## FIXME: OLD: User Guide for the SPEX Software Package

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## Contents

1 SPEX Overview			4	
2	SPI	EX Ut	ilities	6
	2.1	Overv	<i>v</i> iew	6
	2.2	Licens	sing	7
	2.3	Instal	lation	7
	2.4	Mana	ging the SPEX environment	8
		2.4.1	SPEX_UTIL_VERSION: the software package version	8
		2.4.2	SPEX_info: status codes returned by SPEX	8
		2.4.3	SPEX_initialize: initialize the working environment	9
		2.4.4	SPEX_initialize_expert: initialize environment (expert ver-	
			sion)	9
		2.4.5	SPEX_finalize: free the working environment	10
	2.5	Memo	ory Management	10
		2.5.1	SPEX_calloc: allocate initialized memory	10
		2.5.2	SPEX_malloc: allocate uninitialized memory	11
		2.5.3	SPEX_realloc: resize allocated memory	11
		2.5.4	SPEX_free: free allocated memory	12
	2.6	The S	SPEX_options structure: parameter settings for SPEX	12
		2.6.1	SPEX_pivot: enum for pivoting schemes	12
		2.6.2	SPEX_col_order: enum for column ordering schemes	13
		2.6.3	SPEX_options structure	14
		2.6.4	SPEX_create_default_options: create default SPEX_options	
			structure	15
	2.7	The S	SPEX_matrix structure	16
		2.7.1	SPEX_kind: enum for matrix formats	16
		2.7.2	SPEX_type: enum for data types of matrix entries	16
		2.7.3	SPEX matrix structure	16

		2.7.4	${\tt SPEX\_matrix\_allocate: allocate \ an \ } m\hbox{-by-}n {\tt SPEX\_matrix}  .  .$	19
		2.7.5	SPEX_matrix_free: free a SPEX_matrix	20
		2.7.6	SPEX_matrix_copy: make a copy of a SPEX_matrix with a	
			potentially different matrix-format and data-type	20
		2.7.7	SPEX_matrix_nnz: get the number of entries in a SPEX_matrix	21
		2.7.8	SPEX_matrix_check: check and optionally print a SPEX_matrix	
				21
		2.7.9	SPEX_matrix_div: Divide dense matrix by scalar	22
		2.7.10	SPEX_matrix_mul: Multiply dense matrix by scalar	22
	2.8	SPEX_	lu_analysis structure	22
		2.8.1	SPEX_lu_analyze: perform symbolic analysis	23
		2.8.2	SPEX_lu_analysis_free: free SPEX_lu_analysis structure .	24
	2.9		wrapper functions for GMP and MPFR	24
	2.10		onal Useful SPEX Utility Functions	28
			SPEX_cumsum: Cumulative sum of a vector	28
		2.10.2	SPEX_check_solution: Validate solution vector (for debug-	
			$\operatorname{ging}$ )	28
3	SPE	X Lef	t LU	29
	3.1	Overvi	iew	29
	3.2	Licens	ing	30
	3.3	Install	ation	31
	3.4	SPEX_	VERSION: the software package version	31
	3.5		ization and Solve Routines	32
		3.5.1	SPEX_lu_factorize: perform LU factorization	32
		3.5.2	SPEX_lu_solve: solve the linear system $Ax = b \dots \dots$	33
		3.5.3	SPEX_lu_backslash: solve $Ax = b$	34
	3.6	Using	SPEX Left LU in C	34
		3.6.1	SPEX Left LU initialization and population of data structures	35
		3.6.2	Simple SPEX Left LU routines for solving linear systems	37
		3.6.3	Expert SPEX Left LU routines	37
		3.6.4	Freeing memory	39
		3.6.5	Examples	39
	3.7		SPEX Left LU in MATLAB	40
		3.7.1	Optional parameter settings	40
		3.7.2	SPEX_lu_backslash.m	42

## Chapter 1

## SPEX Overview

SPEX is a software package comprising several state-of-the-art SParse EXact linear algebra routines. It currently is comprised of the following:

SPEX Utilities Utility and auxiliary functions for all SPEX routines: interface to the GMP/MPFR library, memory management functions, the SPEX\_matrix data structure, and various functions that are auxiliary to the factorization and solve functions. Please refer to Chapter 2 for further details.

