



Science and
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GALAHAD

ICFS

USER DOCUMENTATION

GALAHAD Optimization Library version 4.1

1 SUMMARY

Given a symmetric matrix \mathbf{A} , this package **computes a symmetric, positive-definite approximation \mathbf{LL}^T using an incomplete Cholesky factorization**; the resulting matrix \mathbf{L} is lower triangular. Subsequently, the solution \mathbf{x} to the either of the linear systems $\mathbf{Lx} = \mathbf{b}$ and $\mathbf{L}^T \mathbf{x} = \mathbf{b}$ may be found for a given vector \mathbf{b} .

ATTRIBUTES — Versions: GALAHAD_ICFS_single, GALAHAD_ICFS_double. **Uses:** GALAHAD_SYMBOLS, GALAHAD_SPECFILE and GALAHAD_SPACE. **Date:** May 1998/December 2022. **Origin:** C.-J. Lin and J. J. Moré, Argonne National Laboratory, enhanced for modern fortran by N. I. M. Gould, Rutherford Appleton Laboratory. **Language:** Fortran 2003.

2 HOW TO USE THE PACKAGE

Access to the package requires a USE statement such as

Single precision version

```
USE GALAHAD_ICFS_single
```

Double precision version

```
USE GALAHAD_ICFS_double
```

The user is **strongly advised** to use the double precision version unless single precision corresponds to 8-byte arithmetic.

If it is required to use both modules at the same time, the derived types ICFS_control_type, ICFS_inform_type, ICFS_data_type and NLPT_userdata_type, (Section 2.1) and the subroutines ICFS_initialize, ICFS_factorize, ICFS_solve, ICFS_terminate, (Section 2.2) and ICFS_read_specfile (Section 2.4) must be renamed on one of the USE statements.

2.1 The derived data types

Four derived data types are accessible from the package.

2.1.1 The derived data type for holding control parameters

The derived data type ICFS_control_type is used to hold controlling data. Default values may be obtained by calling ICFS_initialize (see Section 2.2.1), while components may also be changed by calling GALAHAD_ICFS_read_spec (see Section 2.4.1). The components of ICFS_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 ICFS_analyse, ICFS_estimate and ICFS_terminate is suppressed if `error` ≤ 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 ICFS_analyse and ICFS_estimate 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 ≤ 0`. If `print_level > 01`, details of any data errors encountered will be reported. The default is `print_level = 0`.

`icfs_vectors` is a scalar variable of type default `INTEGER`, that holds the number of extra vectors of length n required by the incomplete Cholesky preconditioner. Usually, the larger the number, the better the preconditioner, but the more space and effort required to use it. Any negative value will be regarded as 0. The default is `icfs_vectors = 10`.

`shift` is a scalar variable of type default `REAL` (double precision in `GALAHAD_ICFS_double`), that holds an initial estimate of the shift α used so that the incomplete factorization of $\mathbf{A} + \mathbf{D}$ is positive definite, where \mathbf{D} is a diagonal matrix whose entries are no larger than α . This value α may subsequently be increased, as necessary, by the package, see `inform%shift`. The default is `shift = 0.0`.

`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 = ""`.

2.1.2 The derived data type for holding timing information

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

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

`factorize` is a scalar variable of type default `REAL` (double precision in `GALAHAD_ICFS_double`), that gives the CPU time spent factorizing the required matrices.

`solve` is a scalar variable of type default `REAL` (double precision in `GALAHAD_ICFS_double`), that gives the CPU time spent solving the resulting triangular systems.

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

`clock_factorize` is a scalar variable of type default `REAL` (double precision in `GALAHAD_ICFS_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_ICFS_double`), that gives the elapsed system clock time spent solving the resulting triangular systems.

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2.1.3 The derived data type for holding informational parameters

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

`status` is a scalar variable of type default `INTEGER`, that gives the exit status of the algorithm. See Section 2.3 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`.

`shift` is a scalar variable of type default `REAL` (double precision in `GALAHAD_ICFS_double`), that holds the final value of the shift α used so that the incomplete factorization of $\mathbf{A} + \mathbf{D}$ is positive definite, where \mathbf{D} is a diagonal matrix whose entries are no larger than α .

