

## C interfaces to GALAHAD SLS

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GALAHAD C package sha	1
1.1 Introduction	1
1.1.1 Purpose	1
1.1.2 Authors	1
1.1.3 Originally released	1
File Index	3
2.1 File List	3
File Documentation	5
3.1 galahad_sha.h File Reference	5
3.1.1 Data Structure Documentation	5
3.1.1.1 struct sha_control_type	5
3.1.1.2 struct sha_inform_type	6

# **Chapter 1**

# GALAHAD C package sls

#### 1.1 Introduction

#### 1.1.1 Purpose

This package solves dense or sparse symmetric systems of linear equations using variants of Gaussian elimination. Given a sparse symmetric  $n \times n$  matrix A, and an n-vector b, this subroutine solves the system Ax = b. The matrix A need not be definite.

The package provides a common interface to a variety of well-known solvers from HSL and elsewhere. Currently supported solvers include MA27/SILS, HSL\_MA57, HSL\_MA77, HSL\_MA86, HSL\_MA87 and HSL\_MA97 from HSL, SSIDS from SPRAL, MUMPS from Mumps Technologies, PARDISO both from the Pardiso Project and Intel's MKL, PaStix from Inria and WSMP from the IBM alpha Works, as well as POTR, SYTR and SBTR from LAPACK. Note that the solvers themselves do not form part of this package and must be obtained separately. Dummy instances are provided for solvers that are unavailable. Also note that additional flexibility may be obtained by calling the solvers directly rather that via this package.

#### 1.1.2 Authors

N. I. M. Gould, STFC-Rutherford Appleton Laboratory, England.

C interface, additionally J. Fowkes, STFC-Rutherford Appleton Laboratory.

Julia interface, additionally A. Montoison and D. Orban, Polytechnique Montréal.

## 1.1.3 Originally released

August 2009, C interface December 2021.

## 1.1.4 Terminology

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

$$A + E = PLDL^T P^T$$
,

where P is a permutation matrix and E is any diagonal perturbation introduced.

## 1.1.5 Supported external solvers

The key features of the external solvers supported by sls are given in the following table.

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

Table 1.1 External solver characteristics

#### 1.1.6 Method

Variants of sparse Gaussian elimination are used.

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

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

The solvers <code>HSL\_MA57</code>, <code>HSL\_MA77</code>, <code>HSL\_MA86</code>, <code>HSL\_MA87</code> and <code>HSL\_MA97</code>, the ordering packages <code>MC61</code> and <code>HSL\_MC68</code>, and the scaling packages <code>HSL\_MC64</code> and <code>MC77</code> are all part of <code>HSL 2011</code>. To obtain <code>HSL 2011</code> packages, see

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

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

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

```
https://mumps-solver.org.
```

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

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

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

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

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

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

1.1 Introduction 3

The solver WSMP is available from the IBM alpha Works; version 10.9 or above is required. To obtain WSMP, see http://www.alphaworks.ibm.com/tech/wsmp.

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

Explicit sparsity re-orderings are obtained by calling the HSL package  ${\tt HSL\_MC68}$ . Both this,  ${\tt HSL\_MA57}$  and  ${\tt PARDISO}$  rely optionally on the ordering package  ${\tt MeTiS}$  (version 4) from the Karypis Lab. To obtain  ${\tt METIS}$ , see

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

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

#### 1.1.7 Reference

The methods used are described in the user-documentation for

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

and papers

- E. Agullo, P. R. Amestoy, A. Buttari, J.-Y. L'Excellent, A. Guermouche and F.-H. Rouet, `Robust memory-aware mappings for parallel multifrontal factorizations'. SIAM Journal on Scientific Computing, **38**(3) (2016), C256–C279,
- P. R. Amestoy, I. S. Duff, J. Koster and J.-Y. L'Excellent. `A fully asynchronous multifrontal solver using distributed dynamic scheduling'. SIAM Journal on Matrix Analysis and Applications **23**(1) (2001) 15-41,
- A. Gupta, `'WSMP: Watson Sparse Matrix Package Part I direct solution of symmetric sparse systems''. IBM Research Report RC 21886, IBM T. J. Watson Research Center, NY 10598, USA (2010),
- P. Henon, P. Ramet and J. Roman, `'PaStiX: A High-Performance Parallel Direct Solver for Sparse Symmetric Definite Systems''. Parallel Computing, **28**(2) (2002) 301–321,
- J.D. Hogg, E. Ovtchinnikov and J.A. Scott. `'A sparse symmetric indefinite direct solver for GPU architectures''. ACM Transactions on Mathematical Software **42**(1) (2014), Article 1,
- O. Schenk and K. Gärtner, `'Solving Unsymmetric Sparse Systems of Linear Equations with PARDISO". Journal of Future Generation Computer Systems , 20(3) (2004) 475–487, and
- O. Schenk and K. Gärtner, `'On fast factorization pivoting methods for symmetric indefinite systems''. Electronic Transactions on Numerical Analysis **23** (2006) 158–179.