**SPEX Left LU** Sparse exact left-looking LU factorization to solve the linear system  $A\mathbf{x} = \mathbf{b}$ . The solution time is proportional to the arithmetic work in the bit-complexity model; this is an asymptotically efficient complexity bound. Please refer to Chapter 3 for further details.

Location: https://github.com/clouren/SPEX and www.suitesparse.com

Required Packages: SPEX depends on the following packages:

- AMD [1, 2], available under a BSD 3-clause license and distributed along with SPEX. May be independently obtained at www.suitesparse.com
- COLAMD [5, 4], available under a BSD 3-clause license and distributed along with SPEX. May be independently obtained at www.suitesparse.com
- SuiteSparse\_config [3], no license restrictions and distributed along with SPEX. May be independently obtained at www.suitesparse.com
- GNU GMP [7] and MPFR [6] libraries. Distributed under the LGPL3 and GPL2 and can be acquired and installed from https://gmplib.org/ and http://www.mpfr.org/, respectively.

Within a Debian/Ubuntu based Linux system, a compatible version of GMP and MPFR can be installed with the following terminal commands:

```
sudo apt-get install libgmp3-dev
sudo apt-get install libmpfr-dev libmpfr-doc libmpfr4 libmpfr4-dbg
```

## Chapter 2

## SPEX Utilities

## 2.1 Overview

SPEX Util is a software package containing utility and auxiliary functions for the SPEX factorizations. Additionally, SPEX Util provides a wrapper class for the GNU Multiple Precision Arithmetic (GMP) [7] and GNU Multiple Precision Floating Point Reliable (MPFR) [6] libraries that prevent memory leaks and improve the overall stability of these external libraries. SPEX Util is written in ANSI C.

SPEX operates on matrices stored in any of the following 15 combinations of matrix formats and entry data-types: {Compressed Sparse Column (CSC), triplet, dense} × { mpz\_t, mpq\_t, mpfr\_t, int64\_t, or double}. Using the SPEX matrix copy function, a matrix of any given form and data-type can be copied and converted into a matrix of any one of the 15 matrix-form and data-type combinations.

Most routines require the matrix to be in CSC form with  $mpz_t$  (i.e., arbitrary-sized integer) data type. This data structure stores the matrix A as a sequence of three arrays:

- A->p: Column pointers; an array of size n+1. The row indices of column j are located in positions A->p[j] to A->p[j+1]-1 of the array A->i. Data type: int64\_t.
- A->i: Row indices; an array of size equal to the number of entries in the matrix. The entry A->i[k] is the row index of the kth nonzero in the matrix. Data type: int64\_t.
- A->x: Numeric entries. The entry A->x[k] is the numeric value of the kth nonzero in the matrix. The array A->x has a union type and must be accessed via a suffix according to the type of A. For details, please refer to Section 2.7.

An example matrix A with  $mpz_t$  type is stored as follows (note that indexing is zero based as per the C convention).

$$A = \begin{bmatrix} 1 & 0 & 0 & 1 \\ 2 & 0 & 4 & 12 \\ 7 & 1 & 1 & 1 \\ 0 & 2 & 3 & 0 \end{bmatrix}$$

$$A \rightarrow p = [0, 3, 5, 8, 11]$$
  
 $A \rightarrow i = [0, 1, 2, 2, 3, 1, 2, 3, 0, 1, 2]$   
 $A \rightarrow x.mpz = [1, 2, 7, 1, 2, 4, 1, 3, 1, 12, 1]$ 

For example, the last column appears in positions 8 to 10 of A->i and A->x.mpz, with row indices 0, 1, and 2, and values  $a_{03} = 1$ ,  $a_{13} = 12$ , and  $a_{23} = 1$ .

