





# **GALAHAD**

**QPC** 

USER DOCUMENTATION

GALAHAD Optimization Library version 4.1

#### 1 SUMMARY

This package uses a crossover method, switching between interior-point and working-set approaches, to solve the **quadratic programming problem** 

minimize 
$$q(\mathbf{x}) = \frac{1}{2}\mathbf{x}^T\mathbf{H}\mathbf{x} + \mathbf{g}^T\mathbf{x} + f$$

subject to the general linear constraints

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

and the simple bound constraints

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

where the *n* by *n* symmetric matrix **H**, the vectors  $\mathbf{g}$ ,  $\mathbf{a}_i$ ,  $\mathbf{c}^l$ ,  $\mathbf{c}^u$ ,  $\mathbf{x}^l$ ,  $\mathbf{x}^u$  and the scalar *f* are given. Full advantage is taken of any zero coefficients in the matrix **H** or the vectors  $\mathbf{a}_i$ . Any of the constraint bounds  $c_i^l$ ,  $c_i^u$ ,  $x_i^l$  and  $x_i^u$  may be infinite.

If the matrix **H** is positive semi-definite, a global solution is found. However, if **H** is indefinite, the procedure may find a (weak second-order) critical point that is not the global solution to the given problem.

ATTRIBUTES — Versions: GALAHAD\_QPC\_single, GALAHAD\_QPC\_double. Uses: GALAHAD\_CLOCK, GALAHAD\_SYMBOLS, GALAHAD\_SPACE, GALAHAD\_NORMS, GALAHAD\_SORT, GALAHAD\_QPT, GALAHAD\_QPP, GALAHAD\_QPD, GALAHAD\_EQP, GALAHAD\_LSQP, GALAHAD\_LSQP, GALAHAD\_QPA, GALAHAD\_QPB, GALAHAD\_SPECFILE, GALAHAD\_FDC. Date: March 2006. Origin: N. I. M. Gould, Rutherford Appleton Laboratory, and Ph. L. Toint, University of Namur, Belgium. Language: Fortran 95 + TR 15581 or Fortran 2003. Parallelism: Some options may use OpenMP and its runtime library.

# 2 HOW TO USE THE PACKAGE

Access to the package requires a USE statement such as

Single precision version

USE GALAHAD\_OPC\_single

Double precision version

USE GALAHAD\_QPC\_double

If it is required to use both modules at the same time, the derived types SMT\_type, QPT\_problem\_type, QPC\_time\_type, QPC\_control\_type, QPC\_inform\_type and QPC\_data\_type (Section 2.4) and the subroutines QPC\_initialize, QPC\_solve, QPC\_terminate, (Section 2.5) and QPC\_read\_specfile (Section 2.7) must be renamed on one of the USE statements.

# 2.1 Matrix storage formats

Both the Hessian matrix **H** and the constraint Jacobian **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.

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#### 2.1.1 Dense storage format

The matrix **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  $i=1,\ldots,m,\ j=1,\ldots,n$ . Since **H** is symmetric, only the lower triangular part (that is the part  $h_{ij}$  for  $1 \le j \le i \le n$ ) need be held. In this case the lower triangle will be stored by rows, that is component i\*(i-1)/2+j of the storage array H%val will hold the value  $h_{ij}$  (and, by symmetry,  $h_{ji}$ ) for  $1 \le j \le i \le n$ .

### 2.1.2 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. The same scheme is applicable to  $\mathbf{H}$  (thus requiring integer arrays H%row, H%col, a real array H%val and an integer value H%ne), except that only the entries in the lower triangle need be stored.

### 2.1.3 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  $\mathsf{A\$ptr}$  holds the position of the first entry in this row, while  $\mathsf{A\$ptr}$  (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  $l = \mathsf{A\$ptr}(i), \ldots, \mathsf{A\$ptr}(i+1) - 1$  of the integer array  $\mathsf{A\$col}$ , and real array  $\mathsf{A\$val}$ , respectively. The same scheme is applicable to  $\mathbf H$  (thus requiring integer arrays  $\mathsf{H\$ptr}$ ,  $\mathsf{H\$col}$ , and a real array  $\mathsf{H\$val}$ ), except that only the entries in the lower triangle need be stored.

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

#### 2.1.4 Diagonal storage format

If **H** is diagonal (i.e.,  $h_{ij} = 0$  for all  $1 \le i \ne j \le n$ ) only the diagonals entries  $h_{ii}$ ,  $1 \le i \le n$ , need be stored, and the first n components of the array H%val may be used for the purpose. There is no sensible equivalent for the non-square **A**.

# 2.2 Integer kinds

We use the term long INTEGER to denote INTEGER (kind=long), where long = selected\_int\_kind(18)).

# 2.3 Parallel usage

OpenMP may be used by the GALAHAD\_QPC 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 <code>-openmp</code>). The number of threads may be controlled at runtime by setting the environment variable <code>OMP\_NUM\_THREADS</code>.

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 <code>-lmpi</code>). 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.

#### 2.4 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 A and H. The components of SMT\_TYPE used here are:

- m is a scalar component of type default INTEGER, that holds the number of rows in the matrix.
- n is a scalar component of type default INTEGER, that holds the number of columns in the matrix.
- ne is a scalar variable of type default INTEGER, 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).
- is a rank-one allocatable array of type default REAL (double precision in GALAHAD\_QPC\_double) and dimension at least ne, that holds the values of the entries. Each pair of off-diagonal entries  $h_{ij} = h_{ji}$  of a *symmetric* matrix **H** is represented as a single entry (see §2.1.1–2.1.3). 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 default INTEGER, and dimension at least ne, that may hold the row indices of the entries. (see §2.1.2).
- is a rank-one allocatable array of type default INTEGER, and dimension at least ne, that may the column indices of the entries (see §2.1.2–2.1.3).
- ptr is a rank-one allocatable array of type default INTEGER, and dimension at least m + 1, that may hold the pointers to the first entry in each row (see §2.1.3).

# 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:

- new\_problem\_structure is a scalar variable of type default LOGICAL, that is .TRUE. if this is the first (or only) problem in a sequence of problems with identical "structure" to be attempted, and .FALSE. if a previous problem with the same "structure" (but different numerical data) has been solved. Here, the term "structure" refers both to the sparsity patterns of the Jacobian matrices  $\bf A$  involved (but not their numerical values), to the zero/nonzero/infinity patterns (a bound is either zero,  $\pm$  infinity, or a finite but arbitrary nonzero) of each of the constraint bounds, and to the variables and constraints that are fixed (both bounds are the same) or free (the lower and upper bounds are  $\pm$  infinity, respectively).
- n is a scalar variable of type default INTEGER, that holds the number of optimization variables, n.
- m is a scalar variable of type default INTEGER, that holds the number of general linear constraints, m.
- H is scalar variable of type SMT\_TYPE that holds the Hessian matrix **H**. The following components are used:
  - H%type is an allocatable array of rank one and type default CHARACTER, that is used to indicate the storage scheme used. If the dense storage scheme (see Section 2.1.1) is used, the first five components of H%type must contain the string DENSE. For the sparse co-ordinate scheme (see Section 2.1.2), the first ten components of H%type must contain the string COORDINATE, for the sparse row-wise storage scheme (see Section 2.1.3), the first fourteen components of H%type must contain the string SPARSE\_BY\_ROWS, and for

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the diagonal storage scheme (see Section 2.1.4), the first eight components of H%type must contain the string DIAGONAL.

For convenience, the procedure SMT\_put may be used to allocate sufficient space and insert the required keyword into H%type. For example, if prob is of derived type QPC\_problem\_type and involves a Hessian we wish to store using the co-ordinate scheme, we may simply

```
CALL SMT_put( prob%H%type, 'COORDINATE' )
```

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

- H%ne is a scalar variable of type default INTEGER, that holds the number of entries in the **lower triangular** part of **H** in the sparse co-ordinate storage scheme (see Section 2.1.2). It need not be set for any of the other three schemes.
- H%val is a rank-one allocatable array of type default REAL (double precision in GALAHAD\_QPC\_double), that holds the values of the entries of the **lower triangular** part of the Hessian matrix **H** in any of the storage schemes discussed in Section 2.1.
- H%row is a rank-one allocatable array of type default INTEGER, that holds the row indices of the **lower triangular** part of **H** in the sparse co-ordinate storage scheme (see Section 2.1.2). It need not be allocated for any of the other three schemes.
- H%col is a rank-one allocatable array variable of type default INTEGER, that holds the column indices of the **lower triangular** part of **H** in either the sparse co-ordinate (see Section 2.1.2), or the sparse row-wise (see Section 2.1.3) storage scheme. It need not be allocated when the dense or diagonal storage schemes are used.
- H%ptr is a rank-one allocatable array of dimension n+1 and type default INTEGER, that holds the starting position of each row of the **lower triangular** part of **H**, as well as the total number of entries plus one, in the sparse row-wise storage scheme (see Section 2.1.3). It need not be allocated when the other schemes are used.
- is a rank-one allocatable array of dimension n and type default REAL (double precision in GALAHAD\_QPC\_double), that holds the gradient  $\mathbf{g}$  of the linear term of the quadratic objective function. The j-th component of  $\mathbf{G}$ ,  $j=1,\ldots,n$ , contains  $\mathbf{g}_j$ .
- is a scalar variable of type default REAL (double precision in GALAHAD\_QPC\_double), that holds the constant term, f, in the objective function.
- A is scalar variable of type SMT\_TYPE that holds the Jacobian matrix 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 storage scheme (see Section 2.1.1) is used, the first five components of A\*type must contain the string DENSE. For the sparse co-ordinate scheme (see Section 2.1.2), the first ten components of A\*type must contain the string COORDINATE, while for the sparse row-wise storage scheme (see Section 2.1.3), the first fourteen components of A\*type must contain the string SPARSE\_BY\_ROWS.

