator_tol_pd = 1.0`.

`indicator_tol_tapia` is a scalar variable of type `REAL(rp_)` that provides the indicator tolerance associated with the test `indicator_type = 3`. The default is `indicator_tol_tapia = 0.9`.

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`cpu_time_limit` is a scalar variable of type `REAL(rp_)`, that is used to specify the maximum permitted CPU time.

Any negative value indicates no limit will be imposed. The default is `cpu_time_limit = - 1.0`.

`clock_time_limit` is a scalar variable of type `REAL(rp_)`, that is used to specify the maximum permitted elapsed system clock time. Any negative value indicates no limit will be imposed. The default is `clock_time_limit = - 1.0`.

`remove_dependencies` is a scalar variable of type default `LOGICAL`, that must be set `.TRUE.` if the algorithm is to attempt to remove any linearly dependent constraints before solving the problem, and `.FALSE.` otherwise. We recommend removing linearly dependencies. The default is `remove_dependencies = .TRUE..`

`treat_zero_bounds_as_general` is a scalar variable of type default `LOGICAL`. If it is set to `.FALSE.`, variables which are only bounded on one side, and whose bound is zero, will be recognised as non-negativities/non-positivities rather than simply as lower- or upper-bounded variables. If it is set to `.TRUE.`, any variable bound  $x_j^l$  or  $x_j^u$  which has the value 0.0 will be treated as if it had a general value. Setting `treat_zero_bounds_as_general` to `.TRUE.` has the advantage that if a sequence of problems are reordered, then bounds which are “accidentally” zero will be considered to have the same structure as those which are nonzero. However, `GALAHAD_CLLS` is able to take special advantage of non-negativities/non-positivities, so if a single problem, or if a sequence of problems whose bound structure is known not to change, is/are to be solved, it will pay to set the variable to `.FALSE..` The default is `treat_zero_bounds_as_general = .FALSE..`

`just_feasible` is a scalar variable of type default `LOGICAL`, that must be set `.TRUE.` if the algorithm should stop as soon as a feasible point of the constraint set is found, and `.FALSE.` otherwise. The default is `just_feasible = .FALSE..`

`getdua` is a scalar variable of type default `LOGICAL`, that must be set `.TRUE.` if the user-provided estimates of the dual variables should be replaced by estimates whose aim is to try to balance the requirements of dual feasibility and complementary slackness, and `.FALSE.` if users estimates are to be used. The default is `getdua = .FALSE..`

`puiseux` is a scalar variable of type default `LOGICAL`, that must be set `.TRUE.` if a Puiseux series will be used when extrapolating along the central path and `.FALSE.` if a Taylor series is preferred. We recommend using the Puiseux series unless the solution is known to be non-degenerate. The default is `puiseux = .TRUE..`

`every_order` is a scalar variable of type default `LOGICAL`, that must be set `.TRUE.` if every order of approximation up to `series_order` will be tried and the best taken, and `.FALSE.` if only the exact order specified by `series_order` will be used. The default is `every_order = .TRUE..`

`feasol` is a scalar variable of type default `LOGICAL`, that should be set `.TRUE.` if the final solution obtained will be perturbed so that variables close to their bounds are moved onto these bounds, and `.FALSE.` otherwise. The default is `feasol = .FALSE..`

`balance_initial_complentarit` is a scalar variable of type default `LOGICAL`, that should be set `.TRUE.` if the initial complementarity is required to be balanced, and `.FALSE.` otherwise. The default is `balance_initial_complentarit = .FALSE..`

`crossover` is a scalar variable of type default `LOGICAL`, that must be set `.TRUE.` if the solution is to be defined in terms of linearly-independent constraints, and `.FALSE.` otherwise. The default is `crossover = .TRUE..`

`reduced_pounce_system` is a scalar variable of type default `LOGICAL`, that should be set `.TRUE.` if fixed variables will be eliminated when solving the linear system required by attempted pounces to the solution, and `.FALSE.` otherwise. The default is `reduced_pounce_system = .TRUE..`

`space_critical` is a scalar variable of type default `LOGICAL`, that must be set `.TRUE.` if space is critical when allocating arrays and `.FALSE.` otherwise. The package may run faster if `space_critical` is `.FALSE.` but at the possible expense of a larger storage requirement. The default is `space_critical = .FALSE..`

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`deallocate_error_fatal` is a scalar variable of type default LOGICAL, that must be set `.TRUE.` if the user wishes to terminate execution if a deallocation fails, and `.FALSE.` if an attempt to continue will be made. The default is `deallocate_error_fatal = .FALSE..`

`symmetric_linear_solver` is a scalar variable of type default CHARACTER and length 30, that specifies the external package to be used to solve any symmetric linear system that might arise. Current possible choices are `'sils'`, `'ma27'`, `'ma57'`, `'ma77'`, `'ma86'`, `'ma97'`, `ssids`, `'pardiso'` and `'wsmp'`, although only `'sils'` and, for OMP 4.0-compliant compilers, `'ssids'` are installed by default. See the documentation for the GALAHAD package SLS for further details. The default is `symmetric_linear_solver = 'sils'`.