## 2.2 Licensing

**Copyright:** The copyright of this software is held by Christopher Lourenco, Jinhao Chen, Erick Moreno-Centeno, and Timothy A. Davis.

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License: This software package is dual licensed under the GNU General Public License version 2 or the GNU Lesser General Public License version 3. Details of this license are in SPEX/License/license.txt. For alternative licenses, please contact the authors.

## 2.3 Installation

Installation of SPEX Util requires the make utility in Linux/MacOS, or Cygwin make in Windows. With the proper compiler, typing make under the main directory will compile AMD, COLAMD and SPEX Util to the respective SPEX/Lib folder. To further install the libraries onto your computer, simply type make install. Thereafter, to use the code inside of your program, precede your code with

#include "SPEX.h". This is done by default in all SPEX factorization routines, thus a user should never have to directly include SPEX\_Utilities.

## 2.4 Managing the SPEX environment

## 2.4.1 SPEX\_UTIL\_VERSION: the software package version

SPEX Util defines the following strings with #define. Refer to the SPEX.h file for details.

Macro	purpose
SPEX_UTIL_VERSION	current version of the code (as a string)
SPEX_UTIL_VERSION_MAJOR	major version of the code
SPEX_UTIL_VERSION_MINOR	minor version of the code
SPEX_UTIL_VERSION_SUB	sub version of the code

## 2.4.2 SPEX\_info: status codes returned by SPEX

Most SPEX functions return their status to the caller as their return value, an enumerated type called SPEX\_info. All current possible values for SPEX\_info are listed as follows:

0	SPEX_OK	The function was successfully executed.
-1	SPEX_OUT_OF_MEMORY	out of memory
-2	SPEX_SINGULAR	The input matrix $A$ is exactly singular.
-3	SPEX_INCORRECT_INPUT	One or more input arguments are incorrect.
-4	SPEX_INCORRECT	The solution is incorrect.
-5	SPEX_UNSYMMETRIC	The input matrix is unsymmetric (for Cholesky)
-5	SPEX_PANIC	SPEX environment error

Either SPEX\_initialize or SPEX\_initialize\_expert (but not both) must be called prior to using any other SPEX function. SPEX\_finalize must be called as the last SPEX function.

Subsequent SPEX sessions can be restarted after a call to SPEX\_finalize, by calling either SPEX\_initialize or SPEX\_initialize\_expert (but not both), followed by a final call to SPEX\_finalize when finished.

## 2.4.3 SPEX\_initialize: initialize the working environment

```
SPEX_info SPEX_initialize
(
    void
);
```

SPEX\_initialize initializes the working environment for SPEX functions. SPEX utilizes a specialized memory management scheme in order to prevent potential memory failures caused by GMP and MPFR libraries. Either this function or SPEX\_initialize\_expert must be called prior to using any other function in the library. Returns SPEX\_PANIC if SPEX has already been initialized, or SPEX\_OK if successful.

# 2.4.4 SPEX\_initialize\_expert: initialize environment (expert version)

SPEX\_initialize\_expert is the same as SPEX\_initialize except that it allows for a redefinition of custom memory functions that are used for SPEX and GMP/MPFR. The four inputs to this function are pointers to four functions with the same signatures as the ANSI C malloc, calloc, realloc, and free functions. That is:

```
#include <stdlib.h>
void *malloc (size_t size) ;
void *calloc (size_t nmemb, size_t size) ;
void *realloc (void *ptr, size_t size) ;
void free (void *ptr) ;
```

Returns SPEX\_PANIC if SPEX has already been initialized, or SPEX\_OK if successful.

## 2.4.5 SPEX\_finalize: free the working environment

```
SPEX_info SPEX_finalize
(
     void
);
```

SPEX\_finalize finalizes the working environment for SPEX library, and frees any internal workspace created by SPEX. It must be called as the last SPEX\_\* function called, except that a subsequent call to SPEX\_initialize\* may be used to start another SPEX session. Returns SPEX\_PANIC if SPEX has not been initialized, or SPEX\_OK if successful.