#### 1.1.8 Call order

To solve a given problem, functions from the sls package must be called in the following order:

- sls initialize provide default control parameters and set up initial data structures
- sls\_read\_specfile (optional) override control values by reading replacement values from a file
- sls\_analyse\_matrix set up matrix data structures and analyse the structure to choose a suitable order for factorization
- sls reset control (optional) possibly change control parameters if a sequence of problems are being solved
- $sls_factorize_matrix$  form and factorize the matrix A
- · one of
  - sls solve system solve the linear system of equations Ax = b
  - sls\_partial\_solve\_system solve a linear system Mx = b involving one of the matrix factors M of A
- sls information (optional) recover information about the solution and solution process
- sls\_terminate deallocate data structures

See Section ?? for examples of use.

## 1.1.9 Symmetric matrix storage formats

The symmetric n by n coefficient matrix A may be presented and stored in a variety of convenient input formats. Crucially symmetry is exploited by only storing values from the lower triangular part (i.e, those entries that lie on or below the leading diagonal).

Both C-style (0 based) and fortran-style (1-based) indexing is allowed. Choose control.f\_indexing as false for C style and true for fortran style; the discussion below presumes C style, but add 1 to indices for the corresponding fortran version.

Wrappers will automatically convert between 0-based (C) and 1-based (fortran) array indexing, so may be used transparently from C. This conversion involves both time and memory overheads that may be avoided by supplying data that is already stored using 1-based indexing.

#### 1.1.9.1 Dense storage format

The matrix A is stored as a compact dense matrix by rows, that is, the values of the entries of each row in turn are stored in order within an appropriate real one-dimensional array. Since A is symmetric, only the lower triangular part (that is the part  $A_{ij}$  for  $0 \le j \le i \le n-1$ ) need be held. In this case the lower triangle should be stored by rows, that is component i\*i/2+j of the storage array val will hold the value  $A_{ij}$  (and, by symmetry,  $A_{ji}$ ) for  $0 \le j \le i \le n-1$ .

#### 1.1.9.2 Sparse co-ordinate storage format

Only the nonzero entries of the matrices are stored. For the l-th entry,  $0 \le l \le ne-1$ , of A, its row index i, column index j and value  $A_{ij}$ ,  $0 \le j \le i \le n-1$ , are stored as the l-th components of the integer arrays row and col and real array val, respectively, while the number of nonzeros is recorded as ne = ne. Note that only the entries in the lower triangle should be stored.

#### 1.1.9.3 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 A the i-th component of the integer array ptr holds the position of the first entry in this row, while ptr(n) holds the total number of entries. The column indices j,  $0 \le j \le i$ , and values  $A_{ij}$  of the entries in the i-th row are stored in components  $I = ptr(i), \ldots, ptr(i+1)-1$  of the integer array col, and real array 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.

# Chapter 2

# File Index

_				
2	1	Fil	ΔI	iet

Here is a list of all files with brief descriptions:	
galahad_sls.h	??

6 File Index

# **Chapter 3**

## **File Documentation**

## 3.1 galahad\_sls.h File Reference

```
#include <stdbool.h>
#include "galahad_precision.h"
#include "galahad_cfunctions.h"
#include "galahad_sils.h"
#include "hsl_ma57.h"
#include "hsl_ma77.h"
#include "hsl_ma86.h"
#include "hsl_ma87.h"
#include "hsl_ma97.h"
#include "spral_ssids.h"
#include "hsl_mc64.h"
#include "hsl_mc68.h"
```

#### **Data Structures**

- struct sls\_control\_type
- struct sls\_time\_type
- struct sls\_inform\_type

#### **Functions**

- void sls\_initialize (const char solver[], void \*\*data, struct sls\_control\_type \*control, int \*status)
- void sls\_read\_specfile (struct sls\_control\_type \*control, const char specfile[])
- void sls\_analyse\_matrix (struct sls\_control\_type \*control, void \*\*data, int \*status, int n, const char type[], int ne, const int row[], const int col[], const int ptr[])
- void sls\_reset\_control (struct sls\_control\_type \*control, void \*\*data, int \*status)
- void sls\_factorize\_matrix (void \*\*data, int \*status, int ne, const real\_wp\_val[])
- void sls\_solve\_system (void \*\*data, int \*status, int n, real\_wp\_ sol[])
- void sls\_partial\_solve\_system (const char part[], void \*\*data, int \*status, int n, real\_wp\_ sol[])
- void sls\_information (void \*\*data, struct sls\_inform\_type \*inform, int \*status)
- void sls\_terminate (void \*\*data, struct sls\_control\_type \*control, struct sls\_inform\_type \*inform)

## 3.1.1 Data Structure Documentation

## 3.1.1.1 struct sls\_control\_type

control derived type as a C struct

## Examples

slst.c, and slstf.c.

