GALAHAD   TRB

USER DOCUMENTATION   GALAHAD Optimization Library version 5.0

1 SUMMARY

This package uses a **trust-region method to find a (local) minimizer of a differentiable objective function $f(\mathbf{x})$ of many variables x, subject to simple bounds $\mathbf{x}^l \leq \mathbf{x} \leq \mathbf{x}^u$ on the variables.** Here, any of the components of the vectors of bounds $\mathbf{x}^l$ and $\mathbf{x}^u$ may be infinite. The method offers the choice of direct and iterative solution of the key trust-region subproblems, and is most suitable for large problems. First derivatives are required, and if second derivatives can be calculated, they will be exploited—if the product of second derivatives with a vector may be found but not the derivatives themselves, that may also be exploited.

ATTRIBUTES — Versions: `GALAHAD_TRB_single`, `GALAHAD_TRB_double`. **Uses:** `GALAHAD_CLOCK`, `GALAHAD_NLPT`, `GALAHAD_SYMBOLS`, `GALAHAD_SPECFILE`, `GALAHAD_SLS`, `GALAHAD_PSLS`, `GALAHAD_GLTR`, `GALAHAD_TRS`, `LANCELOT_CAUCHY`, `LANCELOT_CG`, `GALAHAD_LMS`, `GALAHAD_SHA`, `GALAHAD_MOP`, `GALAHAD_STRINGS`, `GALAHAD_SPACE`, `GALAHAD_NORMS`, `GALAHAD_BLAS_interface`, and `GALAHAD_LAPACK_interface`. **Date:** July 2021. **Origin:** N. I. M. Gould, Rutherford Appleton Laboratory. **Language:** Fortran 95 + TR 15581 or Fortran 2003.

2 HOW TO USE THE PACKAGE

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

        USE GALAHAD_TRB_single

with the obvious substitution `GALAHAD_TRB_double`, `GALAHAD_TRB_single_64` and `GALAHAD_TRB_double_64` for the other variants.

If it is required to use more than one of the modules at the same time, the derived types `SMT_type`, `GALAHAD_userdata_type`, `TRB_time_type`, `TRB_control_type`, `TRB_inform_type`, `TRB_data_type` and `NLPT_problem_type`, (Section 2.3) and the subroutines `TRB_initialize`, `TRB_solve`, `TRB_terminate`, (Section 2.4) and `TRB_read_specfile` (Section 2.8) must be renamed on one of the `USE` statements.

2.1 Matrix storage formats

If available, the Hessian matrix $\mathbf{H} = \nabla_{xx} f(\mathbf{x})$ may be stored in a variety of input formats.

2.1.1 Dense storage format

The matrix $\mathbf{H}$ is stored as a compact dense matrix by rows, that is, the values of the entries of each row in turn are stored in order within an appropriate real one-dimensional array. Since $\mathbf{H}$ is symmetric, only the lower triangular part (that is the part h_{ij} for $1 \leq j \leq i \leq n$) need be held. In this case the lower triangle should 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 $1 \leq j \leq i \leq n$.

2.1.2 Sparse co-ordinate storage format

Only the nonzero entries of the matrices are stored. For the l-th entry, $1 \leq l \leq$ `H%ne`, of $\mathbf{H}$, its row index i, column index j and value h_{ij}, $1 \leq j \leq i \leq n$, are stored in the l-th components of the integer arrays `H%row`, `H%col` and real array `H%val`, respectively. Note that only the entries in the lower triangle should be stored.

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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 **H**, the i-th component of the integer array H%ptr holds the position of the first entry in this row, while H%ptr $(n+1)$ holds the total number of entries plus one. The column indices j, $1 \leq j \leq i$, and values h_{ij} of the entries in the i-th row are stored in components $l = $ H%ptr(i), ...,H%ptr $(i+1)-1$ of the integer array H%col, and real array H%val, respectively. Note that as before only the entries in the lower triangle should 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 $1 \leq i \neq j \leq n$) only the diagonals entries h_{ii}, $1 \leq i \leq n$, need be stored, and the first n components of the array H%val may be used for the purpose.

2.2 Real and integer kinds

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

2.3 The derived data types

Seven derived data types are accessible from the package.

2.3.1 The derived data type for holding matrices

The derived data type SMT_TYPE is used to hold the Hessian matrix **H** if this is available. The components of SMT_TYPE used here are:

n   is a scalar component of type INTEGER(ip_), that holds the dimension of the matrix.

ne   is a scalar variable of type INTEGER(ip_), that holds the number of matrix entries.

type is a rank-one allocatable array of type default CHARACTER, that is used to indicate the matrix storage scheme used. Its precise length and content depends on the type of matrix to be stored (see §2.3.2).

val   is a rank-one allocatable array of type REAL(rp_) and dimension at least ne, that holds the values of the entries. Each pair of off-diagonal entries $h_{ij} = h_{ji}$ of the *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 INTEGER(ip_), and dimension at least ne, that may hold the row indices of the entries. (see §2.1.2).

col   is a rank-one allocatable array of type INTEGER(ip_), and dimension at least ne, that may hold the column indices of the entries (see §2.1.2–2.1.3).

ptr   is a rank-one allocatable array of type INTEGER(ip_), and dimension at least n + 1, that may hold the pointers to the first entry in each row (see §2.1.3).

2.3.2 The derived data type for holding the problem

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

n   is a scalar variable of type `INTEGER(ip_)`, that holds the number of optimization variables, n.

H   is scalar variable of type `SMT_TYPE` that holds the Hessian matrix **H**. The following components are used here:

         `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 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 `nlp` is of derived type `TRB_problem_type` and involves a Hessian we wish to store using the co-ordinate scheme, we may simply

```
CALL SMT_put( nlp%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 `INTEGER(ip_)`, 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 `REAL(rp_)`, 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 `INTEGER(ip_)`, 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 `INTEGER(ip_)`, 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 `INTEGER(ip_)`, 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.

G   is a rank-one allocatable array of dimension n and type `REAL(rp_)`, that holds the gradient **g** of the objective function. The j-th component of G, $j = 1, \ldots, n$, contains $\mathbf{g}_j$. These are equivalently the values **z** of estimates of the dual variables corresponding to the simple bound constraints (see Section 4).

f   is a scalar variable of type `REAL(rp_)`, that holds the value of the objective function.

X_l   is a rank-one allocatable array of dimension n and type `REAL(rp_)`, that holds the vector of lower bounds $\mathbf{x}^l$ on the the variables. The j-th component of X_l, $j = 1, \ldots, n$, contains $\mathbf{x}^l_j$. Infinite bounds are allowed by setting the corresponding components of X_l to any value smaller than `-infinity`, where `infinity` is a component of the control array `control` (see Section 2.3.3).

X_u   is a rank-one allocatable array of dimension n and type `REAL(rp_)`, that holds the vector of upper bounds $\mathbf{x}^u$ on the variables. The j-th component of X_u, $j = 1, \ldots, n$, 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 2.3.3).

X   is a rank-one allocatable array of dimension n and type REAL(rp_), that holds the values **x** of the optimization
        variables. The j-th component of X, $j = 1, \ldots, n$, contains x_j.

pname   is a scalar variable of type default CHARACTER and length 10, which contains the "name" of the problem for
        printing. The default "empty" string is provided.

VNAMES is a rank-one allocatable array of dimension n and type default CHARACTER and length 10, whose j-th entry
        contains the "name" of the j-th variable for printing. This is only used if "debug" printing control%print_level
        > 4) is requested, and will be ignored if the array is not allocated.

2.3.3 The derived data type for holding control parameters

The derived data type TRB_control_type is used to hold controlling data. Default values may be obtained by calling
TRB_initialize (see Section 2.4.1), while components may also be changed by calling GALAHAD_TRB_read_spec
(see Section 2.8.1). The components of TRB_control_type are:

error   is a scalar variable of type INTEGER(ip_), that holds the stream number for error messages. Printing of error
        messages in TRB_solve and TRB_terminate is suppressed if error ≤ 0. The default is error = 6.

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

print_level is a scalar variable of type INTEGER(ip_), that is used to control the amount of informational output
        which is required. No informational output will occur if print_level ≤ 0. If print_level = 1, a single line
        of output will be produced for each iteration of the process. If print_level ≥ 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 INTEGER(ip_), that specifies the first iteration for which printing will occur
        in TRB_solve. If start_print is negative, printing will occur from the outset. The default is start_print =
        -1.

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

print_gap is a scalar variable of type INTEGER(ip_). Once printing has been started, output will occur once every
        print_gap iterations. If print_gap is no larger than 1, printing will be permitted on every iteration. The default
        is print_gap = 1.

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

more_toraldo is a scalar variable of type INTEGER(ip_), that specifies the number of Moré-Toraldo projected
        searches that are to be used to improve upon the Cauchy point when finding the step. Any non-positive value
        results in a standard add-one-at-a-time conjugate-gradient search. The default is more_toraldo = 0.

non_monotone is a scalar variable of type INTEGER(ip_), that specifies the history-length for non-monotone descent
        strategy. Any non-positive value results in standard monotone descent, for which merit function improvement
        occurs at each iteration. There are often definite advantages in using a non-monotone strategy with a modest
        history, since the occasional local increase in the merit function may enable the algorithm to move across (gentle)
        "ripples" in the merit function surface. However, we do not usually recommend large values of non_monotone.
        The default is non_monotone = 1.

model   is a scalar variable of type INTEGER(ip_), that specifies which model to be used to approximate $f(\mathbf{x})$ when
        computing the step. Possible values are:

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    0 the model 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 models may be used at different stages. **Not yet implemented.**

    1 a first-order model, not involving the Hessian, will be used.

    2 a second-order model, using the Hessian, will be used.

    3 a barely-second-order model, in which the Hessian is approximated by the identity matrix, will be used.

    4 a secant-based sparse second-order model, in which the Hessian is approximated within its sparsity pattern using secant formulae will be used.

    5 a secant-based second-order model, in which the Hessian is approximated by a limited-memory BFGS formula, will be used.

    6 a secant-based second-order model, in which the Hessian is approximated by a limited-memory symmetric rank-one (SR1) formula, will be used.

The default is `model = 2`.

norm is a scalar variable of type `INTEGER(ip_)`, that specifies which norm is to be used to define the trust region. In particular the norm $\|\cdot\|$ will be defined by a symmetric, positive-definite matrix $\mathbf{P}$ so that for every vector $\mathbf{v}$, $\|\mathbf{v}\|^2 = \mathbf{v}^T \mathbf{P} \mathbf{v}$. If `%subproblem_direct = .FALSE.`, the same $\mathbf{P}$ also defines the preconditioner to be used to accelerate the generalized-Lanczos inner model minimization. Possible values are:

   -3 the user's own norm will be used.

   -2 a norm based on a limited-memory BFGS formula will be used.

   -1 the Euclidean (ℓ_2-) norm is used.

    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 norms may be used at different stages. **Not yet implemented.**

    1 $\mathbf{P}$ is the diagonal of the Hessian matrix, suitably modified to ensure that it is significantly positive definite, is used.

    2 $\mathbf{P}$ is the Hessian matrix whose entries outside a band of given semi-bandwidth are replaced by zeros (see `nsemib` below).

    3 $\mathbf{P}$ is the Hessian matrix whose entries outside a bandwidth-reduced reordered band of given semi-bandwidth are replaced by zeros (see `nsemib` below).

    4 $\mathbf{P}$ is the (possibly perturbed) Hessian, using the Schnabel-Eskow modification method to ensure that the resultant matrix is positive definite.

    5 $\mathbf{P}$ is the (possibly perturbed) Hessian, using the Gill-Murray-Poncéleon-Saunders modification method to ensure that the resultant matrix is positive definite. **Not yet implemented.**

    6 $\mathbf{P}$ will be that from the incomplete factorization of the Hessian using the Lin-Moré method.

    7 $\mathbf{P}$ will be that from the incomplete factorization of the Hessian using the method implemented by HSL_MI28.

    8 $\mathbf{P}$ will be that from the incomplete factorization of the Hessian using Munksgaars's method. **Not yet implemented.**

    9 $\mathbf{P}$ will be that from an expanding band of the Hessian. **Not yet implemented.**

   10 $\mathbf{P}$ will be that which gives a diagonalising norm as implemented in `TRB_DPS`. Note that this is currently **only** available when `subproblem_direct = .TRUE.` (see below).

The default is `norm = 1`.

semi_bandwidth is a scalar variable of type `INTEGER(ip_)`, that specifies the semi-bandwidth of $\mathbf{P}$ when `norm = 2`, if appropriate. The default is `semi_bandwidth = 5`.

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lbfgs_vectors is a scalar variable of type INTEGER(ip_), that specifies the number of limited-memory vectors used in the model when model = 5 or 6, and/or by the norm when norm = -2, if appropriate. The default is lbfgs_vectors = 10.

max_dxg is a scalar variable of type INTEGER(ip_), that specifies the maximum number of sparse difference vectors used by the model when model = 4. The default is max_dxg = 100.

icfs_vectors is a scalar variable of type INTEGER(ip_), that specifies the number of multiples of the problem dimension n that is available to hold fill-in when computing the Lin-Moré factorization. The default is icfs_vectors = 10.

mi28_lsize is a scalar variable of type INTEGER(ip_), that specifies the maximum number of fill entries within each column of the incomplete factor *L* computed by HSL_MI28. In general, increasing mi28_lsize improves the quality of the preconditioner but increases the time to compute and then it. Values less than 0 are treated as 0. The default is mi28_lsize = 10.

mi28_rsize is a scalar variable of type INTEGER(ip_), that specifies the the maximum number of entries within each column of the strictly lower triangular matrix *R* used in the computation of the preconditioner by HSL_MI28. Rank-1 arrays of size mi28_rsize * n are allocated internally to hold *R*. Thus the amount of memory used, as well as the amount of work involved in computing the preconditioner, depends on mi28_rsize. Setting mi28_rsize > 0 generally leads to a higher quality preconditioner than using mi28_rsize = 0, and choosing mi28_rsize ≥ mi28_lsize is generally recommended. The default is mi28_rsize = 10.

alive_unit is a scalar variable of type INTEGER(ip_). If alive_unit > 0, a temporary file named alive_file (see below) will be created on stream number alive_unit on initial entry to GALAHAD_TRB_solve, and execution of GALAHAD_TRB_solve will continue so long as this file continues to exist. Thus, a user may terminate execution simply by removing the temporary file from this unit. If alive_unit ≤ 0, no temporary file will be created, and execution cannot be terminated in this way. The default is alive_unit = 60.

advanced_start is a scalar variable of type INTEGER(ip_) that specifies the number of evaluations of the objective function that may be performed If the user wishes to try to select a good initial value of the trust-region radius. If the user is content with the initial value provided, advanced_start should be set to 0, and this is the default.

infinity is a scalar variable of type REAL(rp_), that is used to specify which constraint bounds are infinite. Any bound larger than infinity in modulus will be regarded as infinite. The default is infinity = 10^{19}.

stop_pg_absolute is a scalar variable of type REAL(rp_), that is used to specify the maximum permitted (infinity) norm of the projected gradient of the objective function (see Section 4) at the estimate of the solution sought. The default is stop_g_absolute = 10^{-5}.

stop_pg_relative is a scalar variable of type REAL(rp_), that is used to specify the largest relative reduction in the norm of the projected gradient of the objective function that will be permitted (see Section 4) at the estimate of the solution sought compared to that at the initial point. The default is stop_g_relative = 1.

stop_s is a scalar variable of type REAL(rp_), that is used to specify the minimum acceptable correction step **s** relative to the current estimate of the solution **x** The algorithm will be deemed to have converged if $|s_i| \le$ stop_s $* \max(1, |x_i|)$ for all $i = 1, \ldots, n$. The default is stop_s = u, where u is EPSILON(1.0) (EPSILON(1.0D0) in GALAHAD_TRB_double).

initial_radius is a scalar variable of type REAL(rp_), that holds the required initial value of the trust-region radius. If initial_radius ≤ 0, the radius will be chosen automatically by GALAHAD_TRB_solve The default is initial_radius = 100.0.

maximum_radius is a scalar variable of type REAL(rp_), that holds the largest permitted value of the trust-region radius as the algorithm proceeds. The default is maximum_radius = 10^8.

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stop_rel_cg is a scalar variable of type REAL(rp_), that is used to specify the largest relative residual that is tolerated before any conjugate-gradient inner iteration terminates. The default is stop_rel_cg = 0.01.

radius_increase, radius_reduce and radius_reduce_max are scalar variables of type REAL(rp_), that control the maximum amounts by which the trust-region radius can contract or expand during an iteration. The radius will be decreased by powers of radius_reduce, but not in total more than radius_reduce_max, until it is smaller than the norm of the current step. It can be increased by at most a factor radius_increase. The defaults are radius_increase = 2.0, radius_reduce = 0.5 and radius_reduce_max = 0.0625.

eta_successful, eta_very_successful and eta_too_successful are scalar variables of type default REAL(rp_), that control the acceptance and rejection of the trial step and the updates to the trust-region radius. At every iteration, the ratio of the actual reduction in the merit function following the trial step to that predicted by the model is computed. The step is accepted whenever this ratio exceeds eta_successful; otherwise the trust-region radius will be reduced. If, in addition, the ratio exceeds eta_very_successful but not eta_too_successful, the trust-region radius may be increased. The defaults are eta_successful = 10^{-8}, eta_very_successful = 0.9 and eta_too_successful = 2.0.

obj_unbounded is a scalar variable of type default REAL(rp_), 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_TRB_double).

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

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

hessian_available is a scalar variable of type default LOGICAL, that should be set .TRUE. if the user will provide second derivatives (either by providing an appropriate evaluation routine to the solver or by reverse communication, see Section 2.6), and .FALSE. if the second derivatives are not explicitly available. The default is hessian_available = .TRUE..

subproblem_direct is a scalar variable of type default LOGICAL, that should be set .TRUE. if a direct (factorization) method is desired when solving for the step, and .FALSE. if an iterative method suffices. The default is subproblem_direct = .FALSE..

retrospective_trust_region is a scalar variable of type default LOGICAL, that should be set .TRUE. if a retrospective trust-region strategy, based on the model at the next iterate, is to be used, and .FALSE. if the traditional strategy suffices. The default is retrospective_trust_region = .FALSE..

renormalize_radius is a scalar variable of type default LOGICAL, that should be set .TRUE. if the trust-region radius is to be re-normaized to account for the shape of the trust-region norm every iteration, and .FALSE. if no re-normalization is required. The default is renormalize_radius = .FALSE..

two_norm_tr is a scalar variable of type default LOGICAL, that should be set .TRUE. if a two-norm (hyperspherical) trust region is required, and .FALSE. if an infinity-norm (box) trust region is to be used. The default is two_norm_tr = .FALSE..

exact_gcp is a scalar variable of type default LOGICAL, that should be set .TRUE. if the exact generalized Cauchy point, the first estimate of the minimizer of the quadratic model within the feasible box, is required, and .FALSE. if an approximation suffices. The default is exact_gcp = .TRUE..

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accurate_bqp is a scalar variable of type default LOGICAL, that should be set .TRUE. if an accurate minimizer of the quadratic model within the feasible box is required, and .FALSE. if an approximation suffices. The accurate minimizer often requires considerably more work, but occasionally this reduces the overall number of iterations. The default is accurate_bqp = .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..

alive_file is a scalar variable of type default CHARACTER and length 30, that gives the name of the temporary file whose removal from stream number alive_unit terminates execution of GALAHAD_TRB_solve. The default is alive_unit = ALIVE.d.

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 = "".

PSLS_control is a scalar variable of type PSLS_control_type whose components are used to control the preconditioning aspects of the calculation, as performed by the package GALAHAD_PSLS. See the specification sheet for the package GALAHAD_PSLS for details, and appropriate default values (but note that values for PSLS_control%preconditioner, PSLS_control%semi_bandwidth and PSLS_control%icfs_vectors may be overridden by GALAHAD_TRB_solve).

GLTR_control is a scalar variable of type GLTR_control_type whose components are used to control the iterative trust-region step calculation (if any), performed by the package GALAHAD_GLTR. See the specification sheet for the package GALAHAD_GLTR for details, and appropriate default values (but note that value of GLTR_control%unitm may be changed by GALAHAD_TRB_solve).

TRS_control is a scalar variable of type TRS_control_type whose components are used to control the direct trust-region step calculation (if any), performed by the package GALAHAD_TRS. See the specification sheet for the package GALAHAD_TRS for details, and appropriate default values (but note that values of TRS_control%initial_multiplier and TRS_control%new_h may be changed by GALAHAD_TRB_solve).

LMS_control and LMS_control_prec are scalar variables of type LMS_control_type whose components are used to control the limited memory secant approximations for the model Hessian and trust region norm as performed by the package GALAHAD_LMS. See the specification sheet for the package GALAHAD_LMS for details, and appropriate default values.

SHA_control is a scalar variable of type SHA_control_type whose components are used to control the calculation of the sparse model Hessian (if required), performed by the package GALAHAD_SHA. See the specification sheet for the package GALAHAD_SHA for details, and appropriate default values.

2.3.4 The derived data type for holding timing information

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

total is a scalar variable of type default REAL, that gives the CPU total time spent in the package.

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

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

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

solve is a scalar variable of type REAL(rp_), that gives the CPU time spent using the factors to solve relevant linear equations.

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

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

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

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

clock_solve is a scalar variable of type REAL(rp_), that gives the elapsed system clock time spent using the factors to solve relevant linear equations.

2.3.5 The derived data type for holding informational parameters

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

status is a scalar variable of type INTEGER(ip_), that gives the exit status of the algorithm. See Sections 2.6 and 2.7 for details.

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

bad_alloc is a scalar variable of type default CHARACTER and length 80, that gives the name of the last internal array for which there were allocation or deallocation errors. This will be the null string if status = 0.

n_free is a scalar variable of type INTEGER(ip_), that holds the number of variables that are free from their bounds.

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

cg_iter is a scalar variable of type INTEGER(ip_), that gives the total number of conjugate-gradient iterations required.

cg_maxit is a scalar variable of type INTEGER(ip_), that gives the number of conjugate-gradient iterations permitted duriing each major iteration.

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

max_entries_factors is a scalar variable of type INTEGER(int64), that gives the maximum number of entries in any of the matrix factorizations performed during the calculation.

---

factorization_max is a scalar variable of type INTEGER(ip_), that gives the largest number of factorizations required during a subproblem solution.

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

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

f_eval is a scalar variable of type INTEGER(ip_), that gives the total number of objective function evaluations performed.

g_eval is a scalar variable of type INTEGER(ip_), that gives the total number of objective function gradient evaluations performed.

h_eval is a scalar variable of type INTEGER(ip_), that gives the total number of objective function Hessian evaluations performed.

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

norm_pg is a scalar variable of type REAL(rp_), that holds the value of the norm of the projected gradient of the objective function at the best estimate of the solution found.

radius is a scalar variable of type REAL(rp_), that holds the current value of the trust-region radius

factorization_average is a scalar variable of type REAL(rp_), that gives the average number of factorizations per subproblem solved.

time is a scalar variable of type TRB_time_type whose components are used to hold elapsed elapsed CPU and system clock times for the various parts of the calculation (see Section 2.3.4).

PSLS_inform is a scalar variable of type PSLS_inform_type whose components give information about the progress and needs of the preconditioning stages of the algorithm performed by the package GALAHAD_PSLS. See the specification sheet for the package GALAHAD_PSLS for details.

GLTR_inform is a scalar variable of type GLTR_inform_type whose components give information about the progress and needs of the iterative solution stages of the algorithm performed by the package GALAHAD_GLTR. See the specification sheet for the package GALAHAD_GLTR for details.

TRS_inform is a scalar variable of type TRS_inform_type whose components give information about the progress and needs of the direct solution stages of the algorithm performed by the package GALAHAD_TRS. See the specification sheet for the package GALAHAD_TRS for details.

LMS_inform and LMS_inform_prec are scalar variables of type LMS_inform_type whose components give information about the progress and needs of the limited memory secant approximations for the model Hessian and trust region norm as performed by the package GALAHAD_LMS. See the specification sheet for the package GALAHAD_LMS for details.

SHA_inform is a scalar variable of type SHA_inform_type whose components give information about the progress and needs of the sparse model Hessian calculation performed by the package GALAHAD_SHA. See the specification sheet for the package GALAHAD_SHA for details.

2.3.6 The derived data type for holding problem data

The derived data type `TRB_data_type` is used to hold all the data for a particular problem, or sequences of problems with the same structure, between calls of `TRB` procedures. This data should be preserved, untouched (except as directed on return from `GALAHAD_TRB_solve` with positive values of `inform%status`, see Section 2.6), from the initial call to `TRB_initialize` to the final call to `TRB_terminate`.

2.3.7 The derived data type for holding user data

The derived data type `GALAHAD_userdata_type` is available from the package `GALAHAD_userdata` to allow the user to pass data to and from user-supplied subroutines for function and derivative calculations (see Section 2.5). Components of variables of type `GALAHAD_userdata_type` may be allocated as necessary. The following components are available:

`integer` is a rank-one allocatable array of type `INTEGER(ip_)`.

`real` is a rank-one allocatable array of type default `REAL(rp_)`

`complex` is a rank-one allocatable array of type default `COMPLEX` (double precision complex in `GALAHAD_TRB_double`).

`character` is a rank-one allocatable array of type default `CHARACTER`.

`logical` is a rank-one allocatable array of type default `LOGICAL`.

`integer_pointer` is a rank-one pointer array of type `INTEGER(ip_)`.

`real_pointer` is a rank-one pointer array of type default `REAL(rp_)`

`complex_pointer` is a rank-one pointer array of type default `COMPLEX` (double precision complex in `GALAHAD_TRB_double`).

`character_pointer` is a rank-one pointer array of type default `CHARACTER`.

`logical_pointer` is a rank-one pointer array of type default `LOGICAL`.

2.4 Argument lists and calling sequences

There are three procedures for user calls (see Section 2.8 for further features):

1. The subroutine `TRB_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 `TRB_solve` is called to solve the problem.

3. The subroutine `TRB_terminate` is provided to allow the user to automatically deallocate array components of the private data, allocated by `TRB_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 `TRB_initialize` cannot test for this situation, and any existing associated targets will subsequently become unreachable.

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

2.4.1 The initialization subroutine

Default values are provided as follows:

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

data is a scalar `INTENT(INOUT)` argument of type `TRB_data_type` (see Section 2.3.6). It is used to hold data about the problem being solved.

control is a scalar `INTENT(OUT)` argument of type `TRB_control_type` (see Section 2.3.3). On exit, `control` contains default values for the components as described in Section 2.3.3. These values should only be changed after calling `TRB_initialize`.

inform is a scalar `INTENT(OUT)` argument of type `TRB_inform_type` (see Section 2.3.5). A successful call to `TRB_initialize` is indicated when the component `status` has the value 0. For other return values of `status`, see Section 2.7.

2.4.2 The minimization subroutine

The minimization algorithm is called as follows:

```
CALL TRB_solve( nlp, control, inform, data, userdata[, eval_F, eval_G,     &
                eval_H, eval_HPROD, eval_SHPROD, eval_PREC] )
```

nlp is a scalar `INTENT(INOUT)` argument of type `NLPT_problem_type` (see Section 2.3.2). 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 `nlp%n` and the required integer components of `nlp%H` if second derivatives will be used. Users are free to choose whichever of the matrix formats described in Section 2.1 is appropriate for **H** for their application.

The component `nlp%X` must be set to an initial estimate, $\mathbf{x}^0$, of the minimization variables. A good choice will increase the speed of the package, but the underlying method is designed to converge (at least to a local solution) from an arbitrary initial guess.

On exit, the component `nlp%X` will contain the best estimates of the minimization variables **x**, while `nlp%G` will contain the best estimates of the dual variables **z**.

Restrictions: $nlp\%n > 0$ and $nlp\%H\%type \in \{$'DENSE','COORDINATE','SPARSE_BY_ROWS','DIAGONAL'$\}$.

control is a scalar `INTENT(IN)` argument of type `TRB_control_type` (see Section 2.3.3). Default values may be assigned by calling `TRB_initialize` prior to the first call to `TRB_solve`. The arguments `control%PSLS_control-%preconditioner`, `control%PSLS_control%semi_bandwidth`, `control%PSLS_control%lbfgs_vectors` and `control%PSLS_control%icfs_vectors` will be overridden by `control%norm`, `control%semi_bandwidth`, `control%lbfgs_vectors` and `control%icfs_vectors`, respectively.

inform is a scalar `INTENT(INOUT)` argument of type `TRB_inform_type` (see Section 2.3.5). On initial entry, the component `status` must be set to the value 1. Other entries need note be set. A successful call to `TRB_solve` is indicated when the component `status` has the value 0. For other return values of `status`, see Sections 2.6 and 2.7.

data is a scalar `INTENT(INOUT)` argument of type `TRB_data_type` (see Section 2.3.6). It is used to hold data about the problem being solved. With the possible exceptions of the components `eval_status` and `U` (see Section 2.6), it must not have been altered **by the user** since the last call to `TRB_initialize`.

userdata is a scalar `INTENT(INOUT)` argument of type `GALAHAD_userdata_type` whose components may be used to communicate user-supplied data to and from the `OPTIONAL` subroutines `eval_F`, `eval_G`, `eval_H` and `eval_HPROD` (see Section 2.3.7).

---

eval_F is an OPTIONAL user-supplied subroutine whose purpose is to evaluate the value of the objective function $f(\mathbf{x})$ at a given vector $\mathbf{x}$. See Section 2.5.1 for details. If eval_F is present, it must be declared EXTERNAL in the calling program. If eval_F is absent, GALAHAD_TRB_solve will use reverse communication to obtain objective function values (see Section 2.6).

eval_G is an OPTIONAL user-supplied subroutine whose purpose is to evaluate the value of the gradient of the objective function $\nabla_x f(\mathbf{x})$ at a given vector $\mathbf{x}$. See Section 2.5.2 for details. If eval_G is present, it must be declared EXTERNAL in the calling program. If eval_G is absent, GALAHAD_TRB_solve will use reverse communication to obtain gradient values (see Section 2.6).

eval_H is an OPTIONAL user-supplied subroutine whose purpose is to evaluate the value of the Hessian of the objective function $\nabla_{xx} f(\mathbf{x})$ at a given vector $\mathbf{x}$. See Section 2.5.3 for details. If eval_H is present, it must be declared EXTERNAL in the calling program. If eval_H is absent, GALAHAD_TRB_solve will use reverse communication to obtain Hessian function values (see Section 2.6).

eval_HPROD is an OPTIONAL user-supplied subroutine whose purpose is to evaluate the value of the product $\nabla_{xx} f(\mathbf{x})\mathbf{v}$ of the Hessian of the objective function $\nabla_{xx} f(\mathbf{x})$ with a given vector $\mathbf{v}$. See Section 2.5.4 for details. If eval_HPROD is present, it must be declared EXTERNAL in the calling program. If eval_HPROD is absent, GALAHAD_TRB_solve will use reverse communication to obtain Hessian-vector products (see Section 2.6).

eval_SHPROD is an OPTIONAL user-supplied subroutine whose purpose is to evaluate the value of the product $\nabla_{xx} f(\mathbf{x})\mathbf{v}$ of the Hessian of the objective function $\mathbf{u} = \nabla_{xx} f(\mathbf{x})$ with a given *sparse* vector $\mathbf{v}$, and to return the nonzero components of the resulting $\mathbf{u}$. See Section 2.5.5 for details. If eval_SHPROD is present, it must be declared EXTERNAL in the calling program. If eval_SHPROD is absent, GALAHAD_TRB_solve will use reverse communication to obtain Hessian-sparse-vector products (see Section 2.6).

eval_PREC is an OPTIONAL user-supplied subroutine whose purpose is to evaluate the value of the product $\mathbf{P}(\mathbf{x})\mathbf{v}$ of the user's preconditioner with a given vector $\mathbf{v}$. See Section 2.5.6 for details. If eval_PREC is present, it must be declared EXTERNAL in the calling program. If eval_PREC is absent, GALAHAD_TRB_solve will use reverse communication to obtain products with the preconditioner (see Section 2.6).

2.4.3 The termination subroutine

All previously allocated arrays are deallocated as follows:

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

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

control is a scalar INTENT(IN) argument of type TRB_control_type exactly as for TRB_solve.

inform is a scalar INTENT(OUT) argument of type TRB_inform_type exactly as for TRB_solve. Only the component status will be set on exit, and a successful call to TRB_terminate is indicated when this component status has the value 0. For other return values of status, see Section 2.7.

2.5 Function and derivative values

2.5.1 The objective function value via internal evaluation

If the argument eval_F is present when calling GALAHAD_TRB_solve, the user is expected to provide a subroutine of that name to evaluate the value of the objective function $f(\mathbf{x})$. The routine must be specified as