`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, they may use the default `prefix = ""`.

`FDC_control` is a scalar variable of type `FDC_control_type` whose components are used to control any detection of linear dependencies performed by the package GALAHAD\_FDC. See the specification sheet for the package GALAHAD\_FDC for details, and appropriate default values.

`SLS_control` and `SLS_pounce_control` are scalar variables of type `SLS_control_type` whose components are used to control factorizations performed by the package GALAHAD\_SLS for generic and pounce-specific factorizations. See the specification sheet for the package GALAHAD\_SLS for details, and appropriate default values.

`FIT_control` is a scalar variable of type `FIT_control_type` whose components are used to control fitting of data to polynomials performed by the package GALAHAD\_FIT. See the specification sheet for the package GALAHAD\_FIT for details, and appropriate default values.

`ROOTS_control` is a scalar variable of type `ROOTS_control_type` whose components are used to control the polynomial root finding performed by the package GALAHAD\_ROOTS. See the specification sheet for the package GALAHAD\_ROOTS for details, and appropriate default values.

`CRO_control` is a scalar variable of type `CRO_control_type` whose components are used to control crossover performed by the package GALAHAD\_CRO. See the specification sheet for the package GALAHAD\_CRO for details, and appropriate default values.

#### 2.4.4 The derived data type for holding timing information

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

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

`preprocess` is a scalar variable of type `REAL(rp_)`, that gives the CPU time spent preprocess the problem prior to solution.

`find_dependent` is a scalar variable of type `REAL(rp_)`, that gives the CPU time spent detecting and removing dependent constraints prior to solution.

`analyse` is a scalar variable of type `REAL(rp_)`, that gives the CPU time spent analysing the required matrices prior to factorization.

`factorize` is a scalar variable of type `REAL(rp_)`, that gives the CPU time spent factorizing the required matrices.

`solve` is a scalar variable of type `REAL(rp_)`, that gives the CPU time spent computing the search direction.

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

`clock_preprocess` is a scalar variable of type `REAL(rp_)`, that gives the elapsed system clock time spent preprocess the problem prior to solution.

`clock_find_dependent` is a scalar variable of type `REAL(rp_)`, that gives the elapsed system clock time spent detecting and removing dependent constraints prior to solution.

`clock_analyse` is a scalar variable of type `REAL(rp_)`, that gives the elapsed system clock time spent analysing the required matrices prior to factorization.

`clock_factorize` is a scalar variable of type `REAL(rp_)`, that gives the elapsed system clock time spent factorizing the required matrices.

`clock_solve` is a scalar variable of type `REAL(rp_)`, that gives the elapsed system clock time spent computing the search direction.

#### 2.4.5 The derived data type for holding informational parameters

The derived data type `CLLS_inform_type` is used to hold parameters that give information about the progress and needs of the algorithm. The components of `CLLS_inform_type` are:

`status` is a scalar variable of type `INTEGER(ip_)`, that gives the exit status of the algorithm. See Section 2.6 for details.

`alloc_status` is a scalar variable of type `INTEGER(ip_)`, that gives the status of the last attempted array allocation or deallocation. This will be 0 if `status = 0`.

`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 `status = 0`.

`factorization_status` is a scalar variable of type `INTEGER(ip_)`, that gives the return status from the matrix factorization.

`factorization_integer` is a scalar variable of type long `INTEGER(ip_)`, that gives the amount of integer storage used for the matrix factorization.

`factorization_real` is a scalar variable of type `INTEGER(int64)`, that gives the amount of real storage used for the matrix factorization.

`nfacts` is a scalar variable of type `INTEGER(ip_)`, that gives the total number of factorizations performed.

`nbacts` is a scalar variable of type `INTEGER(ip_)`, that gives the total number of backtracks performed during the sequence of line searches.

`threads` is a scalar variable of type `INTEGER(ip_)`, that gives the total number of threads used for parallel execution.

`iter` is a scalar variable of type `INTEGER(ip_)`, that gives the number of iterations performed.

`obj` is a scalar variable of type `REAL(rp_)`, that holds the value of the objective function at the best estimate of the solution found.

`primal_infeasibility` is a scalar variable of type `REAL(rp_)`, that holds the norm of the violation of primal optimality (see Section 2.4.4) at the best estimate of the solution found.