Just as for H%type above, the procedure SMT\_put may be used to allocate sufficient space and insert the required keyword into A%type. Once again, if prob is of derived type QPC\_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' )
```

- A%ne is a scalar variable of type default INTEGER, that holds the number of entries in  $\bf A$  in the sparse co-ordinate storage scheme (see Section 2.1.2). It need not be set for either of the other two schemes.
- A&val is a rank-one allocatable array of type default REAL (double precision in GALAHAD\_QPC\_double), that holds the values of the entries of the Jacobian matrix **A** in any of the storage schemes discussed in Section 2.1.

- Afrow is a rank-one allocatable array of type default INTEGER, that holds the row indices of **A** in the sparse coordinate storage scheme (see Section 2.1.2). It need not be allocated for either of the other two schemes.
- A%col is a rank-one allocatable array variable of type default INTEGER, that holds the column indices of **A** in either the sparse co-ordinate (see Section 2.1.2), or the sparse row-wise (see Section 2.1.3) storage scheme. It need not be allocated when the dense storage scheme is used.
- A%ptr is a rank-one allocatable array of dimension m+1 and type default INTEGER, 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 2.1.3). It need not be allocated when the other schemes are used.
- C\_1 is a rank-one allocatable array of dimension m and type default REAL (double precision in GALAHAD\_QPC\_double), that holds the vector of lower bounds  $\mathbf{c}^l$  on the general constraints. The *i*-th component of C\_1,  $i = 1, \ldots, m$ , contains  $\mathbf{c}^l_i$ . Infinite bounds are allowed by setting the corresponding components of C\_1 to any value smaller than -infinity, where infinity is a component of the control array control (see Section 2.4.7).
- C\_u is a rank-one allocatable array of dimension m and type default REAL (double precision in GALAHAD\_QPC\_double), that holds the vector of upper bounds  $\mathbf{c}^u$  on the general constraints. The *i*-th component of C\_u,  $i = 1, \ldots, m$ , contains  $\mathbf{c}^u_i$ . 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 2.4.7).
- is a rank-one allocatable array of dimension n and type default REAL (double precision in GALAHAD\_QPC\_double), that holds the vector of lower bounds  $\mathbf{x}^l$  on the the variables. The j-th component of X\_1,  $j=1,\ldots,n$ , contains  $\mathbf{x}^l_j$ . Infinite bounds are allowed by setting the corresponding components of X\_1 to any value smaller than -infinity, where infinity is a component of the control array control (see Section 2.4.7).
- X\_u is a rank-one allocatable array of dimension n and type default REAL (double precision in GALAHAD\_QPC\_double), that holds the vector of upper bounds  $\mathbf{x}^u$  on the variables. The *j*-th component of X\_u,  $j = 1, \ldots, n$ , contains  $\mathbf{x}^u_j$ . 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 2.4.7).
- is a rank-one allocatable array of dimension n and type default REAL (double precision in GALAHAD\_QPC\_double), that holds the values  $\mathbf{x}$  of the optimization variables. The j-th component of X, j = 1, ..., n, contains  $x_j$ .
- is a rank-one allocatable array of dimension n and type default REAL (double precision in GALAHAD\_QPC\_double), that holds the values **z** of estimates of the dual variables corresponding to the simple bound constraints (see Section 4). The *j*-th component of  $\mathbb{Z}$ ,  $j = 1, \ldots, n$ , contains  $z_j$ .
- is a rank-one allocatable array of dimension m and type default REAL (double precision in GALAHAD\_QPC\_double), that holds the values  $\mathbf{A}\mathbf{x}$  of the constraints. The *i*-th component of  $\mathbb{C}$ , i = 1, ..., m, contains  $\mathbf{a}_i^T \mathbf{x} \equiv (\mathbf{A}\mathbf{x})_i$ .
- Y is a rank-one allocatable array of dimension m and type default REAL (double precision in GALAHAD\_QPC\_double), 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, ..., m, contains  $y_i$ .

# 2.4.3 The derived data type for holding control parameters specifically for the interior-point phase

The derived data type QPB\_control\_type is used to hold controlling data for the interior-point phase of the calculation, performed by the GALAHAD package GALAHAD\_QPB. Components may be changed by calling QPB\_read\_specfile (see the documentation for GALAHAD\_QPB for details). The components of QPB\_control\_type are:

- error is a scalar variable of type default INTEGER, that holds the stream number for error messages. Printing of error messages in QPB\_solve and QPB\_terminate is suppressed if error  $\leq 0$ . The default is error = 6.
- out is a scalar variable of type default INTEGER, that holds the stream number for informational messages. Printing of informational messages in QPB\_solve is suppressed if out < 0. The default is out = 6.

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print\_level is a scalar variable of type default INTEGER, 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.

- start\_print is a scalar variable of type default INTEGER, that specifies the first iteration for which printing will occur in QPB\_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 default INTEGER, that specifies the last iteration for which printing will occur in QPB\_solve. If stop\_print is negative, printing will occur once it has been started by start\_print. The default is stop\_print = -1.
- maxit is a scalar variable of type default INTEGER, that holds the maximum number of iterations which will be allowed in QPB\_solve. The default is maxit = 1000.
- infeas\_max is a scalar variable of type default INTEGER, 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.
- cg\_maxit is a scalar variable of type default INTEGER, that holds the maximum number of conjugate-gradient inner iterations that may be performed during the computation of each search direction in QPB\_solve. If cg\_maxit is set to a negative number, it will be reset by QPB\_solve to the dimension of the relevant linear system +1. The default is cg\_maxit = 200.
- indicator\_type is a scalar variable of type default INTEGER, that specifies the type of indicator used to assess when a variable or constraint is active. Possible values are:
  - 1 a variable/constraint is active if and only if the distance to its neaerest bound is no larger than indicator\_tol\_p (see below).
  - 2 a variable/constraint is active if and only if the distance to its neaerest bound is no larger than indicator\_tol-\_pd (see below) times the magnitude of its corresponding dual variable.
  - 3 a variable/constraint is active if and only if the distance to its neaerest 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.

- restore\_problem is a scalar variable of type default INTEGER, that specifies how much of the input problem is to be retored on output. Possible values are:
  - 0 nothing is restored.
  - 1 the vector data  $\mathbf{g}, \mathbf{c}^l, \mathbf{c}^u, \mathbf{x}^l$ , and  $\mathbf{x}^u$  will be restored to their input values.
  - 2 the entire problem, that is the above vector data along with the Hessian matrix **H** and the Jacobian matrix **A**, will be restored.

The default is restore\_problem = 2.

- extrapolate is a scalar variable of type default INTEGER, that specifies whether extrapolation should be used to track the central path. Possible values are:
  - 0 no extrapolation should be used.
  - 1 extrapolation should be used after the final update of the barrier parameter.
  - 2 extrapolation should be used after each update of the barrier parameter.

- The default is extrapolate = 2.
- path\_history is a scalar variable of type default INTEGER, that specifies the maximum number of previous path points used when extrapolating to track the central path. The default is path\_history = 1.
- path\_derivatives is a scalar variable of type default INTEGER, that specifies the maximum order of derivatives to use when extrapolating to track the central path. The default is path\_derivatives = 5.
- fit\_order is a scalar variable of type default INTEGER, that specifies the order of (Puiseux or Taylor) series to fit to the available data when building the extrapolant to track the central path. If fit\_order  $\leq 0$ , the order will be such that all available data as specified by path\_history and path\_derivatives will be used. The default is fit\_order = -1.
- infinity is a scalar variable of type default REAL (double precision in GALAHAD\_QPC\_double), 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 =  $10^{19}$ .
- stop\_p is a scalar variable of type default REAL (double precision in GALAHAD\_QPC\_double), that holds the required accuracy for the primal infeasibility (see Section 4). The default is stop\_p =  $u^{1/3}$ , where u is EPSILON(1.0) (EPSILON(1.0D0) in GALAHAD\_QPC\_double).
- stop\_d is a scalar variable of type default REAL (double precision in GALAHAD\_QPC\_double), that holds the required accuracy for the dual infeasibility (see Section 4). The default is stop\_d =  $u^{1/3}$ , where u is EPSILON(1.0) (EPSILON(1.0D0) in GALAHAD\_QPC\_double).
- stop\_c is a scalar variable of type default REAL (double precision in GALAHAD\_QPC\_double), that holds the required accuracy for the violation of complementarity slackness (see Section 4). The default is stop\_c =  $u^{1/3}$ , where u is EPSILON(1.0) (EPSILON(1.0D0) in GALAHAD\_QPC\_double).
- prfeas is a scalar variable of type default REAL (double precision in GALAHAD\_QPC\_double), 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 = 1.0.
- dufeas is a scalar variable of type default REAL (double precision in GALAHAD\_QPC\_double), 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 = 1.0.
- muzero is a scalar variable of type default REAL (double precision in GALAHAD\_QPC\_double), 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.
- reduce\_infeas is a scalar variable of type default REAL (double precision in GALAHAD\_QPC\_double), 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.
- obj\_unbounded is a scalar variable of type default REAL (double precision in GALAHAD\_QPC\_double), that specifies smallest value of the objective function that will be tolerated before the problem is declared to be unbounded from below. The default is obj\_unbounded =  $-u^{-2}$ , where u is EPSILON(1.0) (EPSILON(1.0D0) in GALAHAD\_QPC\_double).
- identical\_bounds\_tol is a scalar variable of type default REAL (double precision in GALAHAD\_QPC\_double). 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\_QPC\_double).

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indicator\_tol\_p is a scalar variable of type default REAL (double precision in GALAHAD\_QPC\_double)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\_QPC\_double).

- indicator\_tol\_pd is a scalar variable of type default REAL (double precision in GALAHAD\_QPC\_double)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 default REAL (double precision in GALAHAD\_QPC\_double)that provides the indicator tolerance associated with the test indicator\_type = 3. The default is indicator\_tol\_tapia = 0.9.
- inner\_stop\_relative and inner\_stop\_absolute are scalar variables of type default REAL (double precision in GALAHAD\_QPC\_double), that hold the relative and absolute convergence tolerances for the inner iteration (search direction) problem using the package GALAHAD\_GLTR, and correspond to the values control%stop\_relative and control%stop\_absolute in that package. The defaults are inner\_stop\_relative = 0.01 and inner\_stop\_absolute =  $\sqrt{u}$ , where u is EPSILON(1.0) (EPSILON(1.0D0) in GALAHAD\_QPC\_double).
- initial\_radius is a scalar variable of type default REAL (double precision in GALAHAD\_QPC\_double), that specifies the initial trust-region radius. If initial\_radius is not positive, it will be reset automatically to an appropriate value. The default is initial\_radius = -1.0.
- inner\_fraction\_opt is a scalar variable of type default REAL (double precision in GALAHAD\_QPC\_double), that specifies the fraction of the optimal value which is acceptable for the solution of the inner iteration (search direction) problem using the package GALAHAD\_GLTR, and corresponds to the value control%fraction\_opt in that package. A negative value is considered to be zero, and a value of larger than one is considered to be one. Reducing fraction\_opt below one will result in a reduction of the computation performed at the expense of an inferior optimal value. The default is inner\_fraction\_opt = 0.1.
- cpu\_time\_limit is a scalar variable of type default REAL (double precision in GALAHAD\_QPC\_double), 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 default REAL (double precision in GALAHAD\_QPC\_double), 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\_QPC 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..
- center is a scalar variable of type default LOGICAL, that must be set .TRUE. if the algorithm will should use the analytic center of the feasible set as its initial feasible point, and .FALSE. otherwise. We recommend using the analytic center. The default is center = .TRUE..

- primal is a scalar variable of type default LOGICAL, that must be set .TRUE. if a primal-barrier Hessian will be used and .FALSE. if the primal-dual Hessian is preferred. We recommend using the primal-dual Hessian. The default is primal = .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..
- 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..
- 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 = "".
- LSQP\_control is a scalar variable of type LSQP\_control\_type whose components are used to control the initial feasible point calculation performed by the package GALAHAD\_LSQP. See the specification sheet for the package GALAHAD\_LSQP for details, and appropriate default values (but note that default value for LSQP\_control%feasol is changed to .FALSE..
- 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.
- SBLS\_control is a scalar variable of type SBLS\_control\_type whose components are used to control preconditioning, needed to accelerate the step calculation, performed by the package GALAHAD\_SBLS. See the specification sheet for the package GALAHAD\_SBLS for details, and appropriate default values (but note that if SBLS\_control%preconditioner = 5, the diagonal matrix used is corresponds to replacing the Hesian matrix by its barrier terms).
- GLTR\_control is a scalar variable of type GLTR\_control\_type whose components are used to control the step calculation performed by the package GALAHAD\_GLTR. See the specification sheet for the package GALAHAD\_GLTR for details, and appropriate default values.

# 2.4.4 The derived data type for holding control parameters specifically for the interior-point phase in the convex case

The derived data type CQP\_control\_type is used to hold controlling data for the interior-point phase of the calculation for convex problems, performed by the GALAHAD package GALAHAD\_CQP. Components may be changed by calling CQP\_read\_specfile (see the documentation for GALAHAD\_CQP for details). The components of CQP\_control\_type are:

- error is a scalar variable of type default INTEGER, that holds the stream number for error messages. Printing of error messages in QPC\_solve and QPC\_terminate is suppressed if error  $\leq 0$ . The default is error = 6.
- out is a scalar variable of type default INTEGER, that holds the stream number for informational messages. Printing of informational messages in QPC\_solve is suppressed if out < 0. The default is out = 6.
- print\_level is a scalar variable of type default INTEGER, 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.