```
SUBROUTINE eval_F( status, X, userdata, f )
```

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whose arguments are as follows:

status is a scalar `INTENT(OUT)` argument of type `INTEGER(ip_)`, that should be set to 0 if the routine has been able to evaluate the objective function and to a non-zero value if the evaluation has not been possible.

X is a rank-one `INTENT(IN)` array argument of type `REAL(rp_)` whose components contain the vector **x**.

userdata is a scalar `INTENT(INOUT)` argument of type `GALAHAD_userdata_type` whose components may be used to communicate user-supplied data to and from the subroutines `eval_F`, `eval_G`, `eval_H`, `eval_HPROD` and `eval_PREC` (see Section 2.3.7).

f is a scalar `INTENT(OUT)` argument of type `REAL(rp_)`, that should be set to the value of the objective function $f(\mathbf{x})$ evaluated at the vector **x** input in X.

2.5.2 Gradient values via internal evaluation

If the argument `eval_G` is present when calling `GALAHAD_TRB_solve`, the user is expected to provide a subroutine of that name to evaluate the value of the gradient the objective function $\nabla_x f(\mathbf{x})$. The routine must be specified as

        SUBROUTINE eval_G(status, X, userdata, G)

whose arguments are as follows:

status is a scalar `INTENT(OUT)` argument of type `INTEGER(ip_)`, that should be set to 0 if the routine has been able to evaluate the gradient of the objective function and to a non-zero value if the evaluation has not been possible.

X is a rank-one `INTENT(IN)` array argument of type `REAL(rp_)` whose components contain the vector **x**.

userdata is a scalar `INTENT(INOUT)` argument of type `GALAHAD_userdata_type` whose components may be used to communicate user-supplied data to and from the subroutines `eval_F`, `eval_G`, `eval_H`, `eval_HPROD` and `eval_PREC` (see Section 2.3.7).

G is a rank-one `INTENT(OUT)` argument of type `REAL(rp_)`, whose components should be set to the values of the gradient of the objective function $\nabla_x f(\mathbf{x})$ evaluated at the vector **x** input in X.

2.5.3 Hessian values via internal evaluation

If the argument `eval_H` is present when calling `GALAHAD_TRB_solve`, the user is expected to provide a subroutine of that name to evaluate the values of the Hessian of the objective function $\nabla_{xx} f(\mathbf{x})$. The routine must be specified as

        SUBROUTINE eval_H(status, X, userdata, Hval)

whose arguments are as follows:

status is a scalar `INTENT(OUT)` argument of type `INTEGER(ip_)`, that should be set to 0 if the routine has been able to evaluate the Hessian of the objective function and to a non-zero value if the evaluation has not been possible.

X is a rank-one `INTENT(IN)` array argument of type `REAL(rp_)` whose components contain the vector **x**.

userdata is a scalar `INTENT(INOUT)` argument of type `GALAHAD_userdata_type` whose components may be used to communicate user-supplied data to and from the subroutines `eval_F`, `eval_G`, `eval_H`, `eval_HPROD` and `eval_PREC` (see Section 2.3.7).

Hval is a scalar `INTENT(OUT)` argument of type `REAL(rp_)`, whose components should be set to the values of the Hessian of the objective function $\nabla_{xx} f(\mathbf{x})$ evaluated at the vector **x** input in X. The values should be input in the same order as that in which the array indices were given in `nlp%H`.

2.5.4 Hessian-vector products via internal evaluation

If the argument `eval_HPROD` is present when calling `GALAHAD_TRB_solve`, the user is expected to provide a subroutine of that name to evaluate the sum $\mathbf{u} + \nabla_{xx} f(\mathbf{x})\mathbf{v}$ involving the product of the Hessian of the objective function $\nabla_{xx} f(\mathbf{x})$ with a given vector $\mathbf{v}$. The routine must be specified as

```
SUBROUTINE eval_HPROD( status, X, userdata, U, V, got_h )
```

whose arguments are as follows:

status   is a scalar `INTENT(OUT)` argument of type `INTEGER(ip_)`, that should be set to 0 if the routine has been able to evaluate the sum $\mathbf{u} + \nabla_{xx} f(\mathbf{x})\mathbf{v}$ and to a non-zero value if the evaluation has not been possible.

X   is a rank-one `INTENT(IN)` array argument of type `REAL(rp_)` whose components contain the vector $\mathbf{x}$.

userdata   is a scalar `INTENT(INOUT)` argument of type `GALAHAD_userdata_type` whose components may be used to communicate user-supplied data to and from the subroutines `eval_F`, `eval_G`, `eval_H`, `eval_HPROD` and `eval_PREC` (see Section 2.3.7).

U   is a rank-one `INTENT(INOUT)` array argument of type `REAL(rp_)` whose components on input contain the vector $\mathbf{u}$ and on output the sum $\mathbf{u} + \nabla_{xx} f(\mathbf{x})\mathbf{v}$.

V   is a rank-one `INTENT(IN)` array argument of type `REAL(rp_)` whose components contain the vector $\mathbf{v}$.

got_h is an `OPTIONAL` scalar `INTENT(IN)` argument of type default `LOGICAL`. If the Hessian has already been evaluated at the current $\mathbf{x}$ `got_h` will be `PRESENT` and set `.TRUE.`; if this is the first time the Hessian is to be accessed at $\mathbf{x}$, either `got_h` will be absent or `PRESENT` and set `.FALSE.`. This gives the user the opportunity to reuse "start-up" computations required for the first instance of $\mathbf{x}$ to speed up subsequent products.

2.5.5 Hessian-sparse-vector products via internal evaluation

If the argument `eval_SHPROD` is present when calling `GALAHAD_TRB_solve`, the user is expected to provide a subroutine of that name to evaluate the product $\mathbf{u} = \nabla_{xx} f(\mathbf{x})\mathbf{v}$ involving the Hessian of the objective function $\nabla_{xx} f(\mathbf{x})$ and a given sparse vector $\mathbf{v}$, and to return the nonzero components of the result $\mathbf{u}$. This routine is **not required** if the user has set `control%hessian_available` to `.TRUE.` and has made the values of $\nabla_{xx} f(\mathbf{x})$ available either by calls to `eval_H` (see §2.5.3) or by reverse communication (see §2.6). If needed, the routine must be specified as