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`dual_infeasibility` is a scalar variable of type `REAL(rp_)`, that holds the norm of the violation of dual optimality (see Section 2.4.4) at the best estimate of the solution found.

`complementary_slackness` is a scalar variable of type `REAL(rp_)`, that holds the norm of the violation of complementary slackness (see Section 2.4.4) at the best estimate of the solution found.

`non_negligible_pivot` is a scalar variable of type `REAL(rp_)`, that holds the value of the smallest pivot which was not judged to be zero when detecting linearly dependent constraints.

`feasible` is a scalar variable of type default `LOGICAL`, that has the value `.TRUE.` if the output value of `x` satisfies the constraints, and the value `.FALSE.` otherwise.

`time` is a scalar variable of type `CLLS_time_type` whose components are used to hold elapsed CPU and system clock times for the various parts of the calculation (see Section 2.4.4).

`FDC_inform` is a scalar variable of type `FDC_inform_type` whose components are used to provide information about any detection of linear dependencies performed by the package `GALAHAD_FDC`. See the specification sheet for the package `GALAHAD_FDC` for details.

`SLS_inform` and `SLS_pounce_inform` are scalar variables of type `SLS_inform_type` whose components are used to provide information about generic and pounce-specific factorizations performed by the package `GALAHAD_SLS`. See the specification sheet for the package `GALAHAD_SLS` for details.

`FIT_inform` is a scalar variable of type `FIT_inform_type` whose components are used to provide information about the fitting of data to polynomials performed by the package `GALAHAD_FIT`. See the specification sheet for the package `GALAHAD_FIT` for details.

`ROOTS_inform` is a scalar variable of type `ROOTS_inform_type` whose components are used to provide information about the polynomial root finding performed by the package `GALAHAD_ROOTS`. See the specification sheet for the package `GALAHAD_ROOTS` for details.

`CRO_inform` is a scalar variable of type `CRO_inform_type` whose components are used to provide information about the crossover performed by the package `GALAHAD_CRO`. See the specification sheet for the package `GALAHAD_CRO` for details.

#### 2.4.6 The derived data type for holding problem data

The derived data type `CLLS_data_type` is used to hold all the data for a particular problem, or sequences of problems with the same structure, between calls of `CLLS` procedures. This data should be preserved, untouched, from the initial call to `CLLS_initialize` to the final call to `CLLS_terminate`.

### 2.5 Argument lists and calling sequences

There are three procedures for user calls (see Section 2.7 for further features):

1. The subroutine `CLLS_initialize` is used to set default values, and initialize private data, before solving one or more problems with the same sparsity and bound structure.
2. The subroutine `CLLS_solve` is called to solve the problem.
3. The subroutine `CLLS_terminate` is provided to allow the user to automatically deallocate array components of the private data, allocated by `CLLS_solve`, at the end of the solution process.

We use square brackets [ ] to indicate `OPTIONAL` arguments.

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### 2.5.1 The initialization subroutine

Default values are provided as follows:

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

`data` is a scalar INTENT(INOUT) argument of type `CLLS_data_type` (see Section 2.4.6). It is used to hold data about the problem being solved.

`control` is a scalar INTENT(OUT) argument of type `CLLS_control_type` (see Section 2.4.3). On exit, `control` contains default values for the components as described in Section 2.4.3. These values should only be changed after calling `CLLS_initialize`.

`inform` is a scalar INTENT(OUT) argument of type `CLLS_inform_type` (see Section 2.4.5). A successful call to `CLLS_initialize` is indicated when the component status has the value 0. For other return values of status, see Section 2.6.

### 2.5.2 The least-squares subroutine

The constrained least-squares solution algorithm is called as follows:

```
CALL CLLS_solve( prob, data, control, inform[, regularization_weight, w] )
```

`prob` is a scalar INTENT(INOUT) argument of type `QPT_problem_type` (see Section 2.4.2). It is used to hold data about the problem being solved. The user must allocate all the array components, and set values for all components except `prob%C`.

The components `prob%X`, `prob%Y` and `prob%Z` must be set to initial estimates of the primal variables,  $\mathbf{x}$ , Lagrange multipliers,  $\mathbf{y}$ , for the general constraints and dual variables for the bound constraints,  $\mathbf{z}$ , respectively. Inappropriate initial values will be altered, so the user should not be overly concerned if suitable values are not apparent, and may be content with merely setting `prob%X=0.0`, `prob%Y=0.0` and `prob%Z=0.0`.

On exit, the components `prob%X`, `prob%C`, `prob%Y`, and `prob%Z` will contain the best estimates of the primal variables  $\mathbf{x}$ , the linear constraints  $\mathbf{Ax}$ , Lagrange multipliers,  $\mathbf{y}$ , for the general constraints and dual variables for the bound constraints  $\mathbf{z}$ , respectively. **Restrictions:** `prob%n > 0`, `prob%m ≥ 0`, `prob%Ao_type` and `prob%A_type`  $\in \{ \text{'DENSE', 'DENSE\_BY\_COLUMNS', 'COORDINATE', 'SPARSE\_BY\_ROWS', 'SPARSE\_BY\_COLUMNS'} \}$ .