#### **Data Fields**

bool	f_indexing	use C or Fortran sparse matrix indexing
int	error	unit for error messages
int	warning	unit for warning messages
int	out	unit for monitor output
int	statistics	unit for statistical output
int	print_level	controls level of diagnostic output
int	print_level_solver	controls level of diagnostic output from external solver
int	bits	number of bits used in architecture
int	block_size_kernel	the target blocksize for kernel factorization
int	block_size_elimination	the target blocksize for parallel elimination
int	blas_block_size_factorize	level 3 blocking in factorize
int	blas_block_size_solve	level 2 and 3 blocking in solve
int	node_amalgamation	a child node is merged with its parent if they both involve fewer than node_amalgamation eliminations
int	initial_pool_size	initial size of task-pool arrays for parallel elimination
int	min_real_factor_size	initial size for real array for the factors and other data
int	min_integer_factor_size	initial size for integer array for the factors and other data
int64_t	max_real_factor_size	maximum size for real array for the factors and other data
int64_t	max_integer_factor_size	maximum size for integer array for the factors and other data
int64_t	max_in_core_store	amount of in-core storage to be used for out-of-core factorization
real_wp_	array_increase_factor	factor by which arrays sizes are to be increased if they are too small
real_wp_	array_decrease_factor	if previously allocated internal workspace arrays are greater than array_decrease_factor times the currently required sizes, they are reset to current requirements
int	pivot_control	pivot control:
		1 Numerical pivoting will be performed.
		<ul> <li>2 No pivoting will be performed and an error exit will occur immediately a pivot sign change is detected.</li> </ul>
		<ul> <li>3 No pivoting will be performed and an error exit will occur if a zero pivot is detected.</li> </ul>
		<ul> <li>4 No pivoting is performed but pivots are changed to all be positive</li> </ul>

## Data Fields

int	ordoring	controls ordering (ignored if explicit DEDM exercises)
int	ordering	controls ordering (ignored if explicit PERM argument present)
		<ul> <li>&lt;0 chosen by the specified solver with its own ordering-selected value -ordering</li> </ul>
		<ul> <li>0 chosen package default (or the AMD ordering if no package default)</li> </ul>
		<ul> <li>1 Approximate minimum degree (AMD) with provisions for "dense" rows/col</li> </ul>
		2 Minimum degree
		3 Nested disection
		<ul> <li>4 indefinite ordering to generate a combination of 1x1 and 2x2 pivots</li> </ul>
		5 Profile/Wavefront reduction
		6 Bandwidth reduction
		<ul> <li>&gt;6 ordering chosen depending on matrix characteristics (not yet implemented)</li> </ul>
int	full_row_threshold	controls threshold for detecting full rows in analyse, registered as percentage of matrix order. If 100, only fully dense rows detected (defa
int	row_search_indefinite	number of rows searched for pivot when using indefinite ordering
int	scaling	controls scaling (ignored if explicit SCALE argument present)
		<ul> <li>&lt;0 chosen by the specified solver with its own scaling-selected value -scaling</li> </ul>
		0 No scaling
		1 Scaling using HSL's MC64
		<ul> <li>2 Scaling using HSL's MC77 based on the row one-norm</li> </ul>
		<ul> <li>3 Scaling using HSL's MC77 based on the row infinity-norm</li> </ul>
int	scale_maxit	the number of scaling iterations performed (default 10 used if .scale_maxit $<$ 0)
real_wp_	scale_thresh	the scaling iteration stops as soon as the row/column norms are less than 1+/scale_thresh
real_wp_	relative_pivot_tolerance	pivot threshold
real_wp_	minimum_pivot_tolerance	smallest permitted relative pivot threshold
real_wp_	absolute_pivot_tolerance	any pivot small than this is considered zero
real_wp_	zero_tolerance	any entry smaller than this is considered zero
real_wp_	zero_pivot_tolerance	any pivot smaller than this is considered zero for positive-definite sol
real_wp_	negative_pivot_tolerance	any pivot smaller than this is considered to be negative for p-d solvers

## **Data Fields**

real_wp_	static_pivot_tolerance	used for setting static pivot level
real_wp_	static_level_switch	used for switch to static
real_wp_	consistency_tolerance	used to determine whether a system is consistent when seeking a Fredholm alternative
int	max_iterative_refinements	maximum number of iterative refinements allowed
real_wp_	acceptable_residual_relative	refinement will cease as soon as the residual $  Ax-b  $ falls below max( acceptable_residual_relative $*$ $  b  $ , acceptable_residual_absolute
real_wp_	acceptable_residual_absolute	see acceptable_residual_relative
bool	multiple_rhs	set .multiple_rhs to .true. if there is possibility that the solver will be required to solve systems with more than one right-hand side. More efficient execution may be possible when .multiple_rhs = .false.
bool	generate_matrix_file	if .generate_matrix_file is .true. if a file describing the current matrix is to be generated
int	matrix_file_device	specifies the unit number to write the input matrix (in co-ordinate form
char	matrix_file_name[31]	name of generated matrix file containing input problem
char	out_of_core_directory[401]	directory name for out of core factorization and additional real workspace in the indefinite case, respectively
char	out_of_core_integer_factor_file[401]	out of core superfile names for integer and real factor data, real works and additional real workspace in the indefinite case, respectively
char	out_of_core_real_factor_file[401]	see out_of_core_integer_factor_file
char	out_of_core_real_work_file[401]	see out_of_core_integer_factor_file
char	out_of_core_indefinite_file[401]	see out_of_core_integer_factor_file
char	out_of_core_restart_file[501]	see out_of_core_integer_factor_file
char	prefix[31]	all output lines will be prefixed by prefix(2:LEN(TRIM(.prefix))-1) where prefix contains the required string enclosed in quotes, e.g. "string" or 'string'