```
SUBROUTINE eval_SHPROD( status, X, userdata, nnz_v, INDEX_nz_v, V,     &
                        nnz_u, INDEX_nz_u, U, got_h )
```

whose arguments are as follows:

status   is a scalar `INTENT(OUT)` argument of type `INTEGER(ip_)`, that should be set to 0 if the routine has been able to evaluate the sum $\mathbf{u} + \nabla_{xx} f(\mathbf{x})\mathbf{v}$ and to a non-zero value if the evaluation has not been possible.

X   is a rank-one `INTENT(IN)` array argument of type `REAL(rp_)` whose components contain the vector $\mathbf{x}$.

userdata   is a scalar `INTENT(INOUT)` argument of type `GALAHAD_userdata_type` whose components may be used to communicate user-supplied data to and from the subroutines `eval_F`, `eval_G`, `eval_H`, `eval_HPROD` and `eval_PREC` (see Section 2.3.7).

nnz_v   is a scalar `INTENT(IN)` argument of type `INTEGER(ip_)`, that specifies the number of nonzeros in the input sparse vector $\mathbf{v}$.

INDEX_nz_v is a rank-one `INTENT(IN)` array argument of length at least `nnz_v` and type `INTEGER(ip_)` whose first `nnz_v` components give the indices of the nonzero components of $\mathbf{v}$.

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V   is a rank-one `INTENT(IN)` array argument of type `REAL(rp_)` whose components `INDEX_nz_v(i)`, $i = 1,\ldots,$ `nnz_v`, hold the nonzero values of **v**. Any other components should be ignored.

`nnz_u` is a scalar `INTENT(OUT)` argument of type `INTEGER(ip_)`, that gives the number of nonzeros in the output vector **u**.

`INDEX_nz_u` is a rank-one `INTENT(OUT)` array argument of length at least `nnz_u` and type `INTEGER(ip_)` whose first `nnz_u` components give the indices of the nonzero components of the computed product **u**.

U   is a rank-one `INTENT(OUT)` array argument of type `REAL(rp_)` whose components `INDEX_nz_u(i)`, $i = 1,\ldots,$ `nnz_u`, hold the nonzero values of **u**. The remaining components should be ignored.

`got_h` is an `OPTIONAL` scalar `INTENT(IN)` argument of type default `LOGICAL`. If the Hessian has already been evaluated at the current **x** `got_h` will be `PRESENT` and set `.TRUE.`; if this is the first time the Hessian is to be accessed at **x**, either `got_h` will be absent or `PRESENT` and set `.FALSE.`. This gives the user the opportunity to reuse "start-up" computations required for the first instance of **x** to speed up subsequent products.

2.5.6   Preconditioner-vector products via internal evaluation

If the argument `eval_PREC` is present when calling `GALAHAD_TRB_solve`, the user is expected to provide a subroutine of that name to evaluate the product $\mathbf{u} = \mathbf{P}(\mathbf{x})\mathbf{v}$ involving the user's preconditioner $\mathbf{P}(\mathbf{x})$ with a given vector **v**. The symmetric matrix $\mathbf{P}(\mathbf{x})$ should ideally be chosen so that the eigenvalues of $\mathbf{P}(\mathbf{x})(\nabla_{xx}f(\mathbf{x}))^{-1}$ are clustered. This subroutine will **only be required** if `control%norm = -3`, and the user prefers a subroutine call to that provided by reverse communication with `inform%status = 6` (see §2.6). The routine must be specified as

```
SUBROUTINE eval_PREC( status, X, userdata, U, V )
```

whose arguments are as follows:

`status` is a scalar `INTENT(OUT)` argument of type `INTEGER(ip_)`, that should be set to 0 if the routine has been able to evaluate the product $\mathbf{P}(\mathbf{x})\mathbf{v}$ and to a non-zero value if the evaluation has not been possible.

X   is a rank-one `INTENT(IN)` array argument of type `REAL(rp_)` whose components contain the vector **x**.

`userdata` is a scalar `INTENT(INOUT)` argument of type `GALAHAD_userdata_type` whose components may be used to communicate user-supplied data to and from the subroutines `eval_F`, `eval_G`, `eval_H` and `eval_PREC` (see Section 2.3.7).

U   is a rank-one `INTENT(OUT)` array argument of type `REAL(rp_)` whose components on output should contain the product sum $\mathbf{u} = \mathbf{P}(\mathbf{x})\mathbf{v}$.

V   is a rank-one `INTENT(IN)` array argument of type `REAL(rp_)` whose components contain the vector **v**.

2.6   Reverse Communication Information

A positive value of `inform%status` on exit from `TRB_solve` indicates that `GALAHAD_TRB_solve` is seeking further information—this will happen if the user has chosen not to evaluate function or derivative values internally (see Section 2.5). The user should compute the required information and re-enter `GALAHAD_TRB_solve` with `inform%status` and all other arguments (except those specifically mentioned below) unchanged.

Possible values of `inform%status` and the information required are

2.   The user should compute the objective function value $f(\mathbf{x})$ at the point **x** indicated in `nlp%X`. The required value should be set in `nlp%f`, and `data%eval_status` should be set to 0. If the user is unable to evaluate $f(\mathbf{x})$—for instance, if the function is undefined at **x**—the user need not set `nlp%f`, but should then set `data%eval_status` to a non-zero value.

---

3.   The user should compute the gradient of the objective function $\nabla_x f(\mathbf{x})$ at the point $\mathbf{x}$ indicated in `nlp%X`. The value of the i-th component of the gradient should be set in `nlp%G(i)`, for $i = 1, \ldots, n$ and `data%eval_status` should be set to 0. If the user is unable to evaluate a component of $\nabla_x f(\mathbf{x})$—for instance, if a component of the gradient is undefined at $\mathbf{x}$—the user need not set `nlp%G`, but should then set `data%eval_status` to a non-zero value.

4.   The user should compute the Hessian of the objective function $\nabla_{xx} f(\mathbf{x})$ at the point $\mathbf{x}$ indicated in `nlp%X`. The value l-th component of the Hessian stored according to the scheme input in the remainder of `nlp%H` (see Section 2.3.2) should be set in `nlp%H%val(l)`, for $l = 1, \ldots,$ `nlp%H%ne` and `data%eval_status` should be set to 0. If the user is unable to evaluate a component of $\nabla_{xx} f(\mathbf{x})$—for instance, if a component of the Hessian is undefined at $\mathbf{x}$—the user need not set `nlp%H%val`, but should then set `data%eval_status` to a non-zero value.

5.   The user should compute the product $\nabla_{xx} f(\mathbf{x})\mathbf{v}$ of the Hessian of the objective function $\nabla_{xx} f(\mathbf{x})$ at the point $\mathbf{x}$ indicated in `nlp%X` with the vector $\mathbf{v}$ and add the result to the vector $\mathbf{u}$. The vectors $\mathbf{u}$ and $\mathbf{v}$ are given in `data%U` and `data%V` respectively, the resulting vector $\mathbf{u} + \nabla_{xx} f(\mathbf{x})\mathbf{v}$ should be set in `data%U` and `data%eval_status` should be set to 0. If the user is unable to evaluate the product—for instance, if a component of the Hessian is undefined at $\mathbf{x}$—the user need not set `nlp%H%val`, but should then set `data%eval_status` to a non-zero value.

6.   The user should compute the product $\mathbf{u} = \mathbf{P}(\mathbf{x})\mathbf{v}$ of their preconditioner $\mathbf{P}(\mathbf{x})$ at the point $\mathbf{x}$ indicated in `nlp%X` with the vector $\mathbf{v}$. The vectors $\mathbf{v}$ is given in `data%V`, the resulting vector $\mathbf{u} = \mathbf{P}(\mathbf{x})\mathbf{v}$ should be set in `data%U` and `data%eval_status` should be set to 0. If the user is unable to evaluate the product—for instance, if a component of the preconditioner is undefined at $\mathbf{x}$—the user need not set `data%U`, but should then set `data%eval_status` to a non-zero value.

This value **can only occur** if the user has set `control%norm = -3`, and has not provided an optional subroutine `eval_PREC` (see §2.5.6) to compute the required product with the preconditioner.

7.   The user should compute the product $\mathbf{h} = \nabla_{xx} f(\mathbf{x})\mathbf{p}$ of the Hessian of the objective function $\nabla_{xx} f(\mathbf{x})$ at the point $\mathbf{x}$ indicated in `nlp%X` with the sparse vector $\mathbf{p}$. The nonzeros of $\mathbf{p}$ are stored in `data%P(data%INDEX_nz_p(data%nnz_p_l:data%nnz_p_u))` while the nonzeros of $\mathbf{h}$ should be returned in `data%HP(data%INDEX_nz_hp(1:data%nnz_hp))`; the user must set `data%nnz_hp` and `data%INDEX_nz_hp` accordingly, and `data%eval_status` should be set to 0. If the user is unable to evaluate the product—for instance, if a component of the Hessian is undefined at $\mathbf{x}$—the user need not set `data%HP`, `data%INDEX_nz_hp` and `data%nnz_hp` but should then set `data%eval_status` to a non-zero value.

This value **will not occur** if the user has set `control%hessian_available` to `.TRUE.` and can provide values of $\nabla_{xx} f(\mathbf{x})$ either by calls to `eval_H` (see §2.5.3) or by reverse communication (see `inform%status = 4`, above).

2.7   Warning and error messages

A negative value of `inform%status` on exit from `TRB_solve` or `TRB_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.   The restriction `nlp%n > 0` or requirement that `nlp%H_type` contains its relevant string `'DENSE'`, `'COORDINATE'`, `'SPARSE_BY_ROWS'` or `'DIAGONAL'` has been violated.

-4.   The bound constraints are inconsistent.

`-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`.

`-11.` The solution of a set of linear equations using factors from the factorization package failed; the return status from the factorization package is given in the component `inform%factor_status`.

`-15.` The preconditioner $\mathbf{P(x)}$ appears not to be positive definite.

`-16.` The problem is so ill-conditioned that further progress is impossible.

`-17.` The step is too small to make further impact.

`-18.` Too many iterations have been performed. This may happen if `control%maxit` is too small, but may also be symptomatic of a badly scaled problem.

`-19.` The elapsed CPU or system clock time limit has been reached. This may happen if either `control%cpu_time_limit` or `control%clock_time_limit` is too small, but may also be symptomatic of a badly scaled problem.

`-82.` The user has forced termination of `GALAHAD_TRB_solve` by removing the file named `control%alive_file` from unit `control%alive_unit`.

2.8 Further features

In this section, we describe an alternative means of setting control parameters, that is components of the variable `control` of type `TRB_control_type` (see Section 2.3.3), by reading an appropriate data specification file using the subroutine `TRB_read_specfile`. This facility is useful as it allows a user to change `TRB` control parameters without editing and recompiling programs that call `TRB`.

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 `TRB_read_specfile` must start with a "`BEGIN TRB`" command and end with an "`END`" command. The syntax of the specfile is thus defined as follows:

```
( .. lines ignored by TRB_read_specfile .. )
  BEGIN TRB
     keyword    value
     .......    .....
     keyword    value
  END
( .. lines ignored by TRB_read_specfile .. )
```

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

and

```
   END TRB SPECIFICATION
```

are acceptable. Furthermore, between the "`BEGIN TRB`" 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 `TRB_read_specfile` is called, and the associated device number passed to the routine in device (see below). Note that the corresponding file is `REWIND`ed, which makes it possible to combine the specifications for more than one program/routine. For the same reason, the file is not closed by `TRB_read_specfile`.

2.8.1 To read control parameters from a specification file

Control parameters may be read from a file as follows:

```
   CALL TRB_read_specfile( control, device )
```

control is a scalar `INTENT(INOUT)` argument of type `TRB_control_type` (see Section 2.3.3). Default values should have already been set, perhaps by calling `TRB_initialize`. On exit, individual components of `control` may have been changed according to the commands found in the specfile. Specfile commands and the component (see Section 2.3.3) of `control` that each affects are given in Table 2.1 on the following page.

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

2.9 Information printed

If `control%print_level` is positive, information about the progress of the algorithm will be printed on unit `control%out`. If `control%print_level` = 1, a single line of output will be produced for each iteration of the process. This will include the values of the objective function and the norm of its gradient, the ratio of actual to predicted decrease following the step, the radius of the trust-region and the time taken so far. In addition, if a direct solution of the subproblem has been attempted, the Lagrange multiplier from the secular equation and the number of factorizations used will be recorded, while if an iterative solution has been used, the numbers of phase 1 and 2 iterations will be given.

If `control%print_level` ≥ 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 variables and gradients. Further details concerning the attempted solution of the models may be obtained by increasing `control%TRS_control%print_level`, `control%PSLS_control%print_level` and `control%GLTR_control%print_level`, while details about factorizations are available by increasing `control%PSLS_control%print_level`. See the specification sheets for the packages `GALAHAD_GLTR`, `GALAHAD_PSLS` and `GALAHAD_TRS` for details.

---

command	component of control	value type
error-printout-device	%error	integer
printout-device	%out	integer
print-level	%print_level	integer
start-print	%start_print	integer
stop-print	%stop_print	integer
iterations-between-printing	%print_gap	integer
maximum-number-of-iterations	%maxit	integer
alive-device	%alive_unit	integer
more-toraldo-search-length	%more_toraldo	integer
history-length-for-non-monotone-descent	%non_monotone	integer
model-used	%model	integer
norm-used	%norm	integer
semi-bandwidth-for-band-norm	%semi_bandwidth	integer
number-of-lbfgs-vectors	%lbfgs_vectors	integer
max-number-of-secant-vectors	%max_dxg	integer
number-of-lin-more-vectors	%icfs_vectors	integer
mi28-l-fill-size	%mi28_lsize	integer
mi28-r-entry-size	%mi28_rsize	integer
advanced-start	%advanced_start	integer
infinity-value	%infinity	real
absolute-gradient-accuracy-required	%stop_g_absolute	real
relative-gradient-reduction-required	%stop_g_relative	real
minimum-relative-step-allowed	%stop_s	real
initial-trust-region-radius	%initial_radius	real
maximum-trust-region-radius	%maximum_radius	real
inner-iteration-relative-accuracy-required	stop_rel_cg	real
successful-iteration-tolerance	%eta_successful	real
very-successful-iteration-tolerance	%eta_very_successful	real
too-successful-iteration-tolerance	%eta_too_successful	real
trust-region-increase-factor	%radius_increase	real
trust-region-decrease-factor	%radius_reduce	real
trust-region-maximum-decrease-factor	%radius_reduce_max	real
minimum-objective-before-unbounded	%obj_unbounded	real
maximum-cpu-time-limit	%cpu_time_limit	real
maximum-clock-time-limit	%clock_time_limit	real
hessian-available	%hessian_available	logical
sub-problem-direct	%subproblem_direct	logical
retrospective-trust-region	%retrospective_trust_region	logical
renormalize-radius	%renormalize_radius	logical
two-norm-trust-region-used	%two_norm_tr	logical
exact-GCP-used	%exact_gcp	logical
subproblem-solved-accurately	%accurate_bqp	logical
space-critical	%space_critical	logical
deallocate-error-fatal	%deallocate_error_fatal	logical
alive-filename	%alive_file	character

Table 2.1: Specfile commands and associated components of control.

3 GENERAL INFORMATION

Use of common: None.

Workspace: Provided automatically by the module.

Other routines called directly: None.

Other modules used directly: `TRB_solve` calls the **GALAHAD** packages `GALAHAD_CLOCK`, `GALAHAD_NLPT`, `GALAHAD_SYMBOLS`, `GALAHAD_SPECFILE`, `GALAHAD_SLS`, `GALAHAD_PSLS`, `GALAHAD_GLTR`, `GALAHAD_TRS`, `LANCELOT_CAUCHY`, `LANCELOT_CG`, `GALAHAD_LMS`, `GALAHAD_SHA`, `GALAHAD_MOP`, `GALAHAD_STRINGS`, `GALAHAD_SPACE`, `GALAHAD_NORMS`, `GALAHAD_BLAS_interface`, and `GALAHAD_LAPACK_interface`.

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

Restrictions: `nlp%n` > 0 and `nlp%H_type` $\in \{$`'DENSE'`,`'COORDINATE'`,`'SPARSE_BY_ROWS'`,`'DIAGONAL'` $\}$.

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

4 METHOD

A trust-region method is used. In this, an improvement to a current estimate of the required minimizer, $\mathbf{x}_k$ is sought by computing a step $\mathbf{s}_k$. The step is chosen to approximately minimize a model $m_k(\mathbf{s})$ of $f(\mathbf{x}_k + \mathbf{s})$ within the intersection of the bound constraints $\mathbf{x}^l \leq \mathbf{x} \leq \mathbf{x}^u$ and a trust region $\|\mathbf{s}_k\| \leq \Delta_k$ for some specified positive "radius" Δ_k. The quality of the resulting step $\mathbf{s}_k$ is assessed by computing the "ratio" $(f(\mathbf{x}_k) - f(\mathbf{x}_k + \mathbf{s}_k))/(m_k(\mathbf{0}) - m_k(\mathbf{s}_k))$. The step is deemed to have succeeded if the ratio exceeds a given $\eta_s > 0$, and in this case $\mathbf{x}_{k+1} = \mathbf{x}_k + \mathbf{s}_k$. Otherwise $\mathbf{x}_{k+1} = \mathbf{x}_k$, and the radius is reduced by powers of a given reduction factor until it is smaller than $\|\mathbf{s}_k\|$. If the ratio is larger than $\eta_v \geq \eta_d$, the radius will be increased so that it exceeds $\|\mathbf{s}_k\|$ by a given increase factor. The method will terminate as soon as $\|\nabla_x f(\mathbf{x}_k)\|$ is smaller than a specified value.

Either linear or quadratic models $m_k(\mathbf{s})$ may be used. The former will be taken as the first two terms $f(\mathbf{x}_k) + \mathbf{s}^T \nabla_x f(\mathbf{x}_k)$ of a Taylor series about $\mathbf{x}_k$, while the latter uses an approximation to the first three terms $f(\mathbf{x}_k) + \mathbf{s}^T \nabla_x f(\mathbf{x}_k) + \frac{1}{2}\mathbf{s}^T \mathbf{B}_k \mathbf{s}$, for which $\mathbf{B}_k$ is a symmetric approximation to the Hessian $\nabla_{xx} f(\mathbf{x}_k)$; possible approximations include the true Hessian, limited-memory secant and sparsity approximations and a scaled identity matrix. Normally a two-norm trust region will be used, but this may change if preconditioning is employed.

The model minimization is carried out in two stages. Firstly, the so-called generalized Cauchy point for the quadratic subproblem is found—the purpose of this point is to ensure that the algorithm converges and that the set of bounds which are satisfied as equations at the solution is rapidly identified. Thereafter an improvement to the quadratic model on the face of variables predicted to be active by the Cauchy point is sought using either a direct approach involving factorization or an iterative (conjugate-gradient/Lanczos) approach based on approximations to the required solution from a so-called Krlov subspace. The direct approach is based on the knowledge that the required solution satisfies the linear system of equations $(\mathbf{B}_k + \lambda_k \mathbf{I})\mathbf{s}_k = -\nabla_x f(\mathbf{x}_k)$, involving a scalar Lagrange multiplier λ_k, on the space of inactive variables. This multiplier is found by uni-variate root finding, using a safeguarded Newton-like process, by `GALAHAD_TRS` or `GALAHAD_DPS` (depending on the norm chosen). The iterative approach uses `GALAHAD_GLTR`, and is best accelerated by preconditioning with good approximations to $\mathbf{B}_k$ using `GALAHAD_PSLS`. The iterative approach has the advantage that only matrix-vector products $\mathbf{B}_k \mathbf{v}$ are required, and thus $\mathbf{B}_k$ is not required explicitly. However when factorizations of $\mathbf{B}_k$ are possible, the direct approach is often more efficient.

The iteration is terminated as soon as the Euclidean norm of the projected gradient,

$$\| \min(\max(\mathbf{x}_k - \nabla_x f(\mathbf{x}_k), \mathbf{x}^l), \mathbf{x}^u) - \mathbf{x}_k \|_2,$$

---

is sufficiently small. At such a point, $\nabla_x f(\mathbf{x}_k) = \mathbf{z}_k$, where the i-th dual variable z_i is non-negative if x_i is on its lower bound x_i^l, non-positive if x_i is on its upper bound x_i^u, and zero if x_i lies strictly between its bounds.

References:

The generic bound-constrained trust-region method is described in detail in

A. R. Conn, N. I. M. Gould and Ph. L. Toint (2000). Trust-region methods. SIAM/MPS Series on Optimization.

5   EXAMPLES OF USE

Suppose we wish to minimize the parametric objective function $f(\mathbf{x}) = (x_1 + x_3 + p)^2 + (x_2 + x_3)^2 + \cos x_1$ when the parameter p takes the value 4, and x is required to satisfy the bounds $x_1 \leq -1.1$, $x_2 \leq -1.1$ and $0 \leq x_3 \leq -1.1$. Starting from the initial guess $\mathbf{x} = (1,1,1)$, we may use the following code:

```
  PROGRAM GALAHAD_TRB_EXAMPLE  !  GALAHAD 4.1 - 2022-12-29 AT 11:15 GMT
  USE GALAHAD_TRB_double                     ! double precision version
  IMPLICIT NONE
  INTEGER, PARAMETER :: wp = KIND( 1.0D+0 )    ! set precision
  TYPE ( NLPT_problem_type ):: nlp
  TYPE ( TRB_control_type ) :: control
  TYPE ( TRB_inform_type ) :: inform
  TYPE ( TRB_data_type ) :: data
  TYPE ( GALAHAD_userdata_type ) :: userdata
  EXTERNAL :: FUN, GRAD, HESS
  INTEGER :: s
  INTEGER, PARAMETER :: n = 3, h_ne = 5
  REAL ( KIND = wp ), PARAMETER :: p = 4.0_wp
  REAL ( KIND = wp ), PARAMETER :: infinity = 10.0_wp ** 20    ! infinity
! start problem data
  nlp%pname = 'TRBSPEC'                       ! name
  nlp%n = n ; nlp%H%ne = h_ne                 ! dimensions
  ALLOCATE( nlp%X( n ), nlp%G( n ), nlp%X_l( n ), nlp%X_u( n ) )
  nlp%X = 1.0_wp                              ! start from one
  nlp%X_l( : n )  = (/ - infinity, - infinity, 0.0_wp /) ; nlp%X_u = 1.1_wp
! sparse co-ordinate storage format
  CALL SMT_put( nlp%H%type, 'COORDINATE', s ) ! Specify co-ordinate storage
  ALLOCATE( nlp%H%val( h_ne ), nlp%H%row( h_ne ), nlp%H%col( h_ne ) )
  nlp%H%row = (/ 1, 3, 2, 3, 3 /)             ! Hessian H
  nlp%H%col = (/ 1, 1, 2, 2, 3 /)             ! NB lower triangle
! problem data complete
  ALLOCATE( userdata%real( 1 ) )              ! Allocate space for parameter
  userdata%real( 1 ) = p                      ! Record parameter, p
  CALL TRB_initialize( data, control, inform ) ! Initialize control parameters
  control%subproblem_direct = .FALSE.         ! Use an iterative method
  control%maxit = 10
! control%print_level = 1
  inform%status = 1                           ! set for initial entry
  CALL TRB_solve( nlp, control, inform, data, userdata, eval_F = FUN,      &
                  eval_G = GRAD, eval_H = HESS )  ! Solve problem
  IF ( inform%status == 0 ) THEN              ! Successful return
    WRITE( 6, "( ' TRB: ', I0, ' iterations -',                           &
  &    ' optimal objective value =',                                      &
  &       ES12.4, /, ' Optimal solution = ', ( 5ES12.4 ) )" )             &
    inform%iter, inform%obj, nlp%X
```

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See `http://galahad.rl.ac.uk/galahad-www/cou.html` **for full details.**

```
ELSE                                    ! Error returns
  WRITE( 6, "( ' TRB_solve exit status = ', I6 ) " ) inform%status
END IF
CALL TRB_terminate( data, control, inform )  ! delete internal workspace
DEALLOCATE( nlp%X, nlp%G, nlp%H%val, nlp%H%row, nlp%H%col, userdata%real )
END PROGRAM GALAHAD_TRB_EXAMPLE

SUBROUTINE FUN( status, X, userdata, f )    ! Objective function
USE GALAHAD_USERDATA_double, ONLY: GALAHAD_userdata_type
INTEGER, PARAMETER :: wp = KIND( 1.0D+0 )
INTEGER, INTENT( OUT ) :: status
REAL ( KIND = wp ), INTENT( OUT ) :: f
REAL ( KIND = wp ), DIMENSION( : ),INTENT( IN ) :: X
TYPE ( GALAHAD_userdata_type ), INTENT( INOUT ) :: userdata
f = ( X( 1 ) + X( 3 ) + userdata%real( 1 ) ) ** 2 +                    &
    ( X( 2 ) + X( 3 ) ) ** 2 + COS( X( 1 ) )
status = 0
RETURN
END SUBROUTINE FUN


SUBROUTINE GRAD( status, X, userdata, G )    ! gradient of the objective
USE GALAHAD_USERDATA_double, ONLY: GALAHAD_userdata_type
INTEGER, PARAMETER :: wp = KIND( 1.0D+0 )
INTEGER, INTENT( OUT ) :: status
REAL ( KIND = wp ), DIMENSION( : ), INTENT( IN ) :: X
REAL ( KIND = wp ), DIMENSION( : ), INTENT( OUT ) :: G
TYPE ( GALAHAD_userdata_type ), INTENT( INOUT ) :: userdata
G( 1 ) = 2.0_wp * ( X( 1 ) + X( 3 ) + userdata%real( 1 ) ) - SIN( X( 1 ) )
G( 2 ) = 2.0_wp * ( X( 2 ) + X( 3 ) )
G( 3 ) = 2.0_wp * ( X( 1 ) + X( 3 ) + userdata%real( 1 ) ) +           &
         2.0_wp * ( X( 2 ) + X( 3 ) )
status = 0
RETURN
END SUBROUTINE GRAD


SUBROUTINE HESS( status, X, userdata, Hval ) ! Hessian of the objective
USE GALAHAD_USERDATA_double, ONLY: GALAHAD_userdata_type
INTEGER, PARAMETER :: wp = KIND( 1.0D+0 )
INTEGER, INTENT( OUT ) :: status
REAL ( KIND = wp ), DIMENSION( : ), INTENT( IN ) :: X
REAL ( KIND = wp ), DIMENSION( : ), INTENT( OUT ) :: Hval
TYPE ( GALAHAD_userdata_type ), INTENT( INOUT ) :: userdata
Hval( 1 ) = 2.0_wp - COS( X( 1 ) )
Hval( 2 ) = 2.0_wp
Hval( 3 ) = 2.0_wp
Hval( 4 ) = 2.0_wp
Hval( 5 ) = 4.0_wp
status = 0
RETURN
END SUBROUTINE HESS
```

Notice how the parameter p is passed to the function evaluation routines via the `real` component of the derived type `userdata`. The code produces the following output:

```
TRB: 5 iterations - optimal objective value = -7.5897E-01
Optimal solution =  -3.7247E+00  0.0000E+00  0.0000E+00
```

If the Hessian is unavailable, but products of the form $\mathbf{u} + \mathbf{Hv}$ are, the same problem may be solved as follows:

```
    PROGRAM GALAHAD_TRB2_EXAMPLE  !  GALAHAD 4.1 - 2022-12-29 AT 11:15 GMT
    USE GALAHAD_TRB_double                     ! double precision version
    IMPLICIT NONE
    INTEGER, PARAMETER :: wp = KIND( 1.0D+0 )    ! set precision
    TYPE ( NLPT_problem_type ):: nlp
    TYPE ( TRB_control_type ) :: control
    TYPE ( TRB_inform_type ) :: inform
    TYPE ( TRB_data_type ) :: data
    TYPE ( GALAHAD_userdata_type ) :: userdata
    EXTERNAL :: FUN, GRAD, HESSPROD,  SHESSPROD
    INTEGER, PARAMETER :: n = 3, h_ne = 5
    REAL ( KIND = wp ), PARAMETER :: p = 4.0_wp
    REAL ( KIND = wp ), PARAMETER :: infinity = 10.0_wp ** 20    ! infinity
! start problem data
    nlp%n = n ; nlp%H%ne = h_ne                ! dimensions
    ALLOCATE( nlp%X( n ), nlp%G( n ), nlp%X_l( n ), nlp%X_u( n ) )
    nlp%X = 1.0_wp                             ! start from one
    nlp%X_l( : n )  = (/ - infinity, - infinity, 0.0_wp /) ; nlp%X_u = 1.1_wp
! problem data complete
    ALLOCATE( userdata%real( 1 ) )             ! Allocate space for parameter
    userdata%real( 1 ) = p                     ! Record parameter, p
    CALL TRB_initialize( data, control, inform ) ! Initialize control parameters
    control%hessian_available = .FALSE.        ! Hessian products will be used
!   control%print_level = 1
    inform%status = 1                          ! Set for initial entry
    CALL TRB_solve( nlp, control, inform, data, userdata, eval_F = FUN,      &
                    eval_G = GRAD, eval_HPROD = HESSPROD,                     &
                    eval_SHPROD = SHESSPROD )    ! Solve problem
    IF ( inform%status == 0 ) THEN             ! Successful return
      WRITE( 6, "( ' TRB: ', I0, ' iterations -',                            &
     &     ' optimal objective value =',                                     &
     &        ES12.4, /, ' Optimal solution = ', ( 5ES12.4 ) )" )            &
      inform%iter, inform%obj, nlp%X
    ELSE                                       ! Error returns
      WRITE( 6, "( ' TRB_solve exit status = ', I6 ) " ) inform%status
    END IF
    CALL TRB_terminate( data, control, inform )  ! delete internal workspace
    DEALLOCATE( nlp%X, nlp%G, userdata%real )
    END PROGRAM GALAHAD_TRB2_EXAMPLE

    SUBROUTINE FUN( status, X, userdata, f )     ! Objective function
    USE GALAHAD_USERDATA_double, ONLY: GALAHAD_userdata_type
    INTEGER, PARAMETER :: wp = KIND( 1.0D+0 )
    INTEGER, INTENT( OUT ) :: status
    REAL ( KIND = wp ), INTENT( OUT ) :: f
    REAL ( KIND = wp ), DIMENSION( : ),INTENT( IN ) :: X
    TYPE ( GALAHAD_userdata_type ), INTENT( INOUT ) :: userdata
    f = ( X( 1 ) + X( 3 ) + userdata%real( 1 ) ) ** 2 +                      &
        ( X( 2 ) + X( 3 ) ) ** 2 + COS( X( 1 ) )
    status = 0
    RETURN
    END SUBROUTINE FUN

    SUBROUTINE GRAD( status, X, userdata, G )    ! gradient of the objective
```

```
USE GALAHAD_USERDATA_double, ONLY: GALAHAD_userdata_type
INTEGER, PARAMETER :: wp = KIND( 1.0D+0 )
INTEGER, INTENT( OUT ) :: status
REAL ( KIND = wp ), DIMENSION( : ), INTENT( IN ) :: X
REAL ( KIND = wp ), DIMENSION( : ), INTENT( OUT ) :: G
TYPE ( GALAHAD_userdata_type ), INTENT( INOUT ) :: userdata
G( 1 ) = 2.0_wp * ( X( 1 ) + X( 3 ) + userdata%real( 1 ) ) - SIN( X( 1 ) )
G( 2 ) = 2.0_wp * ( X( 2 ) + X( 3 ) )
G( 3 ) = 2.0_wp * ( X( 1 ) + X( 3 ) + userdata%real( 1 ) ) +             &
         2.0_wp * ( X( 2 ) + X( 3 ) )
status = 0
RETURN
END SUBROUTINE GRAD