`time` is a scalar variable of type `ICFS_time_type` whose components are used to hold elapsed CPU and system clock times for the various parts of the calculation (see Section 2.1.2).

2.1.4 The derived data type for holding problem data

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

2.2 Argument lists and calling sequences

There are four procedures for user calls (see Section 2.4 for further features):

1. The subroutine `ICFS_initialize` is used to set default values, and initialize private data.
2. The subroutine `ICFS_factorize` is called to form the incomplete Cholesky factor \mathbf{L} from \mathbf{A} .
3. The subroutine `ICFS_triangular_solve` is called to solve either of the triangular systems $\mathbf{L}\mathbf{x} = \mathbf{b}$ or $\mathbf{L}^T\mathbf{x} = \mathbf{b}$ for given vectors \mathbf{b} .
4. The subroutine `ICFS_terminate` is provided to allow the user to automatically deallocate array components of the private data, allocated by `ICFS_factorize`, at the end of the solution process. It is important to do this if the data object is re-used for another matrix **with a different structure** since `ICFS_initialize` cannot test for this situation, and any existing associated targets will subsequently become unreachable.

We note that in addition to the above calls, the user may also call the original fortran 77 subroutines `DICFS` and `DSTRSOL` directly. For details of the necessary argument lists, please see source code for the package.

2.2.1 The initialization subroutine

Default values are provided as follows:

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

`data` is a scalar `INTENT(INOUT)` argument of type `ICFS_data_type` (see Section 2.1.4). It is used to hold data about the matrix and its factors.

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`control` is a scalar `INTENT(OUT)` argument of type `ICFS_control_type` (see Section 2.1.1). On exit, `control` contains default values for the components as described in Section 2.1.1. These values should only be changed after calling `ICFS_initialize`.

`inform` is a scalar `INTENT(OUT)` argument of type `ICFS_inform_type` (see Section 2.1.3). A successful call to `ICFS_initialize` is indicated when the component status has the value 0. For other return values of status, see Section 2.3.

2.2.2 The incomplete factorization subroutine

The factorization phase, in which incomplete Cholesky factors \mathbf{L} of \mathbf{A} are determined, is performed as follows:

```
CALL ICFS_factorize( n, PTR, ROW, DIAG, VAL, data, control, inform )
```

`n` is a scalar `INTENT(IN)` scalar argument of type default `INTEGER`, that must be set to n the dimension of the matrix \mathbf{A} . **Restrictions:** $n > 0$.

`PTR` is a scalar `INTENT(IN)` rank-one array argument of type default `INTEGER` and dimension $n + 1$, whose j -th component gives the starting address for list of nonzero values and their corresponding row indices in column j of the **strict lower triangular part** of \mathbf{A} (The entry $a_{i,j}$ is in the strict lower triangular part of \mathbf{A} if $i > j$). That is, the nonzeros in column j of the strict lower triangle of \mathbf{A} must be in positions `PTR(j) ... PTR(j+1) - 1` for $j = 1, \dots, n$. Note that `PTR(n+1)` points to the first position beyond that needed to store \mathbf{A} .

`ROW` is a scalar `INTENT(IN)` rank-one array argument of type default `INTEGER` and dimension at least `PTR(n+1)-1`, that contains the row indices of the strict lower triangular part of \mathbf{A} in the compressed column storage format described above.

`DIAG` is a scalar `INTENT(IN)` rank-one array argument of type default `REAL` (double precision in `GALAHAD_ICFS_`-double) and dimension n , whose j -th component contains the value of the j -th diagonal of \mathbf{A} .

`VAL` is a scalar `INTENT(IN)` rank-one array argument of type default `REAL` (double precision in `GALAHAD_ICFS_`-double) and dimension at least `PTR(n+1)-1`, that contains the values of the entries strict lower triangular part of \mathbf{A} that correspond to the row indices described above.

`data` is a scalar `INTENT(INOUT)` argument of type `ICFS_data_type` (see Section 2.1.4). 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 `ICFS_initialize`.

`control` is a scalar `INTENT(IN)` argument of type `ICFS_control_type` (see Section 2.1.1). Default values may be assigned by calling `ICFS_initialize` prior to the first call to `ICFS_analyse`.