## 3.1.1.2 struct sls\_time\_type

time derived type as a C struct

## Data Fields

real_wp_	total	the total cpu time spent in the package
real_wp_	analyse	the total cpu time spent in the analysis phase
real_wp_	factorize	the total cpu time spent in the factorization phase
real_wp_	solve	the total cpu time spent in the solve phases
real_wp_	order_external	the total cpu time spent by the external solver in the ordering phase
real_wp_	analyse_external	the total cpu time spent by the external solver in the analysis phase
real_wp_	factorize_external	the total cpu time spent by the external solver in the factorization pha
real_wp_	solve_external	the total cpu time spent by the external solver in the solve phases
real_wp_	clock_total	the total clock time spent in the package
real_wp_	clock_analyse	the total clock time spent in the analysis phase
real_wp_	clock_factorize	the total clock time spent in the factorization phase

## Data Fields

real_wp_	clock_solve	the total clock time spent in the solve phases
real_wp_	clock_order_external	the total clock time spent by the external solver in the ordering phase
real_wp_	clock_analyse_external	the total clock time spent by the external solver in the analysis phase
real_wp_	clock_factorize_external	the total clock time spent by the external solver in the factorization p
real_wp_	clock_solve_external	the total clock time spent by the external solver in the solve phases

## 3.1.1.3 struct sls\_inform\_type

inform derived type as a C struct

## Examples

slst.c, and slstf.c.

## Data Fields

int	status	reported return status: 0 success -1 allocation error -2 deallocation error -3 matrix data faulty (.n < 1, .ne < 0) -20 alegedly +ve definite matrix is not -29 unavailable option -31 input order is not a permutation or is faulty in some other way -32 > control.max_integer_factor_size integer space required for factor -33 > control.max_real_factor_size real space required for factors -40 not possible to alter the diagonals -41 no access to permutation or pivot sequence used -42 no access to diagonal perturbations -43 direct-access file error -50 solver-specific error; see the solver's info parameter -101 unknown solver
int	alloc_status	STAT value after allocate failure.
char	bad_alloc[81]	name of array which provoked an allocate failure
int	more_info	further information on failure
int	entries	number of entries
int	out_of_range	number of indices out-of-range
int	duplicates	number of duplicates
int	upper	number of entries from the strict upper triangle
int	missing_diagonals	number of missing diagonal entries for an allegedly-definite matrix
int	max_depth_assembly_tree	maximum depth of the assembly tree
int	nodes_assembly_tree	nodes in the assembly tree (= number of elimination steps)
int64_t	real_size_desirable	desirable or actual size for real array for the factors and other data
int64_t	integer_size_desirable	desirable or actual size for integer array for the factors and other dat
int64_t	real_size_necessary	necessary size for real array for the factors and other data
int64_t	integer_size_necessary	necessary size for integer array for the factors and other data
int64_t	real_size_factors	predicted or actual number of reals to hold factors

## **Data Fields**

int64_t	integer_size_factors	predicted or actual number of integers to hold
int64_t	entries_in_factors	factors number of entries in factors
int	max_task_pool_size	maximum number of tasks in the factorization task
III	max_task_pool_size	pool
int	max_front_size	forecast or actual size of largest front
int	compresses_real	number of compresses of real data
int	compresses_integer	number of compresses of integer data
int	two_by_two_pivots	number of 2x2 pivots
int	semi_bandwidth	semi-bandwidth of matrix following bandwidth reduction
int	delayed_pivots	number of delayed pivots (total)
int	pivot_sign_changes	number of pivot sign changes if no pivoting is used successfully
int	static_pivots	number of static pivots chosen
int	first_modified_pivot	first pivot modification when static pivoting
int	rank	estimated rank of the matrix
int	negative_eigenvalues	number of negative eigenvalues
int	num_zero	number of pivots that are considered zero (and ignored)
int	iterative_refinements	number of iterative refinements performed
int64_t	flops_assembly	anticipated or actual number of floating-point operations in assembly
int64_t	flops_elimination	anticipated or actual number of floating-point operations in elimination
int64_t	flops_blas	additional number of floating-point operations for BLAS
real_wp_	largest_modified_pivot	largest diagonal modification when static pivoting or ensuring definiten
real_wp_	minimum_scaling_factor	minimum scaling factor
real_wp_	maximum_scaling_factor	maximum scaling factor
real_wp_	condition_number_1	esimate of the condition number of the matrix (category 1 equations)
real_wp_	condition_number_2	estimate of the condition number of the matrix (category 2 equations)
real_wp_	backward_error_1	esimate of the backward error (category 1 equations)
real_wp_	backward_error_2	esimate of the backward error (category 2 equations)
real_wp_	forward_error	estimate of forward error
bool	alternative	has an "alternative" y: A y = 0 and yT b $>$ 0 been found when trying to solve A x = b?
char	solver[21]	name of external solver used to factorize and solve
struct sls_time_type	time	timings (see above)
struct sils_ainfo_type	sils_ainfo	the output structure from sils
struct sils_finfo_type	sils_finfo	see sils_ainfo
struct sils_sinfo_type	sils_sinfo	see sils_ainfo
struct ma57_ainfo	ma57_ainfo	the output structure from ma57
struct ma57_finfo	ma57_finfo	see ma57_ainfo