`data` is a scalar INTENT(INOUT) argument of type `CLLS_data_type` (see Section 2.4.6). It is used to hold data about the problem being solved. It must not have been altered by the user since the last call to `CLLS_initialize`.

`control` is a scalar INTENT(IN) argument of type `CLLS_control_type` (see Section 2.4.3). Default values may be assigned by calling `CLLS_initialize` prior to the first call to `CLLS_solve`.

`inform` is a scalar INTENT(INOUT) argument of type `CLLS_inform_type` (see Section 2.4.5). A successful call to `CLLS_solve` is indicated when the component status has the value 0. For other return values of status, see Section 2.6.

`regularization_weight` is an OPTIONAL scalar variable of type `REAL(rp_)`, that holds the regularization weight,  $\sigma \geq 0$ . It need not be PRESENT if  $\sigma = 0$ .

`W` is an OPTIONAL rank-one allocatable array of dimension `o` and type `REAL(rp_)`, that holds the positive residual weights,  $w$ . If it is PRESENT, its  $i$ -th component must contain the value  $w_i$  for  $i = 1, \dots, o$ . If all the weights are one, `W` need not be PRESENT.

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### 2.5.3 The termination subroutine

All previously allocated arrays are deallocated as follows:

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

`data` is a scalar `INTENT (INOUT)` argument of type `CLLS_data_type` exactly as for `CLLS_solve`, which must not have been altered **by the user** since the last call to `CLLS_initialize`. On exit, array components will have been deallocated.

`control` is a scalar `INTENT (IN)` argument of type `CLLS_control_type` exactly as for `CLLS_solve`.

`inform` is a scalar `INTENT (OUT)` argument of type `CLLS_inform_type` exactly as for `CLLS_solve`. Only the component `status` will be set on exit, and a successful call to `CLLS_terminate` is indicated when this component `status` has the value 0. For other return values of `status`, see Section 2.6.

## 2.6 Warning and error messages

A negative value of `inform%status` on exit from `CLLS_solve` or `CLLS_terminate` 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  $\text{prob}\%n > 0$ ,  $\text{prob}\%o > 0$ ,  $\text{prob}\%m \geq 0$  the requirement that `prob%A_type` contain its relevant string 'DENSE', 'DENSE\_BY\_COLUMNS', 'COORDINATE', 'SPARSE\_BY\_ROWS' or 'SPARSE\_BY\_COLUMNS', has been violated.
- 4. The bound constraints are inconsistent.
- 5. The constraints appear to have no feasible point.
- 7. The objective function appears to be unbounded from below on the feasible set.
- 9. The analysis phase of the factorization failed; the return status from the factorization package is given in the component `inform%factor_status`.
- 10. The factorization failed; the return status from the factorization package is given in the component `inform%factor_status`.
- 16. The problem is so ill-conditioned that further progress is impossible.
- 17. The step is too small to make further impact.
- 18. Too many iterations have been performed. This may happen if `control%maxit` is too small, but may also be symptomatic of a badly scaled problem.
- 19. The elapsed CPU or system clock time limit has been reached. This may happen if either `control%cpu_time_limit` or `control%clock_time_limit` is too small, but may also be symptomatic of a badly scaled problem.

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## 2.7 Further features

In this section, we describe an alternative means of setting control parameters, that is components of the variable control of type `CLLS_control_type` (see Section 2.4.3), by reading an appropriate data specification file using the subroutine `CLLS_read_specfile`. This facility is useful as it allows a user to change CLLS control parameters without editing and recompiling programs that call CLLS.

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", which 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 specfile is limited to 80 characters, including the blanks separating keyword and value.

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

```
( .. lines ignored by CLLS_read_specfile .. )
BEGIN CLLS
    keyword    value
    .....
    keyword    value
END
( .. lines ignored by CLLS_read_specfile .. )
```

where keyword and value are two strings separated by (at least) one blank. The "BEGIN CLLS" 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 CLLS SPECIFICATION
```

and

```
END CLLS SPECIFICATION
```

are acceptable. Furthermore, between the "BEGIN CLLS" 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 manner to "comment out" some specification commands, or to comment specific values of certain control parameters.

The value of a control parameters may be of three different types, namely integer, logical or real. Integer and real values may be expressed in any relevant Fortran integer and floating-point formats (respectively). Permitted values for logical parameters are "ON", "TRUE", ".TRUE.", "T", "YES", "Y", or "OFF", "NO", "N", "FALSE", ".FALSE." and "F". Empty values are also allowed for logical control parameters, and are interpreted as "TRUE".

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

### 2.7.1 To read control parameters from a specification file

Control parameters may be read from a file as follows:

```
CALL CLLS_read_specfile( control, device )
```

---

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`control` is a scalar `INTENT(INOUT)` argument of type `CLLS_control_type` (see Section 2.4.3). Default values should have already been set, perhaps by calling `CLLS_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 Section 2.4.3) of `control` that each affects are given in Table 2.1.

| command                                   | component of control          | value type |
|-------------------------------------------|-------------------------------|------------|
| error-printout-device                     | %error                        | integer    |
| printout-device                           | %out                          | integer    |
| print-level                               | %print_level                  | integer    |
| maximum-number-of-iterations              | %maxit                        | integer    |
| start-print                               | %start_print                  | integer    |
| stop-print                                | %stop_print                   | integer    |
| indicator-type-used                       | %indicator_type               | integer    |
| arc-used                                  | %arc                          | integer    |
| series-order                              | %series_order                 | integer    |
| infinity-value                            | %infinity                     | real       |
| identical-bounds-tolerance                | %identical_bounds_tol         | real       |
| absolute-primal-accuracy                  | %stop_abs_p                   | real       |
| relative-primal-accuracy                  | %stop_rel_p                   | real       |
| absolute-dual-accuracy                    | %stop_abs_d                   | real       |
| relative-dual-accuracy                    | %stop_rel_d                   | real       |
| absolute-complementary-slackness-accuracy | %stop_abs_c                   | real       |
| relative-complementary-slackness-accuracy | %stop_rel_c                   | real       |
| initial-barrier-parameter                 | %muzero                       | real       |
| feasibility-vs-complementarity-weight     | %tao                          | real       |
| balance-complementarity-factor            | %gamma_c                      | real       |
| balance-feasibility-factor                | %gamma_f                      | real       |
| poor-iteration-tolerance                  | %reduce_infeas                | real       |
| identical-bounds-tolerance                | %identical_bounds_tol         | real       |
| required-barrier-value-before-pounce      | mu_pounce                     | real       |
| primal-indicator-tolerance                | %indicator_tol_p              | real       |
| primal-dual-indicator-tolerance           | %indicator_tol_pd             | real       |
| tapia-indicator-tolerance                 | %indicator_tol_tapia          | real       |
| maximum-cpu-time-limit                    | %cpu_time_limit               | real       |
| maximum-clock-time-limit                  | %clock_time_limit             | real       |
| remove-linear-dependencies                | %remove_dependencies          | logical    |
| treat-zero-bounds-as-general              | %treat_zero_bounds_as_general | logical    |
| just-find-feasible-point                  | %just_feasible                | logical    |
| puiseux-series                            | %puiseux                      | logical    |
| try-every-order-of-series                 | %every_order                  | logical    |
| cross-over-solution                       | %crossover                    | logical    |
| solve-reduced-pounce-system               | %reduced_pounce_system        | logical    |
| space-critical                            | %space_critical               | logical    |
| deallocate-error-fatal                    | %deallocate_error_fatal       | logical    |
| symmetric-linear-equation-solver          | %symmetric_linear_solver      | character  |
| output-line-prefix                        | %prefix                       | character  |

Table 2.1: Specfile commands and associated components of `control`.

`device` is a scalar `INTENT(IN)` argument of type `INTEGER(ip_)`, that must be set to the unit number on which the

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specfile 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.

## 2.8 Information printed

If control%print\_level is positive, information about the progress of the algorithm will be printed on unit control%out. If control%print\_level = 1, a single line of output will be produced for each iteration of the process. For the initial-feasible-point phase, this will include values of the current primal and dual infeasibility, and violation of complementary slackness, the feasibility-phase objective value, the current steplength, the value of the barrier parameter, the number of backtracks in the linesearch and the elapsed CPU time in seconds. Once a suitable feasible point has been found, the iteration is divided into major iterations, at which the barrier parameter is reduced, and minor iterations, and which the barrier function is approximately minimized for the current value of the barrier parameter. For the major iterations, the value of the barrier parameter, the required values of dual feasibility and violation of complementary slackness, and the current constraint infeasibility are reported. Each minor iteration of the optimality phase results in a line giving the current dual feasibility and violation of complementary slackness, the objective function value, the ratio of predicted to achieved reduction of the objective function, the trust-region radius, the number of backtracks in the linesearch, the number of conjugate-gradient iterations taken, and the elapsed CPU time in seconds.

If control%print\_level  $\geq 2$  this output will be increased to provide significant detail of each iteration. This extra output includes residuals of the linear systems solved, and, for larger values of control%print\_level, values of the primal and dual variables and Lagrange multipliers.