SUBROUTINE HESSPROD( status, X, userdata, U, V, got_h ) ! Hess-vector product
USE GALAHAD_USERDATA_double, ONLY: GALAHAD_userdata_type
INTEGER, PARAMETER :: wp = KIND( 1.0D+0 )
INTEGER, INTENT( OUT ) :: status
REAL ( KIND = wp ), DIMENSION( : ), INTENT( INOUT ) :: U
REAL ( KIND = wp ), DIMENSION( : ), INTENT( IN ) :: X, V
TYPE ( GALAHAD_userdata_type ), INTENT( INOUT ) :: userdata
LOGICAL, OPTIONAL, INTENT( IN ) :: got_h
U( 1 ) = U( 1 ) + 2.0_wp * ( V( 1 ) + V( 3 ) ) - COS( X( 1 ) ) * V( 1 )
U( 2 ) = U( 2 ) + 2.0_wp * ( V( 2 ) + V( 3 ) )
U( 3 ) = U( 3 ) + 2.0_wp * ( V( 1 ) + V( 2 ) + 2.0_wp * V( 3 ) )
status = 0
RETURN
END SUBROUTINE HESSPROD

SUBROUTINE SHESSPROD( status, X, userdata, nnz_v, INDEX_nz_v, V,          &
                      nnz_u, INDEX_nz_u, U, got_h )
USE GALAHAD_USERDATA_double, ONLY: GALAHAD_userdata_type
INTEGER, PARAMETER :: wp = KIND( 1.0D+0 )
INTEGER, INTENT( IN ) :: nnz_v
INTEGER, INTENT( OUT ) :: nnz_u
INTEGER, INTENT( OUT ) :: status
INTEGER, DIMENSION( : ), INTENT( IN ) :: INDEX_nz_v
INTEGER, DIMENSION( : ), INTENT( OUT ) :: INDEX_nz_u
REAL ( KIND = wp ), DIMENSION( : ), INTENT( IN ) :: X
REAL ( KIND = wp ), DIMENSION( : ), INTENT( OUT ) :: U
REAL ( KIND = wp ), DIMENSION( : ), INTENT( IN ) :: V
TYPE ( GALAHAD_userdata_type ), INTENT( INOUT ) :: userdata
LOGICAL, OPTIONAL, INTENT( IN ) :: got_h
INTEGER :: i, j
REAL ( KIND = wp ), DIMENSION( 3 ) :: P
LOGICAL, DIMENSION( 3 ) :: USED
P = 0.0_wp
USED = .FALSE.
DO i = 1, nnz_v
  j = INDEX_nz_v( i )
  SELECT CASE( j )
  CASE( 1 )
    P( 1 ) = P( 1 ) + 2.0_wp * V( 1 ) - COS( X( 1 ) ) * V( 1 )
    USED( 1 ) = .TRUE.
    P( 3 ) = P( 3 ) + 2.0_wp * V( 1 )
```

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See `http://galahad.rl.ac.uk/galahad-www/cou.html` **for full details.**

```
        USED( 3 ) = .TRUE.
      CASE( 2 )
        P( 2 ) = P( 2 ) + 2.0_wp * V( 2 )
        USED( 2 ) = .TRUE.
        P( 3 ) = P( 3 ) + 2.0_wp * V( 2 )
        USED( 3 ) = .TRUE.
      CASE( 3 )
        P( 1 ) = P( 1 ) + 2.0_wp * V( 3 )
        USED( 1 ) = .TRUE.
        P( 2 ) = P( 2 ) + 2.0_wp * V( 3 )
        USED( 2 ) = .TRUE.
        P( 3 ) = P( 3 ) + 4.0_wp * V( 3 )
        USED( 3 ) = .TRUE.
      END SELECT
    END DO
    nnz_u = 0
    DO j = 1, 3
      IF ( USED( j ) ) THEN
        U( j ) = P( j )
        nnz_u = nnz_u + 1
        INDEX_nz_u( nnz_u ) = j
      END IF
    END DO
    status = 0
    RETURN
    END SUBROUTINE SHESSPROD
```

Notice that storage for the Hessian is now not needed. This produces the same output.

If the user prefers to provide function and gradient information and Hessian-vector products without calls to specified routines, the following code is appropriate. Note the product with the user-provided preconditioner

$$\mathbf{P}(\mathbf{x}) = \left(\begin{array}{ccc} \frac{1}{2} & 0 & 0 \\ 0 & \frac{1}{2} & 0 \\ 0 & 0 & \frac{1}{4} \end{array} \right)$$

which is a suitable approximation to the inverse of the Hessian:

```
    PROGRAM GALAHAD_TRB3_EXAMPLE  !  GALAHAD 4.1 - 2022-12-29 AT 11:15 GMT
    USE GALAHAD_TRB_double                     ! double precision version
    IMPLICIT NONE
    INTEGER, PARAMETER :: wp = KIND( 1.0D+0 )    ! set precision
    TYPE ( NLPT_problem_type ):: nlp
    TYPE ( TRB_control_type ) :: control
    TYPE ( TRB_inform_type ) :: inform
    TYPE ( TRB_data_type ) :: data
    TYPE ( GALAHAD_userdata_type ) :: userdata
    INTEGER :: s
    INTEGER, PARAMETER :: n = 3, h_ne = 5
    REAL ( KIND = wp ), PARAMETER :: p = 4.0_wp
    REAL ( KIND = wp ), PARAMETER :: infinity = 10.0_wp ** 20    ! infinity
! start problem data
    nlp%n = n ; nlp%H%ne = h_ne                  ! dimensions
    ALLOCATE( nlp%X( n ), nlp%G( n ), nlp%X_l( n ), nlp%X_u( n ) )
    nlp%X = 1.0_wp                               ! start from one
    nlp%X_l( : n )  = (/ - infinity, - infinity, 0.0_wp /) ; nlp%X_u = 1.1_wp
! sparse co-ordinate storage format
```

```
   CALL SMT_put( nlp%H%type, 'COORDINATE', s )  ! Specify co-ordinate storage
   ALLOCATE( nlp%H%val( h_ne ), nlp%H%row( h_ne ), nlp%H%col( h_ne ) )
   nlp%H%row = (/ 1, 3, 2, 3, 3 /)              ! Hessian H
   nlp%H%col = (/ 1, 1, 2, 2, 3 /)              ! NB lower triangle
! problem data complete
   CALL TRB_initialize( data, control, inform ) ! Initialize control parameters
!  control%hessian_available = .FALSE.          ! Hessian products will be used
!  control%psls_control%preconditioner = - 3    ! Apply uesr's preconditioner
   inform%status = 1                            ! Set for initial entry
   DO                                           ! Loop to solve problem
     CALL TRB_solve( nlp, control, inform, data, userdata )
     SELECT CASE ( inform%status )              ! reverse communication
     CASE ( 2 )                                 ! Obtain the objective function
       nlp%f = ( nlp%X( 1 ) + nlp%X( 3 ) + p ) ** 2 +                       &
               ( nlp%X( 2 ) + nlp%X( 3 ) ) ** 2 + COS( nlp%X( 1 ) )
       data%eval_status = 0                     ! record successful evaluation
     CASE ( 3 )                                 ! Obtain the gradient
       nlp%G( 1 ) = 2.0_wp * ( nlp%X( 1 ) + nlp%X( 3 ) + p ) - SIN( nlp%X( 1 ) )
       nlp%G( 2 ) = 2.0_wp * ( nlp%X( 2 ) + nlp%X( 3 ) )
       nlp%G( 3 ) = 2.0_wp * ( nlp%X( 1 ) + nlp%X( 3 ) + p ) +             &
                    2.0_wp * ( nlp%X( 2 ) + nlp%X( 3 ) )
       data%eval_status = 0                     ! record successful evaluation
     CASE ( 4 )                                 ! Obtain Hessian evaluation
       nlp%H%val( 1 ) = 2.0_wp - COS( nlp%X( 1 ) )
       nlp%H%val( 2 ) = 2.0_wp
       nlp%H%val( 3 ) = 2.0_wp
       nlp%H%val( 4 ) = 2.0_wp
       nlp%H%val( 5 ) = 4.0_wp
       data%eval_status = 0                     ! record successful evaluation
     CASE ( 5 )                                 ! Obtain Hessian-vector product
       data%U( 1 ) = data%U( 1 ) + 2.0_wp * ( data%V( 1 ) + data%V( 3 ) ) -   &
                     COS( nlp%X( 1 ) ) * data%V( 1 )
       data%U( 2 ) = data%U( 2 ) + 2.0_wp * ( data%V( 2 ) + data%V( 3 ) )
       data%U( 3 ) = data%U( 3 ) + 2.0_wp * ( data%V( 1 ) + data%V( 2 ) +     &
                     2.0_wp * data%V( 3 ) )
       data%eval_status = 0                     ! record successful evaluation
     CASE ( 6 )                                 ! Apply the preconditioner
       data%U( 1 ) = 0.5_wp * data%V( 1 )
       data%U( 2 ) = 0.5_wp * data%V( 2 )
       data%U( 3 ) = 0.25_wp * data%V( 3 )
       data%eval_status = 0                     ! record successful evaluation
     CASE DEFAULT                               ! Terminal exit from loop
       EXIT
     END SELECT
   END DO
   IF ( inform%status == 0 ) THEN               ! Successful return
     WRITE( 6, "( ' TRB: ', I0, ' iterations -',                          &
    &   ' optimal objective value =',                                     &
    &     ES12.4, /, ' Optimal solution = ', ( 5ES12.4 ) )" )             &
     inform%iter, inform%obj, nlp%X
   ELSE                                         ! Error returns
     WRITE( 6, "( ' TRB_solve exit status = ', I6 ) " ) inform%status
   END IF
   CALL TRB_terminate( data, control, inform )  ! Delete internal workspace
   END PROGRAM GALAHAD_TRB3_EXAMPLE
```

This produces the following output:

```
TRB: 5 iterations - optimal objective value = -7.5897E-01
Optimal solution =  -3.7247E+00  0.0000E+00  0.0000E+00
```