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maxit is a scalar variable of type default INTEGER, that holds the maximum number of iterations which will be allowed in OPC\_solve. The default is maxit = 1000.

- start\_print is a scalar variable of type default INTEGER, that specifies the first iteration for which printing will occur in QPC\_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 default INTEGER, that specifies the last iteration for which printing will occur in QPC\_solve. If stop\_print is negative, printing will occur once it has been started by start\_print. The default is stop\_print = -1.
- infeas\_max is a scalar variable of type default INTEGER, 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 default INTEGER, that specifies the number of iterations before the initial barrier parameter (see muzero) may be altered. The default is muzero\_fixed = 1.
- indicator\_type is a scalar variable of type default INTEGER, that specifies the type of indicator used to assess when a variable or constraint is active. Possible values are:
  - 1 a variable/constraint is active if and only if the distance to its neaerest bound is no larger than indicator—tol-p (see below).
  - 2 a variable/constraint is active if and only if the distance to its neaerest bound is no larger than indicator—tol\_pd (see below) times the magnitude of its corresponding dual variable.
  - 3 a variable/constraint is active if and only if the distance to its neaerest 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 default INTEGER, 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 default INTEGER, 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 default REAL (double precision in GALAHAD\_QPC\_double), 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 =  $10^{19}$ .
- stop\_abs\_p and stop\_rel\_p are scalar variables of type default REAL (double precision in GALAHAD\_QPC\_double), 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\_QPC\_double).

- stop\_abs\_d and stop\_rel\_d are scalar variables of type default REAL (double precision in GALAHAD\_QPC\_double), 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\_QPC\_double).
- stop\_abs\_c and stop\_rel\_c are scalar variables of type default REAL (double precision in GALAHAD\_QPC\_double), 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\_QPC\_double).
- perturb\_h is a scalar variable of type default REAL (double precision in GALAHAD\_QPC\_double), that specifies any perturbation that is to be added to the diagonal of **H**. The default is perturb\_h = 0.0.
- prfeas is a scalar variable of type default REAL (double precision in GALAHAD\_QPC\_double), 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<sup>4</sup>.
- dufeas is a scalar variable of type default REAL (double precision in GALAHAD\_QPC\_double), 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<sup>4</sup>.
- muzero is a scalar variable of type default REAL (double precision in GALAHAD\_QPC\_double), 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 default REAL (double precision in GALAHAD\_QPC\_double), 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 default REAL (double precision in GALAHAD\_QPC\_double), 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 default REAL (double precision in GALAHAD\_QPC\_double), 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 default REAL (double precision in GALAHAD\_QPC\_double), 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.
- obj\_unbounded is a scalar variable of type default REAL (double precision in GALAHAD\_QPC\_double), that specifies smallest value of the objective function that will be tolerated before the problem is declared to be unbounded from below. The default is obj\_unbounded =  $-u^{-2}$ , where u is EPSILON(1.0) (EPSILON(1.0D0) in GALAHAD\_QPC\_double).
- potential\_unbounded is a scalar variable of type default REAL (double precision in GALAHAD\_QPC\_double), that specifies smallest value of the potential function divided by the number of one-sided variable and constraint bounds that will be tolerated before the analytic center is declared to be unbounded. The default is potential\_unbounded = -10.0.

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identical\_bounds\_tol is a scalar variable of type default REAL (double precision in GALAHAD\_QPC\_double). 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\_QPC\_double).

- indicator\_tol\_p is a scalar variable of type default REAL (double precision in GALAHAD\_QPC\_double)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\_QPC\_double).
- indicator\_tol\_pd is a scalar variable of type default REAL (double precision in GALAHAD\_QPC\_double)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 default REAL (double precision in GALAHAD\_QPC\_double)that provides the indicator tolerance associated with the test indicator\_type = 3. The default is indicator\_tol\_tapia = 0.9.
- cpu\_time\_limit is a scalar variable of type default REAL (double precision in GALAHAD\_QPC\_double), 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 default REAL (double precision in GALAHAD\_QPC\_double), 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\_QPC 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..
- 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..
- 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..
- 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..
- 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.
- SBLS\_control is a scalar variable of type SBLS\_control\_type whose components are used to control factorizations performed by the package GALAHAD\_SBLS. See the specification sheet for the package GALAHAD\_SBLS 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.

# 2.4.5 The derived data type for holding control parameters specifically for the working-set phase

The derived data type <code>QPA\_control\_type</code> is used to hold controlling data for the working-set phase of the calculation performed by the GALAHAD package <code>GALAHAD\_QPA</code>. Components may be changed by calling <code>QPA\_read\_specfile</code> (see the documentation for <code>GALAHAD\_QPA</code> for details). The components of <code>QPA\_control\_type</code> are:

- error is a scalar variable of type default INTEGER, that holds the stream number for error messages. Printing of error messages in QPA\_solve and QPA\_terminate is suppressed if error  $\leq 0$ . The default is error = 6.
- out is a scalar variable of type default INTEGER, that holds the stream number for informational messages. Printing of informational messages in QPA\_solve is suppressed if out < 0. The default is out = 6.
- print\_level is a scalar variable of type default INTEGER, 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.

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maxit is a scalar variable of type default INTEGER, that holds the maximum number of iterations which will be allowed in OPA\_solve. The default is maxit = 1000.

- start\_print is a scalar variable of type default INTEGER, that specifies the first iteration for which printing will occur in QPA\_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 default INTEGER, that specifies the last iteration for which printing will occur in QPA\_solve. If stop\_print is negative, printing will occur once it has been started by start\_print. The default is stop\_print = -1.
- factor is a scalar variable of type default INTEGER, that indicates the type of factorization of the preconditioner to be used. Possible values are:
  - 0 the type is chosen automatically on the basis of which option looks likely to be the most efficient.
  - 1 a Schur-complement factorization will be used.
  - 2 an augmented-system factorization will be used.

The default is factor = 0.

- max\_col is a scalar variable of type default INTEGER, that specifies the maximum number of nonzeros in a column of **A** which is permitted by the Schur-complement factorization. The default is max\_col = 35.
- max\_sc is a scalar variable of type default INTEGER, that specifies the maximum number of columns permitted in the Schur complement of the reference matrix (see Section 4) before a refactorization is triggered. The default is max\_sc = 75.
- itref\_max is a scalar variable of type default INTEGER, that specifies the maximum number of iterative refinements allowed with each application of the preconditioner. The default is itref\_max = 1.
- cg\_maxit is a scalar variable of type default INTEGER, that holds the maximum number of conjugate-gradient inner iterations that may be performed during the computation of each search direction in QPA\_solve. If cg\_itmax is set to a negative number, it will be reset by QPA\_solve to the dimension of the relevant linear system +1. The default is cg\_itmax = -1.
- precon is a scalar variable of type default INTEGER, that specifies which preconditioner to be used to accelerate the conjugate-gradient inner iteration. Possible values are:
  - 0 the type is chosen automatically on the basis of which option looks likely to be the most efficient at any given stage of the solution process. Different preconditioners may be used at different stages.
  - 1 a full factorization using the Hessian, which is equivalent to replacing the conjugate gradient inner iteration by a direct method. The Hessian may be perturbed to ensure that the resultant matrix is a preconditioner.
  - 2 the Hessian matrix is replaced by the identity matrix.
  - 3 the Hessian matrix is replaced by a band of given semi-bandwidth (see nsemib below).
  - 4 the Hessian matrix terms in the current reference matrix (see Section 4) are replaced by the identity matrix.
  - 5 the Hessian matrix terms outside a band of given semi-bandwidth in the current reference matrix are replaced by zeros (see nsemib below).

The default is precon = 0.

nsemib is a scalar variable of type default INTEGER, that specifies the semi-bandwidth of the band preconditioner when precon = 3, if appropriate. The default is nsemib = 5.

- full\_max\_fill is a scalar variable of type default INTEGER. If the ratio of the number of nonzeros in the factors of the reference matrix (see Section 4) to the number of nonzeros in the matrix itself exceeds full\_max\_fil, and the preconditioner is being selected automatically (precon = 0), a banded approximation (see precon = 3) will be used instead. The default is full\_max\_fill = 10.
- deletion\_strategy is a scalar variable of type default INTEGER, that specifies the rules used to determine which constraint to remove from the working set (see Section 4) when necessary to ensure further progress towards the solution. Possible values are:
  - 0 the constraint whose Lagrange multiplier most violates its required optimality bound will be removed.
  - 1 the most-recently added constraint whose Lagrange multiplier violates its required optimality bound will be removed.
  - k > 1 among the k most-recently added constraints whose Lagrange multipliers violates their required optimality bounds, the one which most violates its bound will be removed.

The default is deletion\_strategy = 0.

- restore\_problem is a scalar variable of type default INTEGER, that specifies how much of the input problem is to be retored on output. Possible values are:
  - 0 nothing is restored.
  - 1 the vector data  $\mathbf{g}$ ,  $\mathbf{c}^l$ ,  $\mathbf{c}^u$ ,  $\mathbf{x}^l$ , and  $\mathbf{x}^u$  will be restored to their input values.
  - 2 the entire problem, that is the above vector data along with the Hessian matrix **H** and the Jacobian matrix **A**, will be restored.

The default is restore\_problem = 2.

- monitor\_residuals is a scalar variable of type default INTEGER, that specifies the frequency at which working constraint residuals will be monitored to ensure feasibility. The residuals will be monitored every monitor\_residual at iterations. The default is monitor\_residuals = 1.
- cold\_start is a scalar variable of type default INTEGER, that controls the initial working set (see Section 4)). Possible values are:
  - 0 a "warm start" will be performed. The values set in C\_stat and B\_stat indicate which constraints will be included in the initial working set. (see C\_stat and B\_stat in Section 2.5.2).
  - 1 the constraints "active" at p%X (see Section 2.5.2) will determine the initial working set.
  - 2 the initial working set will be empty.
  - 3 the initial working set will only contain equality constraints.
  - 4 the initial working set will contain as many active constraints as possible, chosen (in order) from equality constraints, simple bounds, and finally general linear constraints.

The default is cold\_start = 3.

- infeas\_check\_interval is a scalar variable of type default INTEGER, that gives the number of iterations that are permitted before the infeasibility is checked for improvement. The default is infeas\_check\_interval = 100.
- infinity is a scalar variable of type default REAL (double precision in GALAHAD\_QPC\_double), 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 =  $10^{19}$ .
- feas\_tol is a scalar variable of type default REAL (double precision in GALAHAD\_QPC\_double), that specifies the maximum amount by which a constraint may be violated and yet still be considered to be satisfied. The default is feas\_tol =  $u^{3/4}$ , where u is EPSILON(1.0) (EPSILON(1.0D0) in GALAHAD\_QPC\_double).

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obj\_unbounded is a scalar variable of type default REAL (double precision in GALAHAD\_QPC\_double), that specifies smallest value of the objective function that will be tolerated before the problem is declared to be unbounded from below. The default is potential\_unbounded =  $-u^{-2}$ , where u is EPSILON(1.0) (EPSILON(1.0D0) in GALAHAD\_QPC\_double).

- increase\_rho\_g\_factor is a scalar variable of type default REAL (double precision in GALAHAD\_QPC\_double), that gives the factor by which the current penalty parameter  $\rho_g$  for the general constraints may be increased when solving quadratic programs. The default is increase\_rho\_g\_factor = 2.
- increase\_rho\_b\_factor is a scalar variable of type default REAL (double precision in GALAHAD\_QPC\_double), that gives the factor by which the current penalty parameter  $\rho_b$  for the simple bound constraints may be increased when solving quadratic programs. The default is increase\_rho\_b\_factor = 2.
- infeas\_g\_improved\_by\_factor is a scalar variable of type default REAL (double precision in GALAHAD\_QPC\_double), that specifies the relative improvement in the infeasibility that must be achieved when solving quadratic programs if the current value of  $\rho_g$  is to be maintained. Specifically if the infeasibility of the general constraints has not fallen by at least a factor infeas\_g\_improved\_by\_factor during the previous infeas\_check\_interval iterations, the penalty parameter will be increased by a factor increase\_rho\_g\_factor. The default is infeas\_improved\_q\_by\_factor = 0.75.
- infeas\_b\_improved\_by\_factor is a scalar variable of type default REAL (double precision in GALAHAD\_QPC\_double), that specifies the relative improvement in the infeasibility that must be achieved when solving quadratic programs if the current value of  $\rho_b$  is to be maintained. Specifically if the infeasibility of the simple bound constraints has not fallen by at least a factor infeas\_b\_improved\_by\_factor during the previous infeas\_check\_interval iterations, the penalty parameter will be increased by a factor increase\_rho\_b\_factor. The default is infeas\_improved\_b\_by\_factor = 0.75.
- pivot\_tol\_for\_dependencies is a scalar variable of type default REAL (double precision in GALAHAD\_QPC\_double), that holds the relative threshold pivot tolerance used by the matrix factorization when attempting to detect linearly dependent constraints. A value larger than pivot\_tol is appropriate. See the documentation for the package SLS for details. The default is pivot\_tol\_for\_dependencies = 0.5.