## 3 GENERAL INFORMATION

**Use of common:** None.

**Workspace:** Provided automatically by the module.

**Other routines called directly:** None.

**Other modules used directly:** CLLS\_solve calls the GALAHAD packages GALAHAD\_CLOCK, GALAHAD\_SYMBOLS, GALAHAD\_SPACE, GALAHAD\_TOOLS, GALAHAD\_SPECFILE, GALAHAD\_SMT, GALAHAD\_QPT, GALAHAD\_LSP, GALAHAD\_QPD, GALAHAD\_FIT, GALAHAD\_ROOTS, GALAHAD\_NORMS, GALAHAD\_SLS, GALAHAD\_CRO and GALAHAD\_FDC.

**Input/output:** Output is under control of the arguments control%error, control%out and control%print\_level.

**Restrictions:** prob%n > 0, , prob%o > 0, prob%m  $\geq$  0, prob%Ao-type and prob%A-type  $\in \{ \text{'DENSE'}, \text{'DENSE-BY-COLUMNS'}, \text{'COORDINATE'}, \text{'SPARSE-BY-ROWS'}, \text{'SPARSE-BY-COLUMNS'} \}$ .

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

## 4 METHOD

The required solution  $\mathbf{x}$  necessarily satisfies the primal optimality conditions

$$\mathbf{Ax} = \mathbf{c} \quad (4.1)$$

and

$$\mathbf{c}^l \leq \mathbf{c} \leq \mathbf{c}^u, \quad \mathbf{x}^l \leq \mathbf{x} \leq \mathbf{x}^u, \quad (4.2)$$

the dual optimality conditions

$$\mathbf{A}_o^T \mathbf{W}(\mathbf{A}_o \mathbf{x} - \mathbf{b}) + \sigma \mathbf{x} = \mathbf{A}^T \mathbf{y} + \mathbf{z}, \quad (4.3)$$

---

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where

$$\mathbf{y} = \mathbf{y}^l + \mathbf{y}^u, \mathbf{z} = \mathbf{z}^l + \mathbf{z}^u, \mathbf{y}^l \geq 0, \mathbf{y}^u \leq 0, \mathbf{z}^l \geq 0 \text{ and } \mathbf{z}^u \leq 0, \quad (4.4)$$

and the complementary slackness conditions

$$(\mathbf{Ax} - \mathbf{c}^l)^T \mathbf{y}^l = 0, (\mathbf{Ax} - \mathbf{c}^u)^T \mathbf{y}^u = 0, (\mathbf{x} - \mathbf{x}^l)^T \mathbf{z}^l = 0 \text{ and } (\mathbf{x} - \mathbf{x}^u)^T \mathbf{z}^u = 0, \quad (4.5)$$

where the diagonal matrix  $\mathbf{W}$  has diagonal entries  $w_i, i = 1, \dots, o$ , where the vectors  $\mathbf{y}$  and  $\mathbf{z}$  are known as the Lagrange multipliers for the general linear constraints, and the dual variables for the bounds, respectively, and where the vector inequalities hold component-wise.

Primal-dual interior point methods iterate towards a point that satisfies these conditions by ultimately aiming to satisfy (4.1), (4.3) and (4.5), while ensuring that (4.2) and (4.4) are satisfied as strict inequalities at each stage. Appropriate norms of the amounts by which (4.1), (4.3) and (4.5) fail to be satisfied are known as the primal and dual infeasibility, and the violation of complementary slackness, respectively. The fact that (4.2) and (4.4) are satisfied as strict inequalities gives such methods their other title, namely interior-point methods.

The method aims at each stage to reduce the overall violation of (4.1), (4.3) and (4.5), rather than reducing each of the terms individually. Given an estimate  $\mathbf{v} = (\mathbf{x}, \mathbf{c}, \mathbf{y}, \mathbf{y}^l, \mathbf{y}^u, \mathbf{z}, \mathbf{z}^l, \mathbf{z}^u)$  of the primal-dual variables, a correction  $\Delta \mathbf{v} = \Delta(\mathbf{x}, \mathbf{c}, \mathbf{y}, \mathbf{y}^l, \mathbf{y}^u, \mathbf{z}, \mathbf{z}^l, \mathbf{z}^u)$  is obtained by solving a suitable linear system of Newton equations for the nonlinear systems (4.1), (4.3) and a parameterized “residual trajectory” perturbation of (4.5); residual trajectories proposed by Zhang (1994) and Zhao and Sun (1999) are possibilities. An improved estimate  $\mathbf{v} + \alpha \Delta \mathbf{v}$  is then used, where the step-size  $\alpha$  is chosen as close to 1.0 as possible while ensuring both that (4.2) and (4.4) continue to hold and that the individual components which make up the complementary slackness (4.5) do not deviate too significantly from their average value. The parameter that controls the perturbation of (4.5) is ultimately driven to zero.

If the algorithm believes that it is close to the solution, it may take a speculative “pounce” extrapolation, based on an estimate of the ultimate active set, to avoid further costly iterations. If the pounce is unsuccessful, the iteration continues, but further pounces may be attempted later.

The Newton equations are solved by applying the GALAHAD matrix factorization package `GALAHAD_SLS`. Optionally, the problem may be pre-processed temporarily to eliminate dependent constraints using the package `GALAHAD_FDC`. This may improve the performance of the subsequent iteration.

## References:

The basic algorithm is a generalisation of those of

Y. Zhang (1994). On the convergence of a class of infeasible interior-point methods for the horizontal linear complementarity problem. *SIAM J. Optimization* **4** (1) 208-227,

and

G. Zhao and J. Sun (1999). On the rate of local convergence of high-order infeasible path-following algorithms for  $P_*$  linear complementarity problems. *Computational Optimization and Applications* **14** (1) 293-307,

with many enhancements described by

N. I. M. Gould, D. Orban and D. P. Robinson (2013). Trajectory-following methods for large-scale degenerate convex quadratic programming, *Mathematical Programming Computation* **5**(2) 113-142.

## 5 EXAMPLE OF USE

Suppose we wish to minimize

$$\frac{1}{2} \left\| \begin{pmatrix} x_1 + x_2 - 2 \\ x_2 + x_3 - 2 \\ x_1 + x_3 - 3 \\ \sqrt{2}(x_2 - 1) \end{pmatrix} \right\|^2$$

---

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subject to the general linear constraints  $1 \leq 2x_1 + x_2 \leq 2$  and  $x_2 + x_3 = 2$ , and simple bounds  $-1 \leq x_1 \leq 1$  and  $x_3 \leq 2$ . Then, on writing the data for this problem as

$$\mathbf{A}_o = \begin{pmatrix} 1 & 1 & \\ & 1 & 1 \\ 1 & & 1 \\ & & 1 \end{pmatrix}, \mathbf{b} = \begin{pmatrix} 2 \\ 2 \\ 3 \\ 1 \end{pmatrix}, \mathbf{w} = \begin{pmatrix} 1 \\ 1 \\ 1 \\ 2 \end{pmatrix}, \mathbf{x}^l = \begin{pmatrix} -1 \\ -\infty \\ -\infty \end{pmatrix}, \mathbf{x}^u = \begin{pmatrix} 1 \\ \infty \\ 2 \end{pmatrix}$$

and

$$\mathbf{A} = \begin{pmatrix} 2 & 1 & \\ & 1 & 1 \end{pmatrix}, \mathbf{c}^l = \begin{pmatrix} 1 \\ 2 \end{pmatrix}, \text{ and } \mathbf{c}^u = \begin{pmatrix} 2 \\ 2 \end{pmatrix}$$

in sparse co-ordinate format, we may use the following code:

```
! THIS VERSION: GALAHAD 4.2 - 2023-08-31 AT 10:15 GMT.
PROGRAM GALAHAD_CLLS_EXAMPLE
USE GALAHAD_CLLS_double          ! double precision version
IMPLICIT NONE
INTEGER, PARAMETER :: wp = KIND( 1.0D+0 ) ! set precision
REAL ( KIND = wp ), PARAMETER :: infinity = 10.0_wp ** 20
TYPE ( QPT_problem_type ) :: p
TYPE ( CLLS_data_type ) :: data
TYPE ( CLLS_control_type ) :: control
TYPE ( CLLS_inform_type ) :: inform
INTEGER :: s
INTEGER, PARAMETER :: n = 3, o = 4, m = 2, ao_ne = 7, a_ne = 4
REAL ( KIND = wp ), DIMENSION( o ) :: W
! start problem data
ALLOCATE( p%B( o ), p%R( o ) )
ALLOCATE( p%X_l( n ), p%X_u( n ) )
ALLOCATE( p%C_l( m ), p%C_u( m ) )
ALLOCATE( p%X( n ), p%Y( m ), p%Z( n ) )
ALLOCATE( p%C_status( m ), p%X_status( n ) )
p%new_problem_structure = .TRUE.          ! new structure
p%n = n ; p%o = o ; p%m = m ;           ! dimensions
p%B = (/ 2.0_wp, 2.0_wp, 3.0_wp, 1.0_wp /) ! observations
p%C_l = (/ 1.0_wp, 2.0_wp /)             ! constraint lower bound
p%C_u = (/ 2.0_wp, 2.0_wp /)             ! constraint upper bound
p%X_l = (/ -1.0_wp, -infinity, -infinity /) ! variable lower bound
p%X_u = (/ 1.0_wp, infinity, 2.0_wp /)    ! variable upper bound
p%X = 0.0_wp ; p%Y = 0.0_wp ; p%Z = 0.0_wp ! start from zero
W = (/ 1.0_wp, 1.0_wp, 1.0_wp, 1.0_wp /) ! weights
! sparse co-ordinate storage format
CALL SMT_put( p%Ao%type, 'COORDINATE', s ) ! Specify co-ordinate
CALL SMT_put( p%A%type, 'COORDINATE', s ) ! storage for Ao and A
ALLOCATE( p%Ao%row( ao_ne ), p%Ao%col( ao_ne ), p%Ao%val( ao_ne ) )
ALLOCATE( p%A%col( a_ne ), p%A%val( a_ne ), p%A%row( a_ne ) )
p%Ao%row = (/ 1, 1, 2, 2, 3, 3, 4 /) ; p%Ao%ne = ao_ne ! Ao
p%Ao%col = (/ 1, 2, 2, 3, 1, 3, 2 /)
p%Ao%val = (/ 1.0_wp, 1.0_wp, 1.0_wp, 1.0_wp, 1.0_wp, 1.0_wp, 1.0_wp /)
p%A%row = (/ 1, 1, 2, 2 /) ; p%A%ne = a_ne ! A
p%A%col = (/ 1, 2, 2, 3 /)
p%A%val = (/ 2.0_wp, 1.0_wp, 1.0_wp, 1.0_wp /)
! problem data complete
CALL CLLS_initialize( data, control, inform ) ! Initialize control parameters
control%symmetric_linear_solver = 'sytr '
```

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```

control%FDC_control%symmetric_linear_solver = 'sytr '
control%infinity = infinity          ! Set infinity
CALL CLLS_solve( p, data, control, inform, W = W ) ! Solve
IF ( inform%status == 0 ) THEN      ! Successful return
    WRITE( 6, "( ' CLLS: ', I0, ' iterations ', /,
    &      ' Optimal objective value =',
    &      ES12.4, /, ' Optimal solution = ', ( 5ES12.4 ) )" )
    inform%iter, inform%obj, p%X
ELSE
    ! Error returns
    WRITE( 6, "( ' CLLS_solve exit status = ', I6 ) " ) inform%status
END IF
CALL CLLS_terminate( data, control, inform ) ! delete internal workspace
END PROGRAM GALAHAD_CLLS_EXAMPLE