## 2.5 Memory Management

The routines in this section are used to allocate and free memory for the data structures used in SPEX. By default, SPEX relies on the SuiteSparse memory management functions, SuiteSparse\_malloc, SuiteSparse\_calloc, SuiteSparse\_realloc, and SuiteSparse\_free. By default, those functions rely on the ANSI C malloc, calloc, realloc, and free, but this may be changed by initializing the SPEX environment with SPEX\_initialize\_expert.

## 2.5.1 SPEX\_calloc: allocate initialized memory

SPEX\_calloc allocates a block of memory for an array of nitems elements, each of them size bytes long, and initializes all its bits to zero. If any input is less than 1, it is treated as if equal to 1. If the function failed to allocate the requested block of memory, then a NULL pointer is returned. Returns NULL if SPEX has not been initialized.

#### 2.5.2 SPEX\_malloc: allocate uninitialized memory

```
void *SPEX_malloc
(
    size_t size  // size of memory space to allocate
);
```

SPEX\_malloc allocates a block of size bytes of memory, returning a pointer to the beginning of the block. The content of the newly allocated block of memory is not initialized, remaining with indeterminate values. If size is less than 1, it is treated as if equal to 1. If the function fails to allocate the requested block of memory, then a NULL pointer is returned. Returns NULL if SPEX has not been initialized.

#### 2.5.3 SPEX\_realloc: resize allocated memory

SPEX\_realloc is a wrapper for realloc. If p is non-NULL on input, it points to a previously allocated array of size nitems\_old × size\_of\_item. The array is reallocated to be of size nitems\_new × size\_of\_item. If p is NULL on input, then a new array of that size is allocated. On success, a pointer to the new array is returned. Returns ok as false if SPEX has not been initialized.

If the reallocation fails, p is not modified, and ok is returned as false to indicate that the reallocation failed. If the size decreases or remains the same, then the method always succeeds (ok is returned as true), unless SPEX has not been initialized.

Typical usage: the following code fragment allocates an array of 10 int's, and then increases the size of the array to 20 int's. If the SPEX\_malloc succeeds but the SPEX\_realloc fails, then the array remains unmodified, of size 10.

```
int *p;
p = SPEX_malloc (10 * sizeof (int));
if (p == NULL) { error here ... }
printf ("p points to an array of size 10 * sizeof (int)\n");
```

```
bool ok ;
p = SPEX_realloc (20, 10, sizeof (int), p, &ok) ;
if (ok) printf ("p has size 20 * sizeof (int)\n") ;
else printf ("realloc failed; p still has size 10 * sizeof (int)\n") ;
SPEX_free (p) ;
```

### 2.5.4 SPEX\_free: free allocated memory

```
void SPEX_free
(
    void *p  // Pointer to memory space to free
);
```

SPEX\_free deallocates the memory previously allocated by a call to SPEX\_calloc, SPEX\_malloc, or SPEX\_realloc. If p is NULL on input, then no action is taken (this is not an error condition). To guard against freeing the same memory space twice, the following macro SPEX\_FREE is provided, which calls SPEX\_free and then sets the freed pointer to NULL.

```
#define SPEX_FREE(p)
{
          SPEX_free (p);
          (p) = NULL;
}
```

No action is taken if SPEX has not been initialized.

# 2.6 The SPEX\_options structure: parameter settings for SPEX

The SPEX\_options structure contains numerous parameters that may be modified to change the behavior of the SPEX functions. Default values of these parameters will lead to good performance in most cases. Modifying this struct provides control of column orderings, pivoting schemes, and other components of the factorization.