## **Data Fields**

struct ma57 sinfo	ma57 sinfo	see ma57 ainfo
struct ma77_info	ma77_info	the output structure from ma77
struct ma86_info	ma86_info	the output structure from ma86
struct ma87_info	ma87_info	the output structure from ma87
struct ma97_info	ma97_info	the output structure from ma97
struct spral_ssids_inform	ssids_inform	the output structure from ssids
int	mc61_info[10]	the integer and real output arrays from mc61
real_wp_	mc61_rinfo[15]	see mc61_info
struct mc64_info	mc64_info	the output structure from mc64
struct mc68_info	mc68_info	the output structure from mc68
int	mc77_info[10]	the integer output array from mc77
real_wp_	mc77_rinfo[10]	the real output status from mc77
int	mumps_error	the output scalars and arrays from mumps
int	mumps_info[80]	see mumps_error
real_wp_	mumps_rinfo[40]	see mumps_error
int	pardiso_error	the output scalars and arrays from pardiso
int	pardiso_IPARM[64]	see pardiso_error
real_wp_	pardiso_DPARM[64]	see pardiso_error
int	mkl_pardiso_error	the output scalars and arrays from mkl_pardiso
int	mkl_pardiso_IPARM[64]	see mkl_pardiso_error
int	pastix_info	the output flag from pastix
int	wsmp_error	the output scalars and arrays from wsmp
int	wsmp_iparm[64]	see wsmp_error
real_wp_	wsmp_dparm[64]	see wsmp_error
int	mpi_ierr	the output flag from MPI routines
int	lapack_error	the output flag from LAPACK routines

## 3.1.2 Function Documentation

## 3.1.2.1 sls\_initialize()

Select solver, set default control values and initialize private data

#### **Parameters**

in	$ \begin{array}{c} \textit{solver} \\ \textit{is a one-dimensional array of type char that specifies the solver package tha} \\ \textit{used to factorize the matrix } A. \textit{ It should be one of 'sils', 'ma27', 'ma57', 'ma77'} \\ \textit{'ma87', 'ma97', 'ssids', 'mumps', 'pardiso', 'mkl pardiso', 'pastix', 'wsmp', 'potr' 'pbtr'; lower or upper case variants are allowed. \\ \end{array} $	
in,out	data	holds private internal data
out	control	is a struct containing control information (see sls_control_type)
out	status	is a scalar variable of type int, that gives the exit status from the package. Possible values are:  • 0. The import was succesful.  • -26. The requested solver is not available.

#### **Examples**

slst.c, and slstf.c.

#### 3.1.2.2 sls\_read\_specfile()

Read the content of a specification file, and assign values associated with given keywords to the corresponding control parameters. By default, the spcification file will be named RUNSLS.SPC and lie in the current directory. Refer to Table 2.1 in the fortran documentation provided in \$GALAHAD/doc/sls.pdf for a list of keywords that may be set.

## **Parameters**

in, out   control		is a struct containing control information (see sls_control_type)	
in	specfile	is a character string containing the name of the specification file	

## 3.1.2.3 sls\_analyse\_matrix()

```
const int col[],
const int ptr[] )
```

Import structural matrix data into internal storage prior to solution

## **Parameters**

in	control	is a struct whose members provide control paramters for the remaining prcedures (see sls_control_type)
in,out	data	holds private internal data
in,out out	status status	is a scalar variable of type int, that gives the exit status from the package.  Possible values are:  • 0. The import and analysis were conducted succesfully.  • -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 restrictions n > 0 or requirement that the matrix type must contain the relevant string 'dense', 'coordinate' or 'sparse_by_rows has been violated.  • -20. The matrix is not positive definite while the solver used expected it to be.  • -26. The requested solver is not available.  • -29. This option is not available with this solver.  • -32. More than control.max integer factor size words of internal integer storage are required for in-core factorization.  • -34. The package PARDISO failed; check the solver-specific information components inform.pardiso iparm and inform.pardiso_dparm along with PARDISO's documentation for more details.  • -35. The package WSMP failed; check the solver-specific information components inform.wsmp_iparm and inform.wsmp dparm along with WSMP's documentation for more details.  • -36. The scaling package HSL MC64 failed; check the solver-specific information components inform.mc64_info along with HSL MC64's documentation for more details.  • -37. The scaling package MC77 failed; check the solver-specific information components inform.mc77_info along with MC77's documentation for more details.
		component of inform along with the solver's documentation for more details.
in	n	is a scalar variable of type int, that holds the number of rows in the symmetric matrix $A$ .
in	type	is a one-dimensional array of type char that specifies the symmetric storage scheme used for the matrix $A$ . It should be one of 'coordinate', 'sparse_by_rows' or 'dense'; lower or upper case variants are allowed.
in	ne	is a scalar variable of type int, that holds the number of entries in the lower triangular part of $A$ in the sparse co-ordinate storage scheme. It need not be set for any of the other schemes.

#### **Parameters**

in	row	is a one-dimensional array of size ne and type int, that holds the row indices of the lower triangular part of $A$ in the sparse co-ordinate storage scheme. It need not be set for any of the other three schemes, and in this case can be NULL.
in	col	is a one-dimensional array of size ne and type int, that holds the column indices of the lower triangular part of $A$ in either the sparse co-ordinate, or the sparse row-wise storage scheme. It need not be set when the dense storage scheme is used, and in this case can be NULL.
in	ptr	is a one-dimensional array of size $n+1$ and type int, that holds the starting position of each row of the lower triangular part of $A$ , as well as the total number of entries, in the sparse row-wise storage scheme. It need not be set when the other schemes are used, and in this case can be NULL.