`inform` is a scalar `INTENT(INOUT)` argument of type `ICFS_inform_type` (see Section 2.1.3). A successful call to `ICFS_analyse` is indicated when the component status has the value 0. For other return values of status, see Section 2.3.

2.2.3 The triangular solution subroutine

The solution phase, in which one of the triangular systems $\mathbf{Lx} = \mathbf{b}$ or $\mathbf{L}^T \mathbf{x} = \mathbf{b}$ for given vectors \mathbf{b} , is performed as follows:

```
CALL ICFS_triangular_solve( n, X, transpose, data, control, inform )
```

`n`, `data`, `control` and `inform` are exactly as described and input to `ICFS_factorize`, and must not have been changed in the interim.

`X` is a scalar `INTENT(INOUT)` rank-one array argument of type default `REAL` (double precision in `GALAHAD_ICFS_`-double), and dimension n , that must be set on input so that `X(i)` contains the component b_i , $i = 1, \dots, n$ of the vector \mathbf{b} . On output, this will have been overwritten by the desired vector \mathbf{x} .

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`transpose` is a scalar `INTENT(IN)` argument of type default `LOGICAL`, that must be set `.FALSE.` if the user wishes to solve $\mathbf{Lx} = \mathbf{b}$ and `.TRUE.` if instead the solution to $\mathbf{L}^T \mathbf{x} = \mathbf{b}$ is sought.

2.2.4 The termination subroutine

All previously allocated arrays are deallocated as follows:

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

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

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

`inform` is a scalar `INTENT(OUT)` argument of type `ICFS_inform_type` exactly as for `ICFS_factorize`. Only the component `status` will be set on exit, and a successful call to `ICFS_terminate` is indicated when this component `status` has the value 0. For other return values of `status`, see Section 2.3.

2.3 Warning and error messages

A negative value of `inform%status` on exit from `ICFS_factorize`, `ICFS_triangular_solve` or `ICFS_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 $0 < n$ has been violated.

2.4 Further features

In this section, we describe an alternative means of setting control parameters, that is components of the variable `control` of type `ICFS_control_type` (see Section 2.1.1), by reading an appropriate data specification file using the subroutine `ICFS_read_specfile`. This facility is useful as it allows a user to change ICFS control parameters without editing and recompiling programs that call ICFS.

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

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```
( .. lines ignored by ICFS_read_specfile .. )
BEGIN ICFS
  keyword      value
  .....      .....
  keyword      value
END
( .. lines ignored by ICFS_read_specfile .. )
```

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

and

```
END ICFS SPECIFICATION
```

are acceptable. Furthermore, between the “BEGIN ICFS” 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 `ICFS_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 `ICFS_read_specfile`.

2.4.1 To read control parameters from a specification file

Control parameters may be read from a file as follows:

```
CALL ICFS_read_specfile( control, device )
```

`control` is a scalar `INTENT(INOUT)` argument of type `ICFS_control_type` (see Section 2.1.1). Default values should have already been set, perhaps by calling `ICFS_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 2.1.1) of `control` that each affects are given in Table 2.1.

`device` is a scalar `INTENT(IN)` argument of type default `INTEGER`, 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`.

2.5 Information printed

If `control%print_level` is positive, information about errors encountered will be printed on unit `control%out`.

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command	component of control	value type
error-printout-device	%error	integer
printout-device	%out	integer
print-level	%print_level	integer
number-of-icfs-vectors	icfs_vectors	integer
initial-shift	shift	real
space-critical	%space_critical	logical
deallocate-error-fatal	%deallocate_error_fatal	logical
output-line-prefix	%prefix	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: The module uses the GALAHAD packages `GALAHAD_SYMBOLS`, `GALAHAD_SPECFILE` and `GALAHAD_SPACE`.

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

Restrictions: $n > 0$.

Portability: ISO Fortran 2003. The package is thread-safe.

4 METHOD

The package computes incomplete Cholesky factors \mathbf{L} of \mathbf{A} so that

$$\mathbf{A} + \mathbf{D} = \mathbf{L}\mathbf{L} + \mathbf{E}.$$

The pattern of entries in \mathbf{L} match those in \mathbf{A} with additional “fill-ins” controlled by the extra storage provided. The shifted diagonal \mathbf{D} whose values do not exceed a scalar shift α allows for indefinite \mathbf{A} , and also guarantees stable factors \mathbf{L} . Increasing the extra storage provided generally decreases the size of the error matrix \mathbf{E} , but increases the cost of the algorithm.

Reference:

The method is described in detail in

C.J. Lin and J. J. Moreé. “Incomplete Cholesky factorizations with limited memory”. *SIAM J. Sci. Computing*. **21** (1999) 24–45.

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5 EXAMPLES OF USE

Suppose that

$$\mathbf{A} = \begin{pmatrix} 2 & 1 & & & \\ 1 & 5 & 1 & & 1 \\ & 1 & 1 & 1 & \\ & & 1 & 7 & \\ 1 & & & & 2 \end{pmatrix} \quad \text{and} \quad \mathbf{b} = \begin{pmatrix} 3 \\ 8 \\ 3 \\ 8 \\ 3 \end{pmatrix},$$

where the missing entries in \mathbf{A} are structural zeros. Then we may find suitable incomplete factors \mathbf{L} , and subsequently solve $\mathbf{L}\mathbf{y} = \mathbf{b}$ and $\mathbf{L}^T\mathbf{x} = \mathbf{y}$ using the following code; notice that we initialize \mathbf{b} in \mathbf{x} , overwrite this with \mathbf{y} in the first triangular solve, and finally recover \mathbf{x} from \mathbf{y} in the second solve:

```
PROGRAM ICFS_EXAMPLE ! GALAHAD 4.1 - 2022-12-04 AT 09:30 GMT.
USE GALAHAD_ICFS_double
IMPLICIT NONE
INTEGER, PARAMETER :: wp = KIND( 1.0D+0 )
TYPE ( ICFS_data_type ) :: data
TYPE ( ICFS_control_type ) control
TYPE ( ICFS_inform_type ) :: inform
INTEGER, PARAMETER :: n = 5
INTEGER, PARAMETER :: ne = 5
INTEGER, ALLOCATABLE, DIMENSION( : ) :: PTR, ROW
REAL ( KIND = wp ), ALLOCATABLE, DIMENSION( : ) :: DIAG, VAL
REAL ( KIND = wp ) :: X( n )
! allocate and set lower triangle of matrix in sparse by column form
ALLOCATE( PTR( n + 1 ), DIAG( n ), VAL( ne ), ROW( ne ) )
PTR = (/ 1, 2, 4, 5, 5, 5 /)
ROW = (/ 2, 3, 5, 4 /)
DIAG = (/ 2.0_wp, 5.0_wp, 1.0_wp, 7.0_wp, 2.0_wp /)
VAL = (/ 1.0_wp, 1.0_wp, 1.0_wp, 1.0_wp /)
! problem setup complete
CALL ICFS_initialize( data, control, inform )
control%icfs_vectors = 1
! form and factorize the preconditioner, P = L L^T
CALL ICFS_factorize( n, PTR, ROW, DIAG, VAL, data, control, inform )
IF ( inform%status < 0 ) THEN
    WRITE( 6, '( A, I0 )' )
    ' Failure of ICFS_factorize with status = ', inform%status
    STOP
END IF
! use the factors to solve L L^T x = b, with b input in x
X( : n ) = (/ 3.0_wp, 8.0_wp, 3.0_wp, 8.0_wp, 3.0_wp /)
CALL ICFS_triangular_solve( n, X, .FALSE., data, control, inform )
CALL ICFS_triangular_solve( n, X, .TRUE., data, control, inform )
IF ( inform%status == 0 ) THEN
    WRITE( 6, "( ' ICFS - Preconditioned solution is ', 5F6.2 )" ) X
ELSE
    WRITE( 6, "( ' ICFS - exit status = ', I0 )" ) inform%status
END IF
! clean up
CALL ICFS_terminate( data, control, inform )
DEALLOCATE( DIAG, VAL, ROW, PTR )
STOP
END PROGRAM ICFS_EXAMPLE
```

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The code produces the following output:

```
ICFS - Preconditioned solution is  1.00  1.00  1.00  1.00  1.00
```

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