- multiplier\_tol is a scalar variable of type default REAL (double precision in GALAHAD\_QPC\_double). Any dual variable or Lagrange multiplier which is less than multiplier\_tol outside its optimal interval will be regarded as being acceptable when checking for optimality. The default is zero\_pivot =  $\sqrt{u}$ , where u is EPSILON(1.0) (EPSILON(1.0D0) in GALAHAD\_QPC\_double).
- inner\_stop\_relative and inner\_stop\_absolute are scalar variables of type default REAL (double precision in GALAHAD\_QPC\_double), that hold the relative and absolute convergence tolerances for the inner iteration (search direction) problem. and correspond to the values control%stop\_relative and control%stop\_absolute in the GALAHAD package GALAHAD\_GLTR. The defaults are inner\_stop\_relative = 0.0 and inner\_stop\_absolute =  $\sqrt{u}$ , where u is EPSILON(1.0) (EPSILON(1.0D0) in GALAHAD\_QPC\_double).
- cpu\_time\_limit is a scalar variable of type default REAL (double precision in GALAHAD\_QPC\_double), 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 default REAL (double precision in GALAHAD\_QPC\_double), 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.
- 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  $x_i^l$  or  $x_i^u$

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\_QPC 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..

- ramdomize is a scalar variable of type default LOGICAL, that must be set .TRUE. if the user wishes to perturb the constraint bounds by small random quantities during the first stage of the solution process, and .FALSE. otherwise. Any randomization will ultimately be removed. Randomization helps when solving degenerate problems and is usually to be recommended. The default is randomize = .TRUE..
- 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'.
- definite\_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 positive-definite linear system that might arise. Current possible choices are 'sils', 'ma27', 'ma57', 'ma77', 'ma86', 'ma87', '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 definite\_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 = "".
- SLS\_control is a scalar variable argument of type SLS\_control\_type that is used to pass control options to external packages used to factorize relevant symmetric matrices that arise. See the documentation for the GALAHAD package SLS for further details. In particular, default values are as for SLS, except that SLS\_control%relative\_pivot\_tolerance is reset to pivot\_tol.

# 2.4.6 The derived data type for holding control parameters specifically for the equality-constrained phase

The derived data type EQP\_control\_type is used to hold controlling data for the equality-constrained QP phase of the calculation (if any), performed by the GALAHAD package GALAHAD\_EQP. Components may be changed by calling EQP\_read\_specfile (see the documentation for GALAHAD\_EQP for details). The components of EQP\_control\_type are:

- error is a scalar variable of type default INTEGER, that holds the stream number for error messages. Printing of error messages in QPC\_solve and QPC\_terminate is suppressed if error  $\leq 0$ . The default is error = 6.
- out is a scalar variable of type default INTEGER, that holds the stream number for informational messages. Printing of informational messages in QPC\_solve is suppressed if out < 0. The default is out = 6.
- print\_level is a scalar variable of type default INTEGER, 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.

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new\_h is a scalar variable of type default INTEGER, that is used to indicate how **H** has changed (if at all) since the previous call to QPC\_solve. Possible values are:

- 0 H is unchanged
- 1 the values in **H** have changed, but its nonzero structure is as before.
- 2 both the values and structure of **H** have changed.

The default is new\_h = 2.

- new\_a is a scalar variable of type default INTEGER, that is used to indicate how A has changed (if at all) since the previous call to QPC\_solve. Possible values are:
  - 0 A is unchanged
  - 1 the values in **A** have changed, but its nonzero structure is as before.
  - 2 both the values and structure of **A** have changed.

The default is new\_a = 2.

- cg\_maxit is a scalar variable of type default INTEGER, that is used to limit the number of conjugate-gradient iterations performed in the optimality phase. If cg\_maxit is negative, no limit will be impossed. The default is cg\_maxit = 200.
- radius is a scalar variable of type default REAL (double precision in GALAHAD\_QPC\_double), that may be used to specify an upper bound on the norm of the allowed solution (a "trust-region" constraint) during the iterative solution of the optimality phase of the problem. This is particularly useful if the problem is unbounded from below. If radius is set too small, there is a possibility that this will preclude the package from finding the actual solution. If initial\_radius is not positive, it will be reset to the default value, initial\_radius = SQRT(0.1\*HUGE(1.0)) (SQRT(0.1\*HUGE(1.0D0)) in GALAHAD\_QPC\_double).
- inner\_stop\_relative and inner\_stop\_absolute are scalar variables of type default REAL (double precision in GALAHAD\_QPC\_double), that hold the relative and absolute convergence tolerances for the iterative solution of the optimality phase of the problem using the package GALAHAD\_GLTR, and correspond to the values control%stop\_relative and control%stop\_absolute in that package. The defaults are inner\_stop\_relative = 0.01 and inner\_stop\_absolute =  $\sqrt{u}$ , where u is EPSILON(1.0) (EPSILON(1.0D0) in GALAHAD\_QPC\_double).
- max\_infeasibility\_relative and max\_infeasibility\_absolute are scalar variables of type default REAL (double precision in GALAHAD\_QPC\_double), that hold the relative and absolute tolerances for assessing infeasibility in the feasibility phase. If the constraints are believed to be rank defficient and the norm of the residual  $\mathbf{A}\mathbf{x}_T + \mathbf{c}$  at a "typical" feasiblke point is larger than  $\max(\max_i nfeasibility_relative*||A||, \max_i nfeasibility_absolute)$ , the problem will be marked as infeasible, The defaults are  $\max_i nfeasibility_relative = \max_i nfeasibility_absolute = <math>u^{0.75}$  where u is EPSILON(1.0) (EPSILON(1.000) in  $\text{GALAHAD\_QPC\_double}$ ).
- remove\_dependencies is a scalar variable of type default LOGICAL, that must be set .TRUE. if linear dependent constraints Ax + c = 0 should be removed and .FALSE. otherwise. The default is remove\_dependencies = .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..
- 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..

- 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.
- GLTR\_control is a scalar variable argument of type GLTR\_control\_type that is used to pass control options to the conjugate-gradient solver used to solve linear systems that arise. See the documentation for the GALAHAD package GLTR for further details. In particular, default values are as for GLTR.
- SBLS\_control is a scalar variable argument of type SBLS\_control\_type that is used to pass control options to the symmetric block linear equation preconditioner used to help solve linear systems that arise. See the documentation for the GALAHAD package SBLS for further details. In particular, default values are as for SBLS.
- 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 ignoreing 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 = "".

## 2.4.7 The derived data type for holding control parameters

The derived data type QPC\_control\_type is used to hold controlling data. Default values may be obtained by calling QPC\_initialize (see Section 2.5.1), while components may also be changed by calling QPC\_read\_specfile (see Section 2.7.1). The components of QPC\_control\_type are:

- error is a scalar variable of type default INTEGER, that holds the stream number for error messages. Printing of error messages in QPC\_solve and QPC\_terminate is suppressed if error  $\leq 0$ . The default is error = 6.
- out is a scalar variable of type default INTEGER, that holds the stream number for informational messages. Printing of informational messages in QPC\_solve is suppressed if out < 0. The default is out = 6.
- print\_level is a scalar variable of type default INTEGER, 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.
- restore\_problem is a scalar variable of type default INTEGER, that specifies how much of the input problem is to be retored on output. Possible values are:
  - 0 nothing is restored.
  - 1 the vector data  $\mathbf{g}, \mathbf{c}^l, \mathbf{c}^u, \mathbf{x}^l$ , and  $\mathbf{x}^u$  will be restored to their input values.
  - 2 the entire problem, that is the above vector data along with the Hessian matrix **H** and the Jacobian matrix **A**, will be restored.

The default is restore\_problem = 2.

- infinity is a scalar variable of type default REAL (double precision in GALAHAD\_QPC\_double), 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 =  $10^{19}$ .
- identical\_bounds\_tol is a scalar variable of type default REAL (double precision in GALAHAD\_QPC\_double). 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\_QPC\_double).

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rho\_g is a scalar variable of type default REAL (double precision in GALAHAD\_QPC\_double), that holds the initial values of the parameter,  $\rho_g$ , used to weight the infeasibility term  $v_g(\mathbf{x})$  for the working-set phase (see Section 4).

- rho\_b is a scalar variable of type default REAL (double precision in GALAHAD\_QPC\_double), that holds the initial values of the parameter,  $\rho_b$ , used to weight the infeasibility term  $v_b(\mathbf{x})$  for the working-set phase (see Section 4).
- on\_bound\_tol is a scalar variable of type default REAL (double precision in GALAHAD\_QPC\_double)that specifies the furthest a variable or constraint may be from one of its bounds to be regarded as active. The default is on\_bound\_tol = u, where u is EPSILON(1.0) (EPSILON(1.0D0) in GALAHAD\_QPC\_double).
- cpu\_time\_limit is a scalar variable of type default REAL (double precision in GALAHAD\_QPC\_double), 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 default REAL (double precision in GALAHAD\_QPC\_double), 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.
- convex is a scalar variable of type default LOGICAL, that must be set .TRUE. if the problem is convex (i.e., if the matrix **H** is positive semi-definite) and the user wishes to take advantage of the fact, and .FALSE. otherwise. The package will usually run faster for convex problems if convex is .TRUE., but convex must be set .FALSE. if the user is uncertain as otherwise the package may fail. The default is convex = .FALSE.
- 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\_QPC 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..
- 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..
- 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..
- no\_qpa is a scalar variable of type default LOGICAL, that must be set .TRUE. if the user wishes to skip the working-set phase of the computation, and .FALSE. if this phase is required. The default is no\_qpa = .FALSE..
- no\_qpb is a scalar variable of type default LOGICAL, that must be set .TRUE. if the user wishes to skip the interior-point phase of the computation, and .FALSE. if this phase is required. The default is no\_qpa = .FALSE..
- qpb\_or\_qpa is a scalar variable of type default LOGICAL, that must be set .TRUE. if the user wishes to use the interiorpoint phase of the computation, but only to follow this with the working-set phase if the former is unsuccessful,
  and to .FALSE. if both phases are to be used (subject to the requests made in no\_qpa and no\_qpb). The default
  is qpb\_or\_qpa = .FALSE..
- 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 = "".

- QPA\_control is a scalar variable of type QPA\_control\_type (see Section 2.4.5 whose components are used to control the working-set phase of the calculation, performed by the package GALAHAD\_QPA.
- QPB\_control is a scalar variable of type QPB\_control\_type (see Section 2.4.3 whose components are used to control the interior-point phase of the calculation, performed by the package GALAHAD\_QPB.
- CQP\_control is a scalar variable of type CQP\_control\_type (see Section 2.4.4 whose components are used to control the convex primal-dual phase of the calculation, performed by the package GALAHAD\_CQP.
- EQP\_control is a scalar variable of type EQP\_control\_type (see Section 2.4.6 whose components are used to control the equality-constrained phase of the calculation (if any), performed by the package GALAHAD\_EQP.
- 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.

# 2.4.8 The derived data type for holding timing information

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

- total is a scalar variable of type default REAL (double precision in GALAHAD\_QPC\_double), that gives the total CPU time spent in the package.
- preprocess is a scalar variable of type default REAL (double precision in GALAHAD\_QPC\_double), that gives the CPU time spent reordering the problem to standard form prior to solution.
- find\_dependent is a scalar variable of type default REAL (double precision in GALAHAD\_QPC\_double), that gives the CPU time spent detecting and removing linearly-dependent equality constraints
- analyse is a scalar variable of type default REAL (double precision in GALAHAD\_QPC\_double), that gives the CPU time spent analysing the required matrices prior to factorization.
- factorize is a scalar variable of type default REAL (double precision in GALAHAD\_QPC\_double), that gives the CPU time spent factorizing the required matrices.
- solve is a scalar variable of type default REAL (double precision in GALAHAD\_QPC\_double), that gives the CPU time spent computing the search direction.
- clock\_total is a scalar variable of type default REAL (double precision in GALAHAD\_QPC\_double), that gives the total elapsed system clock time spent in the package.
- clock\_preprocess is a scalar variable of type default REAL (double precision in GALAHAD\_QPC\_double), that gives the elapsed system clock time spent reordering the problem to standard form prior to solution.
- clock\_find\_dependent is a scalar variable of type default REAL (double precision in GALAHAD\_QPC\_double), that gives the elapsed system clock time spent detecting and removing linearly-dependent equality constraints
- clock\_analyse is a scalar variable of type default REAL (double precision in GALAHAD\_QPC\_double), that gives the elapsed system clock time spent analysing the required matrices prior to factorization.
- clock\_factorize is a scalar variable of type default REAL (double precision in GALAHAD\_QPC\_double), that gives the elapsed system clock time spent factorizing the required matrices.
- clock\_solve is a scalar variable of type default REAL (double precision in GALAHAD\_QPC\_double), that gives the elapsed system clock time spent computing the search direction.

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## 2.4.9 The derived data type for holding informational parameters specifically for the interior-point phase

The derived data type QPB\_inform\_type is used to hold parameters that give information about the progress of the working-set phase of the algorithm performed by the GALAHAD package GALAHAD\_QPB. The components of QPB\_inform\_type are:

- status is a scalar variable of type default INTEGER, that gives the exit status of the algorithm. See Section 2.6 for details
- alloc\_status is a scalar variable of type default INTEGER, 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.