## Examples

slst.c, and slstf.c.

## 3.1.2.4 sls\_reset\_control()

Reset control parameters after import if required.

## **Parameters**

in	control	is a struct whose members provide control paramters for the remaining proedures (see sls_control_type)
in,out	out data holds private internal data	
in,out	status	is a scalar variable of type int, that gives the exit status from the package. Possible values are:
		0. The import was succesful.

## Examples

slst.c, and slstf.c.

## 3.1.2.5 sls\_factorize\_matrix()

```
int * status,
int ne,
const real_wp_ val[] )
```

Form and factorize the symmetric matrix  $\boldsymbol{A}.$ 

## **Parameters**

in,out	data	holds private internal data
out	status	is a scalar variable of type int, that gives the exit status from the package.  Possible values are:
		0. The factors were generated succesfully.
		<ul> <li>-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.</li> </ul>
		<ul> <li>-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.</li> </ul>
		<ul> <li>-3. The restrictions n &gt; 0 or requirement that the matrix type must contain the relevant string 'dense', 'coordinate' or 'sparse_by_rows has been violated.</li> </ul>
		-20. The matrix is not positive definite while the solver used expected it to be.
		-26. The requested solver is not available.
		-29. This option is not available with this solver.
		<ul> <li>-32. More than control.max integer factor size words of internal integer storage are required for in-core factorization.</li> </ul>
		<ul> <li>-34. The package PARDISO failed; check the solver-specific information components inform.pardiso iparm and inform.pardiso_dparm along with PARDISO's documentation for more details.</li> </ul>
		<ul> <li>-35. The package WSMP failed; check the solver-specific information components inform.wsmp_iparm and inform.wsmp dparm along with WSMP's documentation for more details.</li> </ul>
		<ul> <li>-36. The scaling package HSL MC64 failed; check the solver-specific information component inform.mc64_info along with HSL MC64's documentation for more details.</li> </ul>
		<ul> <li>-37. The scaling package MC77 failed; check the solver-specific information components inform.mc77 info and inform.mc77_rinfo along with MC77's documentation for more details.</li> </ul>
		<ul> <li>-43. A direct-access file error occurred. See the value of inform.ma77_info.flag for more details.</li> </ul>
		<ul> <li>-50. A solver-specific error occurred; check the solver-specific information component of inform along with the solver's documentation for more details.</li> </ul>
in	ne	is a scalar variable of type int, that holds the number of entries in the lower triangular part of the symmetric matrix ${\cal A}.$
in	val	is a one-dimensional array of size ne and type double, that holds the values of the entries of the lower triangular part of the symmetric matrix $A$ in any of the supported storage schemes.

## Examples

slst.c, and slstf.c.

## 3.1.2.6 sls\_solve\_system()

Solve the linear system Ax = b.

#### **Parameters**

in,out	data	holds private internal data
in, out	status	is a scalar variable of type int, that gives the exit status from the package.  Possible values are:  • 0. The required solution was obtained.  • -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.  • -34. The package PARDISO failed; check the solver-specific information components inform.pardiso iparm and inform.pardiso_dparm along with PARDISO's documentation for more details.  • -35. The package WSMP failed; check the solver-specific information components inform.wsmp_iparm and inform.wsmp dparm along with WSMP's documentation for more details.
in	n	is a scalar variable of type int, that holds the number of entries in the vectors $\boldsymbol{b}$ and $\boldsymbol{x}$ .
in,out	sol	is a one-dimensional array of size n and type double. On entry, it must hold the vector $b$ . On a successful exit, its contains the solution $x$ .

## Examples

slst.c, and slstf.c.

## 3.1.2.7 sls\_partial\_solve\_system()

```
void ** data,
int * status,
int n,
real_wp_ sol[] )
```

Given the factorization A=LDU with  $U=L^T$ , solve the linear system Mx=b, where M is one of L, D, U or  $S=L\sqrt{D}$ .

## **Parameters**

in	part	is a one-dimensional array of type char that specifies the component $M$ of the factorization that is to be used. It should be one of "L", "D", "U" or "S", and these correspond to the parts $L,D,U$ and $S$ ; lower or upper case variants are allowed.
in,out	data	holds private internal data
in,out	status	is a scalar variable of type int, that gives the entry and exit status from the package.  On initial entry, status must be set to 1.  Possible exit are:  • 0. The required solution was obtained.  • -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.  • -34. The package PARDISO failed; check the solver-specific information components inform.pardiso iparm and inform.pardiso_dparm along with PARDISO's documentation for more details.  • -35. The package WSMP failed; check the solver-specific information components
		inform.wsmp_iparm and inform.wsmp dparm along with WSMP's documentation for more details.
in	n	is a scalar variable of type int, that holds the number of entries in the vectors $\boldsymbol{b}$ and $\boldsymbol{x}$ .
in,out	sol	is a one-dimensional array of size n and type double. On entry, it must hold the vector $b$ . On a successful exit, its contains the solution $x$ .

## **Examples**

slst.c, and slstf.c.

## 3.1.2.8 sls\_information()

## Provide output information

## **Parameters**

in, out	data	holds private internal data
out	inform is a struct containing output information (see sls_inform_type)	
out	status	is a scalar variable of type int, that gives the exit status from the package. Possible values are (currently):
		0. The values were recorded succesfully

## Examples

slst.c, and slstf.c.