```

This produces the following output:

```

CLLS: 9 iterations
Optimal objective value =  6.7857E-01
Optimal solution =   7.8571E-01  4.2857E-01  1.5714E+00

```

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

```

! sparse co-ordinate storage format
...
! problem data complete

```

by

```

! sparse row-wise storage format
CALL SMT_put( p%Ao%type, 'SPARSE_BY_ROWS', s ) ! Specify sparse row
CALL SMT_put( p%A%type, 'SPARSE_BY_ROWS', s ) ! storage for Ao and A
ALLOCATE( p%Ao%col( ao_ne ), p%Ao%ptr( o + 1 ), p%Ao%val( ao_ne ) )
ALLOCATE( p%A%col( a_ne ), p%A%ptr( m + 1 ), p%A%val( a_ne ) )
p%Ao%col = (/ 1, 2, 2, 3, 1, 3, 2 /) ! design matrix Ao
p%Ao%ptr = (/ 1, 3, 5, 7, 8 /)
p%Ao%val = (/ 1.0_wp, 1.0_wp, 1.0_wp, 1.0_wp, 1.0_wp, 1.0_wp, 1.0_wp /)
p%A%col = (/ 1, 2, 2, 3 /) ! Jacobian A
p%A%ptr = (/ 1, 3, 5 /)
p%A%val = (/ 2.0_wp, 1.0_wp, 1.0_wp, 1.0_wp /)
! problem data complete

```

or using a dense storage format with the replacement lines

```

! dense storage format
CALL SMT_put( p%Ao%type, 'DENSE', s ) ! Specify dense
CALL SMT_put( p%A%type, 'DENSE', s ) ! storage for Ao and A
ALLOCATE( p%Ao%val( o * n ), p%A%val( n * m ) )
p%Ao%val = (/ 1.0_wp, 1.0_wp, 0.0_wp, 0.0_wp, 1.0_wp, 1.0_wp, &
    1.0_wp, 0.0_wp, 1.0_wp, 0.0_wp, 1.0_wp, 0.0_wp /) ! Ao
p%A%val = (/ 2.0_wp, 1.0_wp, 0.0_wp, 0.0_wp, 1.0_wp, 1.0_wp /) ! A
! problem data complete

```

respectively.

---

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