- iter is a scalar variable of type default INTEGER, that gives the total number of iterations required.
- factorization\_status is a scalar variable of type default INTEGER, that gives the return status from the matrix factorization.
- factorization\_integer is a scalar variable of type long INTEGER, that gives the amount of integer storage used for the matrix factorization.
- factorization\_real is a scalar variable of type long INTEGER, that gives the amount of real storage used for the matrix factorization.
- nfacts is a scalar variable of type default INTEGER, that gives the total number of factorizations performed.
- nbacts is a scalar variable of type default INTEGER, that gives the total number of backtracks performed during the sequence of linesearches.
- nmods is a scalar variable of type default INTEGER, that gives the total number of factorizations which were modified to ensure that the matrix is an appropriate preconditioner.
- obj is a scalar variable of type default REAL (double precision in GALAHAD\_QPC\_double), that holds the value of the objective function at the best estimate of the solution found.
- non\_negligible\_pivot is a scalar variable of type default REAL (double precision in GALAHAD\_QPC\_double), that holds the value of the smallest pivot larger than control%zero\_pivot when searching for dependent linear constraints. If non\_negligible\_pivot is close to control%zero\_pivot, this may indicate that there are further dependent constraints, and it may be worth increasing control%zero\_pivot above non\_negligible\_pivot and solving again.
- feasible is a scalar variable of type default LOGICAL, that has the value . TRUE. if the output value of  $\boldsymbol{x}$  satisfies the constraints, and the value . FALSE. otherwise.
- time is a scalar variable of type QPC\_time\_type whose components are used to hold elapsed CPU and system clock times for the various parts of the calculation (see Section 2.4.8).
- LSQP\_inform is a scalar variable of type LSQP\_inform\_type whose components are used to provide information about the initial feasible point calculation performed by the package GALAHAD\_LSQP. See the specification sheet for the package GALAHAD\_LSQP for details, and appropriate default values.
- 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.

- SBLS\_inform is a scalar variable of type SBLS\_inform\_type whose components are used to provide information about factorizations performed by the package GALAHAD\_SBLS. See the specification sheet for the package GALAHAD\_SBLS for details.
- GLTR\_inform is a scalar variable of type GLTR\_inform\_type whose components are used to provide information about the step calculation performed by the package GALAHAD\_GLTR. See the specification sheet for the package GALAHAD\_GLTR for details.

# 2.4.10 The derived data type for holding informational parameters specifically for the interior-point phase in the convex case

The derived data type CQP\_inform\_type is used to hold parameters that give information about the progress of the working-set phase of the algorithm performed by the GALAHAD package GALAHAD\_CQP. The components of CQP\_inform\_type are:

- status is a scalar variable of type default INTEGER, that gives the exit status of the algorithm. See Section 2.6 for details
- alloc\_status is a scalar variable of type default INTEGER, 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 default INTEGER, that gives the return status from the matrix factorization.
- factorization\_integer is a scalar variable of type long INTEGER, that gives the amount of integer storage used for the matrix factorization.
- factorization\_real is a scalar variable of type long INTEGER, that gives the amount of real storage used for the matrix factorization.
- nfacts is a scalar variable of type default INTEGER, that gives the total number of factorizations performed.
- nbacts is a scalar variable of type default INTEGER, that gives the total number of backtracks performed during the sequence of linesearches.
- threads is a scalar variable of type default INTEGER, that gives the total number of threads used for parallel execution.
- iter is a scalar variable of type default INTEGER, that gives the number of iterations performed.
- obj is a scalar variable of type default REAL (double precision in GALAHAD\_QPC\_double), that holds the value of the objective function at the best estimate of the solution found.
- primal\_infeasibility is a scalar variable of type default REAL (double precision in GALAHAD\_QPC\_double), that holds the norm of the violation of primal optimality (see Section 2.4.8) at the best estimate of the solution found.
- dual\_infeasibility is a scalar variable of type default REAL (double precision in GALAHAD\_QPC\_double), that holds the norm of the violation of dual optimality (see Section 2.4.8) at the best estimate of the solution found.
- complementary\_slackness is a scalar variable of type default REAL (double precision in GALAHAD\_QPC\_double), that holds the norm of the violation of complementary slackness (see Section 2.4.8) at the best estimate of the solution found.

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

- time is a scalar variable of type QPC\_time\_type whose components are used to hold elapsed CPU and system clock times for the various parts of the calculation (see Section 2.4.8).
- 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.
- SBLS\_inform is a scalar variable of type SBLS\_inform\_type whose components are used to provide information about factorizations performed by the package GALAHAD\_SBLS. See the specification sheet for the package GALAHAD\_SBLS 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.

# 2.4.11 The derived data type for holding informational parameters specifically from the working-set phase

The derived data type <code>QPA\_inform\_type</code> is used to hold parameters that give information about the progress of the working-set phase of the algorithm performed by the GALAHAD package <code>GALAHAD\_QPA</code>. The components of <code>QPA\_inform\_type</code> are:

- status is a scalar variable of type default INTEGER, that gives the exit status of the algorithm. See Section 2.6 for details
- alloc\_status is a scalar variable of type default INTEGER, 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.
- major\_iter is a scalar variable of type default INTEGER, that gives the total number of major iterations required.
- iter is a scalar variable of type default INTEGER, that gives the total number of iterations required.
- cg\_iter is a scalar variable of type default INTEGER, that gives the total number of conjugate-gradient inner iterations required.
- factorization\_status is a scalar variable of type default INTEGER, that gives the return status from the matrix factorization.
- factorization\_integer is a scalar variable of type long INTEGER, that gives the amount of integer storage used for the matrix factorization.
- factorization\_real is a scalar variable of type long INTEGER, that gives the amount of real storage used for the matrix factorization.

- nfacts is a scalar variable of type default INTEGER, that gives the total number of factorizations performed.
- nmods is a scalar variable of type default INTEGER, that gives the total number of factorizations which were modified to ensure that the matrix is an appropriate preconditioner.
- num\_g\_infeas is a scalar variable of type default INTEGER, that gives the total number of general constraints that are violated.
- num\_b\_infeas is a scalar variable of type default INTEGER, that gives the total number of simple bound constraints that are violated.
- obj is a scalar variable of type default REAL (double precision in GALAHAD\_QPC\_double), that holds the value of the objective function at the best estimate of the solution found.
- infeas\_g is a scalar variable of type default REAL (double precision in GALAHAD\_QPC\_double), that holds the value of the infeasibility  $v_g(\mathbf{x})$ .
- infeas\_b is a scalar variable of type default REAL (double precision in GALAHAD\_QPC\_double), that holds the value of the infeasibility  $v_b(\mathbf{x})$ .
- merit is a scalar variable of type default REAL (double precision in GALAHAD\_QPC\_double), that holds the value of the merit function  $q(\mathbf{x}) + \rho_{\varrho} v_{\varrho}(\mathbf{x}) + \rho_{b} v_{b}(\mathbf{x})$  at the best estimate of the solution found.
- time is a scalar variable of type QPC\_time\_type whose components are used to hold elapsed CPU and system clock times for the various parts of the calculation (see Section 2.4.8).
- SLS\_inform is a scalar variable argument of type SLS\_inform\_type that is used to pass information concerning the progress of the external packages used to factorize relevant symmetric matrices that arise. See the documentation for the GALAHAD package SLS for further details.

# 2.4.12 The derived data type for holding informational parameters specifically for the equality-constrained phase

The derived data type EQP\_inform\_type is used to hold parameters that give information about the progress of the equality-constrained phase of the algorith (if any) performed by the GALAHAD package GALAHAD\_EQP. The components of EQP\_inform\_type are:

- status is a scalar variable of type default INTEGER, that gives the exit status of the algorithm. See Section 2.6 for details.
- alloc\_status is a scalar variable of type default INTEGER, 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.
- cg\_iter is a scalar variable of type default INTEGER, that gives the total number of conjugate-gradient iterations required.
- factorization\_integer is a scalar variable of type long INTEGER, that gives the amount of integer storage used for the matrix factorization.
- factorization\_real is a scalar variable of type long INTEGER, that gives the amount of real storage used for the matrix factorization.
- obj is a scalar variable of type default REAL (double precision in GALAHAD\_QPC\_double), that holds the value of the objective function at the best estimate of the solution found.

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time is a scalar variable of type QPC\_time\_type whose components are used to hold elapsed CPU and system clock times for the various parts of the calculation (see Section 2.4.8).

- 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.
- SBLS\_inform is a scalar variable of type SBLS\_inform\_type whose components are used to hold information relating to the formation and factorization of the preconditioner. See the documentation for the GALAHAD package SBLS for further details.
- GLTR\_inform is a scalar variable of type GLTR\_inform\_type whose components are used to hold information relating to the computation of the solution via the conjugate-gradient method. See the documentation for the GALAHAD package GLTR for further details.

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

The derived data type QPC\_inform\_type is used to hold parameters that give information about the progress and needs of the algorithm. The components of QPC\_inform\_type are:

- status is a scalar variable of type default INTEGER, that gives the exit status of the algorithm. See Section 2.6 for details.
- alloc\_status is a scalar variable of type default INTEGER, 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 default INTEGER, that gives the return status from the matrix factorization.
- factorization\_integer is a scalar variable of type long INTEGER, that gives the amount of integer storage used for the matrix factorization.
- factorization\_real is a scalar variable of type long INTEGER, that gives the amount of real storage used for the matrix factorization.
- nfacts is a scalar variable of type default INTEGER, that gives the total number of factorizations performed.
- nmods is a scalar variable of type default INTEGER, that gives the total number of factorizations which were modified to ensure that the matrix is an appropriate preconditioner.
- obj is a scalar variable of type default REAL (double precision in GALAHAD\_QPC\_double), that holds the value of the objective function at the best estimate of the solution found.
- non\_negligible\_pivot is a scalar variable of type default REAL (double precision in GALAHAD\_QPC\_double), that holds the value of the smallest pivot larger than control%zero\_pivot when searching for dependent linear constraints. If non\_negligible\_pivot is close to control%zero\_pivot, this may indicate that there are further dependent constraints, and it may be worth increasing control%zero\_pivot above non\_negligible\_pivot and solving again.
- p\_found is a scalar variable of type default LOGICAL, that has the value . TRUE. if the active-set predictions have been computed, and the value . FALSE. otherwise.

- time is a scalar variable of type QPC\_time\_type whose components are used to hold elapsed CPU and system clock times for the various parts of the calculation (see Section 2.4.8).
- QPA\_inform is a scalar variable of type QPA\_inform\_type (see Section 2.4.11 whose components provide information about the progress and needs of the working-set phase of the calculation performed by the package GALAH-AD\_QPA.
- QPB\_inform is a scalar variable of type QPB\_inform\_type (see Section 2.4.9 whose components provide information about the progress and needs of the interior-point phase of the calculation performed by the package GALAH-AD\_QPB.
- CQP\_inform is a scalar variable of type CQP\_inform\_type (see Section 2.4.10 whose components provide information about the progress and needs of the primal-dual phase of the calculation performed by the package GALAHAD\_CQP.
- EQP\_inform is a scalar variable of type EQP\_inform\_type (see Section 2.4.12 whose components provide information about the progress and needs of the equality-constrained phase of the calculation (if any) performed by the package GALAHAD\_EQP.
- 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.

# 2.4.14 The derived data type for holding problem data

The derived data type QPC\_data\_type is used to hold all the data for a particular problem, or sequences of problems with the same structure, between calls of QPC procedures. This data should be preserved, untouched, from the initial call to QPC\_initialize to the final call to QPC\_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 QPC\_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 QPC\_solve is called to solve the problem.
- 3. The subroutine QPC\_terminate is provided to allow the user to automatically deallocate array components of the private data, allocated by QPC\_solve, at the end of the solution process. It is important to do this if the data object is re-used for another problem with a different structure since QPC\_initialize cannot test for this situation, and any existing associated targets will subsequently become unreachable.

We use square brackets [ ] to indicate OPTIONAL arguments.

# 2.5.1 The initialization subroutine

Default values are provided as follows:

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

- data is a scalar INTENT (INOUT) argument of type QPC\_data\_type (see Section 2.4.14). It is used to hold data about the problem being solved.
- control is a scalar INTENT (OUT) argument of type QPC\_control\_type (see Section 2.4.7). On exit, control contains default values for the components as described in Section 2.4.7. These values should only be changed after calling QPC\_initialize.

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inform is a scalar INTENT (OUT) argument of type QPC\_inform\_type (see Section 2.4.13). A successful call to QPC\_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 quadratic programming subroutine

The quadratic programming solution algorithm is called as follows:

```
CALL QPC_solve(p, C_stat, B_stat, data, control, inform)
```

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. For a new problem, the user must allocate all the array components, and set values for all components except p%C. p%new\_problem\_structure must be set .TRUE., but will have been reset to .FALSE. on exit from QPC\_solve. Users are free to choose whichever of the matrix formats described in Section 2.1 is appropriate for A and H for their application—different formats may be used for the two matrices.

For a problem with the same structure as one that has just been solved, the user may set p%new\_problem\_structure to .FALSE., so long as QPC\_terminate has not been called in the interim. The INTEGER components must be unaltered since the previous call to QPC\_solve, but the REAL (double precision in GALAHAD\_QPC\_double) may be altered to reflect the new problem.

The components p%X, p%Y and p%Z must be set to initial estimates,  $\mathbf{x}^0$ , of the primal variables,  $\mathbf{x}$ , Lagrange multipliers for the general constraints,  $\mathbf{y}$ , 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 p%X=0.0, p%Y=0.0 and p%Z=0.0. The component p%C need not be set on entry.

On exit, the components p%X, p%Y, p%Z and p%C will contain the best estimates of the primal variables  $\mathbf{x}$ , Lagrange multipliers for the general constraints  $\mathbf{y}$ , dual variables for the bound constraints  $\mathbf{z}$ , and values of the constraints  $\mathbf{A}\mathbf{x}$  respectively. What of the remaining problem data has been restored depends upon the input value of the control parameter control%restore\_problem. The return format for a restored array component will be the same as its input format. **Restrictions:** p%n > 0, p%M%ne  $\ge -2$  and p%H%ne  $\ge -2$ .

- C\_stat is a rank-one INTENT (INOUT) array argument of dimension p%m and type default INTEGER, that indicates which of the general linear constraints are in the current working set. Possible values for C\_stat(i),  $i=1,\ldots$ , p%m, and their meanings are
  - <0 the *i*-th general constraint is in the working set, on its lower bound,
  - >0 the *i*-th general constraint is in the working set, on its upper bound, and
  - 0 the *i*-th general constraint is not in the working set.

Suitable values must be supplied if control%qpa\_control%cold\_start = 0 on entry, but need not be provided for other input values of control%cold\_start. Inappropriate values will be ignored. On exit, C\_stat will contain values appropriate for the ultimate working set.

- B\_stat is a rank-one INTENT(INOUT) array argument of dimension p%n and type default INTEGER, that indicates which of the simple bound constraints are in the current working set. Possible values for B\_stat(j), j=1,..., p%n, and their meanings are
  - <0 the j-th simple bound constraint is in the working set, on its lower bound,
  - >0 the j-th simple bound constraint is in the working set, on its upper bound, and
  - 0 the *j*-th simple bound constraint is not in the working set.

Suitable values must be supplied if control%qpa\_control%cold\_start = 0 on entry, but need not be provided for other input values of control%cold\_start. Inappropriate values will be ignored. On exit, B\_stat will contain values appropriate for the ultimate working set.

- data is a scalar INTENT (INOUT) argument of type QPC\_data\_type (see Section 2.4.14). 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 QPC\_initialize.
- control is a scalar INTENT (IN) argument of type QPC\_control\_type (see Section 2.4.7). Default values may be assigned by calling QPC\_initialize prior to the first call to QPC\_solve.
- inform is a scalar INTENT (INOUT) argument of type QPC\_inform\_type (see Section 2.4.13). A successful call to QPC\_solve is indicated when the component status has the value 0. For other return values of status, see Section 2.6.

#### 2.5.3 The termination subroutine

All previously allocated arrays are deallocated as follows:

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

- data is a scalar INTENT (INOUT) argument of type QPC\_data\_type exactly as for QPC\_solve, which must not have been altered by the user since the last call to QPC\_initialize. On exit, array components will have been deallocated.
- control is a scalar INTENT (IN) argument of type QPC\_control\_type exactly as for QPC\_solve.
- inform is a scalar INTENT (OUT) argument of type QPC\_inform\_type exactly as for QPC\_solve. Only the component status will be set on exit, and a successful call to QPC\_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 QPC\_solve or QPC\_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 prob%n > 0 or prob%m ≥ 0 or requirements that prob%A\_type and prob%H\_type contain its relevant string 'DENSE', 'COORDINATE', 'SPARSE\_BY\_ROWS' or 'DIAGONAL' 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.

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-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.
- -23. An entry from the strict upper triangle of **H** has been specified.

#### 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 QPC\_control\_type (see Section 2.4.7), by reading an appropriate data specification file using the subroutine QPC\_read\_specifile. This facility is useful as it allows a user to change QPC control parameters without editing and recompiling programs that call QPC.

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 QPC\_read\_specfile must start with a "BEGIN QPC" command and end with an "END" command. The syntax of the specifile is thus defined as follows:

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

and

END QPC SPECIFICATION
```