## 2.6.1 SPEX\_pivot: enum for pivoting schemes

There are six available pivoting schemes provided in SPEX that can be selected with the SPEX\_options structure. If the matrix is non-singular (in an exact sense), then the pivot is always nonzero, and is chosen as the *smallest* nonzero entry, with the smallest magnitude. This may seem counter-intuitive, but selecting a small nonzero pivot leads to smaller growth in the number of digits in the entries of L and U. This choice does not lead to any kind of numerical inaccuracy, since SPEX is guaranteed to find an exact roundoff-error free factorization of a non-singular matrix (unless it runs out of memory), for any nonzero pivot choice.

The pivot tolerance for two of the pivoting schemes is specified by the tol component in SPEX\_options. The pivoting schemes are as follows:

0	SPEX_SMALLEST	The $k$ -th pivot is selected as the smallest entry in the $k$ -th
		column.
1	SPEX_DIAGONAL	The $k$ -th pivot is selected as the diagonal entry. If the di-
		agonal entry is zero, this method instead selects the smallest
		pivot in the column.
2	SPEX_FIRST_NONZERO	The $k$ -th pivot is selected as the first eligible nonzero in the
		column.
3	SPEX_TOL_SMALLEST	The $k$ -th pivot is selected as the diagonal entry if the diagonal
		is within a specified tolerance of the smallest entry in the
		column. Otherwise, the smallest entry in the $k$ -th column is
		selected. This is the default pivot selection strategy.
4	SPEX_TOL_LARGEST	The $k$ -th pivot is selected as the diagonal entry if the diago-
		nal is within a specified tolerance of the largest entry in the
		column. Otherwise, the largest entry in the $k$ -th column is
		selected.
5	SPEX_LARGEST	The $k$ -th pivot is selected as the largest entry in the $k$ -th
		column.

## 2.6.2 SPEX\_col\_order: enum for column ordering schemes

The SPEX library provides three column ordering schemes: no pre-ordering, CO-LAMD, and AMD, selected via the order component in the SPEX\_options structure described in Section 2.6.3.

0	SPEX_NO_ORDERING	No pre-ordering is performed on the matrix $A$ , that is $Q = I$ .
1	SPEX_COLAMD	The columns of $A$ are permuted prior to factorization using
		the COLAMD [4] ordering. This is the default ordering.
2	SPEX_AMD	The nonzero pattern of $A + A^T$ is analyzed and the columns
		of $A$ are permuted prior to factorization based on the AMD
		[2] ordering of $A + A^T$ . This works well if A has a mostly
		symmetric pattern, but tends to be worse than COLAMD on
		matrices with unsymmetric pattern. [5].

#### 2.6.3 SPEX\_options structure

The SPEX\_options struct stores key command parameters for various functions used in the SPEX package. The SPEX\_options option struct contains the following components:

- option->pivot: An enum SPEX\_pivot type (discussed in Section 2.6.1) which controls the type of pivoting used. Default value: SPEX\_TOL\_SMALLEST (3).
- option->order: An enum SPEX\_col\_order type (discussed in Section 2.6.2) which controls what column ordering is used. Default value: SPEX\_COLAMD (1).
- option->tol: A double tolerance for the tolerance-based pivoting scheme, i.e., SPEX\_TOL\_SMALLEST or SPEX\_TOL\_LARGEST. option->tol must be in the range of (0, 1]. Default value: 1 meaning that the diagonal entry will be selected if it has the same magnitude as the smallest entry in the k the column.
- option->print\_level: An int which controls the amount of output: 0: print nothing, 1: just errors, 2: terse, with basic stats from COLAMD/AMD and SPEX, 3: all, with matrices and results. Default value: 0.
- option->prec: An int32\_t which specifies the precision used for multiple precision floating point numbers, (i.e., MPFR). This can be any integer larger than MPFR\_PREC\_MIN (value of 1 in MPFR 4.0.2 and 2 in some legacy versions) and smaller than MPFR\_PREC\_MAX (usually the largest possible integer available in your system). Default value: 128 (quad precision).
- option->round: A mpfr\_rnd\_t which determines the type of MPFR rounding to be used by SPEX. This is a parameter of the MPFR library. The options for this parameter are:
  - MPFR\_RNDN: round to nearest (roundTiesToEven in IEEE 754-2008)
  - MPFR\_RNDZ: round toward zero (roundTowardZero in IEEE 754-2008)
  - MPFR\_RNDU: round toward plus infinity (roundTowardPositive in IEEE 754-2008)
  - MPFR\_RNDD: round toward minus infinity (roundTowardNegative in IEEE 754-2008)
  - MPFR\_RNDA: round away from zero
  - MPFR\_RNDF: faithful rounding. This is not stable.