## 3.1.2.9 sls\_terminate()

## Deallocate all internal private storage

## **Parameters**

in,out	data	holds private internal data
out	control	is a struct containing control information (see sls_control_type)
out	inform	is a struct containing output information (see sls_inform_type)

## Examples

slst.c, and slstf.c.

# **Chapter 4**

# **Example Documentation**

#### 4.1 slst.c

This is an example of how to use the package in conjunction with the sparse linear solver sils. A variety of supported matrix storage formats are illustrated.

Notice that C-style indexing is used, and that this is flaggeed by setting control.f\_indexing to false.

```
/* slst.c */
/* Full test for the SLS C interface using C sparse matrix indexing \star/
#include <stdio.h>
#include <math.h>
#include <stdlib.h>
#include <float.h>
#include "galahad_precision.h"
#include "galahad_cfunctions.h"
#include "galahad_sls.h"
int maxabsarray(double a[],int n, real_wp_ *maxabs);
int main(void)
      // Derived types
      void *data;
      struct sls_control_type control;
struct sls_inform_type inform;
       // Set problem data
      // Set problem data
int n = 5; // dimension of A
int ne = 7; // number of entries of A
int dense_ne = 15; // number of elements of A as a dense matrix
int row[] = {0, 1, 1, 2, 2, 3, 4}; // row indices, NB lower triangle
int col[] = {0, 0, 4, 1, 2, 2, 4}; // column indices
int ptr[] = {0, 1, 3, 5, 6, 7}; // pointers to indices
real_wp_ val[] = {2.0, 3.0, 6.0, 4.0, 1.0, 5.0, 1.0}; // values
real_wp_ dense[] = {2.0, 3.0, 0.0, 0.0, 4.0, 1.0, 0.0,
0.0, 5.0, 0.0, 0.0, 0.0, 0.0, 0.0, 1.0};
      0.0, 5.0, 0.0, 0.0, 6.0, 0.0, 0.0, 1.0);
real_wp_ rhs[] = {8.0, 45.0, 31.0, 15.0, 17.0};
real_wp_ sol[] = {1.0, 2.0, 3.0, 4.0, 5.0};
      int i, status;
      real_wp_ x[n];
      real_wp_ error[n];
      real_wp_ norm_residual;
      real_wp_ good_x = pow( DBL_EPSILON, 0.3333 );
printf(" C sparse matrix indexing\n\n");
      printf(" basic tests of storage formats\n\n");
      printf(" storage
                                                 RHS
                                                           refine partial\n");
       for( int d=1; d <= 3; d++){
              \//\ Initialize SLS - use the sytr solver
             // Initialize SLS - use the syll solver
sls_initialize("sytr", &data, &control, &status);
// Set user-defined control options
control.f_indexing = false; // C sparse matrix indexing
             switch(d) { // import matrix data and factorize
                   case 1: // sparse co-ordinate storage
    printf(" coordinate ");
```

```
case 2: // sparse by rows
                   printf(" sparse by rows ");
                   sls_factorize_matrix( &data, &status, ne, val );
              break;
case 3: // dense
                   printf(" dense
                                                ");
                   sls_factorize_matrix( &data, &status, dense_ne, dense );
         // Set right-hand side and solve the system
         for(i=0; i<n; i++) x[i] = rhs[i];
sls_solve_system( &data, &status, n, x );</pre>
         sls_information( &data, &inform, &status );
if(inform.status == 0){
            for (i=0; i<n; i++) error[i] = x[i]-sol[i];</pre>
            status = maxabsarray( error, n, &norm_residual );
            if(norm_residual < good_x){
  printf(" ok ");</pre>
            lelse(
             printf(" fail ");
         }else{
             printf(" SLS_solve exit status = %1i\n", inform.status);
         //printf("sol: ");
         //for( int i = 0; i < n; i++) printf("%f ", x[i]);
// resolve, this time using iterative refinement</pre>
         control.max_iterative_refinements = 1;
         sls_reset_control( &control, &data, &status );
          for(i=0; i<n; i++) x[i] = rhs[i];</pre>
         sls_solve_system( &data, &status, n, x );
sls_information( &data, &inform, &status );
if(inform.status == 0)(
            for (i=0; i<n; i++) error[i] = x[i]-sol[i];</pre>
            status = maxabsarray( error, n, &norm_residual );
            if(norm_residual < good_x){
  printf(" ok ");</pre>
             printf("
            lelse(
             printf(" fail ");
         }else{
             printf(" SLS_solve exit status = %1i\n", inform.status);
         ^{\prime}// obtain the solution by part solves
         for(i=0; i<n; i++) x[i] = rhs[i];
sls_partial_solve_system( "L", &data, &status, n, x );
sls_partial_solve_system( "D", &data, &status, n, x );
sls_partial_solve_system( "U", &data, &status, n, x );</pre>
         sls_information( &data, &inform, &status );
         if(inform.status == 0){
  for(i=0; i<n; i++) error[i] = x[i]-sol[i];</pre>
            status = maxabsarray( error, n, &norm_residual );
            if(norm_residual < good_x){
  printf(" ok ");</pre>
             printf("
            }else{
             printf(" fail ");
         }else{
             printf(" SLS_solve exit status = %li\n", inform.status);
          // Delete internal workspace
         sls_terminate( &data, &control, &inform );
         printf("\n");
int maxabsarray(double a[],int n, real_wp_ *maxabs)
    real_wp_ b, max;
    max=abs(a[0]);
    for (i=1; i<n; i++)</pre>
         b = abs(a[i]);
    if (max<b)</pre>
           max=b:
    *maxabs=max;
```