are acceptable. Furthermore, between the "BEGIN QPC" 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 QPC\_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 QPC\_read\_specfile.

Control parameters corresponding to the components CQP\_control, QPA\_control and QPB\_control may be changed by including additional sections enclosed by "BEGIN CQP" and "END CQP", "BEGIN QPA" and "END QPA", and "BEGIN QPB" and "END QPB", respectively. See the specification sheets for the packages GALAHAD\_CQP, GALAHAD\_QPA and GALAHAD\_QPB for further details.

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

Control parameters may be read from a file as follows:

```
CALL QPC_read_specfile( control, device )
```

control is a scalar INTENT (INOUT) argument of type QPC\_control\_type (see Section 2.4.7). Default values should have already been set, perhaps by calling QPC\_initialize. On exit, individual components of control may have been changed according to the commands found in the specifile. Specifile commands and the component (see Section 2.4.7) 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
restore-problem-on-output	%restore_problem	integer
infinity-value	%infinity	real
identical-bounds-tolerance	%identical_bounds_tol	real
initial-rho-g	%rho_g	real
initial-rho-b	%rho_b	real
on-bound-tolerance	%on_bound_tol	real
maximum-cpu-time-limit	%cpu_time_limit	real
maximum-clock-time-limit	%clock_time_limit	real
convex	%convex	logical
treat-zero-bounds-as-general	%treat_zero_bounds_as_general	logical
space-critical	%space_critical	logical
deallocate-error-fatal	%deallocate_error_fatal	logical
no-qpa-phase	%no_qpa	logical
no-qpb-phase	%no_qpb	logical

Table 2.1: Specifle commands and associated components of control.

device is a scalar INTENT (IN) argument of type default INTEGER, that must be set to the unit number on which the specifile 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\*cout. 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

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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  $control print_level \ge 2$  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: QPC\_solve calls the GALAHAD packages GALAHAD\_CLOCK, GALAHAD\_SYMBOLS, GALAHAD\_SPACE, GALAHAD\_NORMS, GALAHAD\_SORT, GALAHAD\_QPT, GALAHAD\_QPP, GALAHAD\_QPD, GALAHAD\_EQP, GALAHAD\_LSQP, GALAHAD\_CQP, GALAHAD\_QPA, GALAHAD\_QPB, GALAHAD\_SPECFILE 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%m  $\ge 0$ , prob%A\_type and prob%H\_type  $\in \{' \text{DENSE'}, ' \text{COORDINATE'}, ' \text{SPARSE_BY_-ROWS'}, ' \text{DIAGONAL'} \}$ .

**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

$$\mathbf{A}\mathbf{x} = \mathbf{c} \tag{4.1}$$

and

$$\mathbf{c}^l \le \mathbf{c} \le \mathbf{c}^u, \ \mathbf{x}^l \le \mathbf{x} \le \mathbf{x}^u, \tag{4.2}$$

the dual optimality conditions

$$\mathbf{H}\mathbf{x} + \mathbf{g} = \mathbf{A}^T \mathbf{y} + \mathbf{z}, \ \mathbf{y} = \mathbf{y}^l + \mathbf{y}^u \text{ and } \mathbf{z} = \mathbf{z}^l + \mathbf{z}^u,$$
 (4.3)

and

$$\mathbf{y}^l \ge 0, \ \mathbf{y}^u \le 0, \ \mathbf{z}^l \ge 0 \text{ and } \mathbf{z}^u \le 0,$$
 (4.4)

and the complementary slackness conditions

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

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 problem is solved in three phases. The goal of the first "initial feasible point" phase is to find a strictly interior point which is primal feasible, that is that (4.1) is satisfied. The GALAHAD package GALAHAD\_LSQP is used for this purpose, and offers the options of either accepting the first strictly feasible point found, or preferably of aiming for the so-called "analytic center" of the feasible region. Having found such a suitable initial feasible point, the second "optimality" phase ensures that (4.1) remains satisfied while iterating to satisfy accurately (but not exactly) the dual feasibility (4.3) and complementary slackness (4.5) using the GALAHAD package GALAHAD\_QPB. This optimality phase proceeds by approximately minimizing a sequence of barrier functions

$$q(\mathbf{x}) - \mu \left[ \sum_{i=1}^{m} \log(c_i - c_i^l) + \sum_{i=1}^{m} \log(c_i^u - c_i) + \sum_{j=1}^{n} \log(x_j - x_j^l) + \sum_{j=1}^{n} \log(x_j^u - x_j) \right],$$

for an approriate sequence of positive barrier parameters  $\mu$  converging to zero while ensuring that (4.1) remain satisfied and that  $\mathbf{x}$  and  $\mathbf{c}$  are strictly interior points for (4.2). Note that terms in the above sumations corresponding to infinite bounds are ignored, and that equality constraints are treated specially. See the documentation of GALAHAD\_QPB.for more details.