Refer to the MPFR User Guide available at <a href="https://www.mpfr.org/mpfr-current/mpfr.pdf">https://www.mpfr.org/mpfr-current/mpfr.pdf</a> for details on the MPFR rounding style and any other utilized MPFR convention. Default value: MPFR\_RNDN.

• option->check: A bool which indicates whether the solution to the system should be checked. Intended for debugging only; the SPEX library is guaranteed to return the exact solution. Default value: false.

All SPEX routines except basic memory management routines in Sections 2.4.5-2.5.1 and SPEX\_options allocation routine in 2.6.4 require option as an input argument. The construction of the option struct can be avoided by passing NULL for the default settings. Otherwise, the following functions create and destroy a SPEX\_options structure:

function/macro name	description	section
SPEX_create_default_options	create and return SPEX_options pointer with default parameters upon successful allocation	2.6.4
SPEX_FREE	destroy SPEX_options structure	2.5.4

## 2.6.4 SPEX\_create\_default\_options: create default SPEX\_options structure

```
SPEX_options SPEX_create_default_options
(
    void
);
```

SPEX\_create\_default\_options creates and returns a pointer to a SPEX\_options struct with default parameters upon successful allocation, which are discussed in Section 2.6.3. To safely free the SPEX\_options option structure, simply use SPEX\_FREE(option). All functions that require SPEX\_options option as an input argument can have a NULL pointer passed instead. In this case, the default value of the corresponding command option is used. For example, if a NULL pointer is passed to the symbolic analysis routines, COLAMD is used. As a result, defaults are desired, the SPEX\_options struct need not be allocated. Returns NULL if SPEX has not been initialized.

## 2.7 The SPEX\_matrix structure

All matrices for SPEX are stored as a SPEX\_matrix structure (a pointer to a struct). The matrix can be held in three formats: CSC, triplet or dense matrix (as discussed in Section 2.7.1) with entries stored as 5 different types:  $mpz_t$ ,  $mpq_t$ ,  $mpfr_t$ ,  $int64_t$  and double (as discussed in Section 2.7.2). This gives a total of 15 different combinations of matrix format and entry type. Note that not all functions accept all 15 matrix types. Indeed, most functions expect the input matrix A to be a CSC  $mpz_t$  matrix while vectors (such as x and b) are in dense format.

### 2.7.1 SPEX\_kind: enum for matrix formats

The SPEX library provides three available matrix formats: sparse CSC (compressed sparse column), sparse triplet and dense.

0	SPEX_CSC	Matrix is in compressed sparse column format.
1	SPEX_TRIPLET	Matrix is in sparse triplet format.
2	SPEX_DENSE	Matrix is in dense format.

## 2.7.2 SPEX\_type: enum for data types of matrix entries

The SPEX library provides five data types for matrix entries: mpz\_t, mpq\_t, mpfr\_t, int64\_t and double.

0	SPEX_MPZ	Matrix entries are in mpz_t type: an integer of arbitrary size.
1	SPEX_MPQ	Matrix entries are in mpq_t type: a rational number with
		arbitrary-sized integer numerator and denominator.
$\overline{2}$	SPEX_MPFR	Matrix entries are in mpfr_t type: a floating-point number
		of arbitrary precision.
3	SPEX_INT64	Matrix entries are in int64_t type.
4	SPEX_FP64	Matrix entries are in double type.

## 2.7.3 SPEX\_matrix structure

A matrix SPEX\_matrix A has the following components:

- A->m: Number of rows in the matrix. Data Type: int64\_t.
- A->n: Number of columns in the matrix. Data Type: int64\_t.