4.2 slstf.c 25

#### 4.2 slstf.c

This is the same example, but now fortran-style indexing is used.

```
/* Full test for the SLS C interface using Fortran sparse matrix indexing */
#include <stdio.h>
#include <math.h>
#include <stdlib.h>
#include <float.h>
#include "galahad_precision.h"
#include "galahad_cfunctions.h"
#include "galahad_sls.h"
int maxabsarray( real_wp_ a[],int n, real_wp_ *maxabs);
int main(void) {
    // Derived types
    void *data;
    struct sls_control_type control;
    struct sls_inform_type inform;
    // Set problem data
    int n = 5; // dimension of A
    int ne = 7; // number of entries of A
    int dense_ne = 15; // number of elements of A as a dense matrix
    real_wp_ rhs[] = {8.0, 45.0, 31.0, 15.0, 17.0};
real_wp_ sol[] = {1.0, 2.0, 3.0, 4.0, 5.0};
    int i. status:
    real_wp_ x[n];
    real_wp_ error[n];
real_wp_ norm_residual;
    real_wp_ good_x = pow( DBL_EPSILON, 0.3333 ); printf(" Fortran sparse matrix indexing\n");
    printf(" basic tests of storage formats\n\n");
    printf(" storage
                                RHS refine partial\n");
    for( int d=1; d <= 3; d++){
         // Initialize SLS - use the sytr solver
         sls_initialize( "sytr", &data, &control, &status );
        // Set user-defined control options
control.f_indexing = true; // Fortran sparse matrix indexing
        switch(d){ // import matrix data and factorize
    case 1: // sparse co-ordinate storage
        printf(" coordinate ");
                                           ");
                 sls_analyse_matrix( &control, &data, &status, n,
                                       "coordinate", ne, row, col, NULL);
                 sls_factorize_matrix( &data, &status, ne, val );
             break;
case 2: // sparse by rows
                 printf(" sparse by rows ");
                 sls_analyse_matrix( &control, &data, &status, n,
                                       "sparse_by_rows", ne, NULL, col, ptr );
                 sls_factorize_matrix( &data, &status, ne, val );
             break;
case 3: // dense
                                            ");
                 printf(" dense
                 sls_analyse_matrix( &control, &data, &status, n,
                                        "dense", ne, NULL, NULL, NULL);
                 sls_factorize_matrix( &data, &status, dense_ne, dense );
         // Set right-hand side and solve the system
         for(i=0; i<n; i++) x[i] = rhs[i];</pre>
         sls_solve_system( &data, &status, n, x );
        sls_information( &data, &inform, &status );
         if(inform.status == 0){
           for (i=0; i<n; i++) error[i] = x[i]-sol[i];</pre>
           status = maxabsarray( error, n, &norm_residual );
           if(norm_residual < good_x){
  printf(" ok ");</pre>
            printf(" fail ");
         }else{
            printf(" SLS_solve exit status = %1i\n", inform.status);
         //for( int i = 0; i < n; i++) printf("%f ", x[i]);
         // resolve, this time using iterative refinement
        control.max iterative refinements = 1;
        sls_reset_control( &control, &data, &status );
         for(i=0; i<n; i++) x[i] = rhs[i];</pre>
```

```
sls_solve_system( &data, &status, n, x );
                              sls_information( &data, &inform, &status );
                              if(inform.status == 0){
                                    for(i=0; i<n; i++) error[i] = x[i]-sol[i];
status = maxabsarray( error, n, &norm_residual );</pre>
                                      if(norm_residual < good_x){
  printf(" ok ");</pre>
                                        printf(" fail ");
                               }else{
                                           printf(" SLS_solve exit status = %1i\n", inform.status);
                            }
// obtain the solution by part solves
for(i=0; i<n; i++) x[i] = rhs[i];
sls_partial_solve_system( "L", &data, &status, n, x );
sls_partial_solve_system( "D", &data, &status, n, x );
sls_partial_solve_system( "U", &data, &status, n, x );
sls_information( &data, &inform, &status );
if information that are not set in the set
                               if (inform.status == 0) {
                                    for(i=0; i<n; i++) error[i] = x[i]-sol[i];
status = maxabsarray( error, n, &norm_residual );</pre>
                                     if(norm_residual < good_x){
  printf(" ok ");</pre>
                                      }else{
                                        printf(" fail ");
                               }else{
                                           printf(" SLS_solve exit status = %1i\n", inform.status);
                              // Delete internal workspace
                             sls_terminate( &data, &control, &inform );
                             printf("\n");
int maxabsarray( real_wp_ a[], int n, real_wp_ *maxabs )
               real_wp_ b, max;
               max=abs(a[0]);
               for(i=1; i<n; i++)</pre>
                             b = abs(a[i]);
               if (max<b)</pre>
                                    max=b;
               *maxabs=max;
```