Since GALAHAD\_QPB may not give a fully accurate solution, the last phase uses the GALAHAD package GALAHAD\_QPA to refine this solution. This package uses a active/working-set method to solve the related  $\ell_1$  quadratic programming problem

$$\underset{\mathbf{x} \in \mathbb{R}^n}{\text{minimize}} \quad q(\mathbf{x}) + \rho_g v_g(\mathbf{x}) + \rho_b v_b(\mathbf{x}),$$

where the he infeasibilities

$$v_g(\mathbf{x}) = \sum_{i=1}^m \max(c_i^l - \mathbf{a}_i^T \mathbf{x}, 0) + \sum_{i=1}^m \max(\mathbf{a}_i^T \mathbf{x} - c_i^u, 0)$$

and

$$v_b(\mathbf{x}) = \sum_{i=1}^n \max(x_j^l - x_j, 0) + \sum_{i=1}^n \max(x_j - x_j^u, 0),$$

and  $\rho_g$  and  $\rho_b$  are appropriately chosen positive weights. See the documentation of GALAHAD\_QPA for more details.

In order to make the solution as efficient as possible, the variables and constraints are reordered internally by the GALAHAD package GALAHAD\_QPP prior to solution. In particular, fixed variables, and free (unbounded on both sides) constraints are temporarily removed.

If at any stage only equality constraints remain, a much simpler equality-constrained phase is performed, by GALAHAD package GALAHAD\_EQP, in place of the three inequality-based phases described above.

#### **References:**

The interior-point and working-set methods are described in detail in

A. R. Conn, N. I. M. Gould, D. Orban and Ph. L. Toint (1999). "A primal-dual trust-region algorithm for minimizing a non-convex function subject to general inequality and linear equality constraints". Mathematical Programming 87 215–249.

N. I. M. Gould and Ph. L. Toint (2002). "An iterative working-set method for large-scale non-convex quadratic programming". Applied Numerical Mathematics **43** (1–2) 109–128.

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#### 5 EXAMPLE OF USE

Suppose we wish to minimize  $\frac{1}{2}x_1^2 + x_2^2 + \frac{3}{2}x_3^2 + 4x_1x_3 + 2x_2 + 1$  subject to the general linear constraints  $1 \le 2x_1 + x_2 \le 2$  and  $x_2 + x_3 = 2$ , and simple bounds  $-1 \le x_1 \le 1$  and  $x_3 \le 2$ . Then, on writing the data for this problem as

$$\mathbf{H} = \begin{pmatrix} 1 & 4 \\ 2 & \\ 4 & 3 \end{pmatrix}, \ \mathbf{g} = \begin{pmatrix} 0 \\ 2 \\ 0 \end{pmatrix}, \ \mathbf{x}^l = \begin{pmatrix} -1 \\ -\infty \\ -\infty \end{pmatrix} \text{ and } \mathbf{x}^u = \begin{pmatrix} 1 \\ \infty \\ 2 \end{pmatrix},$$

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 2.2 - 23/04/2008 AT 16:30 GMT.
  PROGRAM GALAHAD QPC EXAMPLE
  USE GALAHAD OPC 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 ( QPC_data_type ) :: data
  TYPE ( QPC_control_type ) :: control
  TYPE ( QPC_inform_type ) :: inform
  INTEGER :: s
  INTEGER, PARAMETER :: n = 3, m = 2, h_ne = 4, a_ne = 4
  INTEGER, ALLOCATABLE, DIMENSION(:):: C_stat, B_stat
! start problem data
  ALLOCATE( p%G( n ), p%X_l( n ), p%X_u( n ) )
  ALLOCATE( p%C( m ), p%C_1( m ), p%C_u( m ) )
  ALLOCATE ( p%X( n ), p%Y( m ), p%Z( n ) )
  ALLOCATE( B_stat( n ), C_stat( m ) )
  p%new_problem_structure = .TRUE.
                                            ! new structure
  p%n = n ; p%m = m ; p%f = 1.0_wp
                                            ! dimensions & objective constant
  p%G = (/ 0.0_wp, 2.0_wp, 0.0_wp /)
                                            ! objective gradient
  p\C_1 = (/ 1.0_wp, 2.0_wp /)
                                            ! constraint lower bound
  p\C_u = (/ 2.0_wp, 2.0_wp /)
                                             ! constraint upper bound
  p%X_1 = (/ - 1.0_wp, - infinity, - infinity /) ! variable lower bound
  pX_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
  sparse co-ordinate storage format
  CALL SMT_put(p%H%type, 'COORDINATE', s)
                                               ! Specify co-ordinate
                                              ! storage for H and A
  CALL SMT_put( p%A%type, 'COORDINATE', s)
  ALLOCATE( p%H%val( h_ne ), p%H%row( h_ne ), p%H%col( h_ne ) )
  ALLOCATE( p%A%val( a_ne ), p%A%row( a_ne ), p%A%col( a_ne ) )
  p%H%val = (/ 1.0_wp, 2.0_wp, 3.0_wp, 4.0_wp /) ! Hessian H
  p%H%row = (/ 1, 2, 3, 3 /)
                                                 ! NB lower triangle
  p%H%col = (/ 1, 2, 3, 1 /) ; p%H%ne = h_ne
  p%A%val = (/ 2.0_wp, 1.0_wp, 1.0_wp, 1.0_wp /) ! Jacobian A
  p%A%row = (/ 1, 1, 2, 2 /)
  p%A%col = (/ 1, 2, 2, 3 /) ; p%A%ne = a_ne
! problem data complete
  CALL QPC_initialize( data, control, inform ) ! Initialize control parameters
  control%infinity = infinity
                                                ! Set infinity
! control%print_level = 1
```

```
control%QPA_control%print_level = 1
! control%QPB_control%print_level = 1
  CALL QPC_solve(p, C_stat, B_stat, data, control, inform) ! Solve problem
  WRITE( 6, "( 'QPC: ', IO, 'QPA and ', IO, 'QPB iterations ', /,
     ' Optimal objective value =',
                                                                       δ
          ES12.4, /, ' Optimal solution = ', ( 5ES12.4 ) )")
                                                                       S.
    inform%QPA_inform%iter, inform%QPB_inform%iter, inform%obj, p%X
  ELSE
                                        ! Error returns
    WRITE( 6, "( ^{\prime} QPC_solve exit status = ^{\prime}, I6 ) " ) inform%status
  END IF
  CALL QPC_terminate( data, control, inform ) ! delete internal workspace
  END PROGRAM GALAHAD_QPC_EXAMPLE
```

#### This produces the following output:

```
QPC: -1 QPA and 7 QPB iterations Optimal objective value = 5.4459E+00 Optimal solution = -5.4054E-02 1.1081E+00 8.9189E-01
```

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

```
! sparse co-ordinate storage format
! problem data complete
by
! sparse row-wise storage format
  CALL SMT_put( p%H%type, 'SPARSE_BY_ROWS', s ) ! Specify sparse-by-row
  CALL SMT_put( p%A%type, 'SPARSE_BY_ROWS', s ) ! storage for H and A
  ALLOCATE( p%H%val(h_ne), p%H%col(h_ne), p%H%ptr(n + 1))
  ALLOCATE( p%A%val( a_ne ), p%A%col( a_ne ), p%A%ptr( m + 1 ) )
  p%H%val = (/ 1.0_wp, 2.0_wp, 3.0_wp, 4.0_wp /) ! Hessian H
  p%H%col = (/ 1, 2, 3, 1 /)
                                                  ! NB lower triangular
  p%H%ptr = (/ 1, 2, 3, 5 /)
                                                  ! Set row pointers
  p%A%val = (/ 2.0_wp, 1.0_wp, 1.0_wp, 1.0_wp /) ! Jacobian A
  p%A%col = (/ 1, 2, 2, 3 /)
  p%A%ptr = (/ 1, 3, 5 /)
                                                  ! Set row pointers
! problem data complete
```

# or using a dense storage format with the replacement lines

```
! dense storage format

CALL SMT_put( p%H%type, 'DENSE', s ) ! Specify dense

CALL SMT_put( p%A%type, 'DENSE', s ) ! storage for H and A

ALLOCATE( p%H%val( n * (n + 1 ) / 2 ) )

ALLOCATE( p%A%val( n * m ) )

p%H%val = (/ 1.0_wp, 0.0_wp, 2.0_wp, 4.0_wp, 0.0_wp, 3.0_wp /) ! Hessian

p%A%val = (/ 2.0_wp, 1.0_wp, 0.0_wp, 0.0_wp, 1.0_wp, 1.0_wp /) ! Jacobian
! problem data complete
```

# respectively.

If instead **H** had been the diagonal matrix

$$\mathbf{H} = \left( \begin{array}{cc} 1 & & \\ & 0 & \\ & & 3 \end{array} \right)$$

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but the other data is as before, the diagonal storage scheme might be used for H, and in this case we would instead

```
CALL SMT_put( prob%H%type, 'DIAGONAL', s ) ! Specify dense storage for H ALLOCATE( p%H%val( n ) ) p%H%val = (/ 1.0_{\rm wp}, 0.0_{\rm wp}, 3.0_{\rm wp} /) ! Hessian values
```

Notice here that zero diagonal entries are stored.