- A->nz: The number of nonzeros in the matrix A, if A is a triplet matrix (ignored for matrices in CSC or dense formats). Data Type: int64\_t.
- A->nzmax: The allocated size of the vectors A->i, A->j and A->x. Note that
   A->nzmax ≥ nnz(A), where nnz(A) is the return value of SPEX\_matrix\_nnz(A,option).
   Data Type: int64\_t.
- A->kind: Indicating the kind of matrix A: CSC, triplet or dense. Data Type: SPEX\_kind.
- A->type: Indicating the type of entries in matrix A: mpz\_t, mpq\_t, mpfr\_t, int64\_t or double. Data Type: SPEX\_type.
- A->p: An array of size A->n+1 which contains column pointers of A, if A is a CSC matrix (NULL for matrices in triplet or dense formats). Data Type: int64\_t\*.
- A->p\_shallow: A boolean indicating whether A->p is shallow. A shallow pointer is one that refers to a component of another matrix or data structure. If A->p is shallow, then it should not be modified as part of the A matrix, and it is not freed if A is freed. Data Type: bool.
- A->i: An array of size A->nzmax which contains the row indices of the nonzeros in A, if A is a CSC or triplet matrix (NULL for dense matrices). The matrix is zero-based, so row indices are in the range of [0, A->m-1]. Data Type: int64\_t\*.
- A->i\_shallow: A boolean indicating whether A->i is shallow. Data Type: bool.
- A->j: An array of size A->nzmax which contains the column indices of the nonzeros in A, if A is a triplet matrix (NULL for matrices in CSC or dense formats). The matrix is zero-based, so column indices are in the range of [0, A->n-1]. Data Type: int64\_t\*.
- A->j\_shallow: A boolean indicating whether A->j is shallow. Data Type: bool.
- A->x: An array of size A->nzmax which contains the numeric values of the matrix. This array is a union, and must be accessed via one of: A->x.mpz, A->x.mpq, A->x.mpfr, A->x.int64, or A->x.fp64, depending on the A->type parameter. Data Type: union.

- A->x\_shallow: A boolean indicating whether A->x is shallow. Data Type: bool.
- A->scale: A scaling parameter for matrix of mpz\_t type. For all matrices whose entries are stored in data type other than mpz\_t, A->scale = 1. This is used to ensure that entry can be represented as an integer in an mpz\_t matrix if these entries are converted from non-integer type data (such as double, variable precision floating point, or rational). Data Type: mpq\_t.

Specifically, for different kinds of A of size  $A->m \times A->n$  with nz nonzero entries, its components are defined as:

- (0) SPEX\_CSC: A sparse matrix in CSC (compressed sparse column) format. A->p is an int64\_t array of size A->n+1, A->i is an int64\_t array of size A->nzmax (with  $nz \leq A->nzmax$ ), and A->x.TYPE is an array of size A->nzmax of matrix entries (TYPE is one of mpz, mpq, mpfr, int64, or fp64). The row indices of column j appear in A->i [A->p [j] ... A->p [j+1]-1], and the values appear in the same locations in A->x.TYPE. The A->j array is NULL. A->nz is ignored; the number of entries in A is given by A->p [A->n]. Row indices need not be sorted in each column, but duplicates cannot appear.
- (1) SPEX\_TRIPLET: A sparse matrix in triplet format. A->i and A->j are both int64\_t arrays of size A->nzmax, and A->x.TYPE is an array of values of the same size. The kth tuple has row index A->i [k], column index A->j [k], and value A->x.TYPE [k], with 0 ≤ k < A->nz. The A->p array is NULL. Triplets can be unsorted, but duplicates cannot appear.
- (2) SPEX\_DENSE: A dense matrix. The integer arrays  $A \rightarrow p$ ,  $A \rightarrow i$ , and  $A \rightarrow j$  are all NULL.  $A \rightarrow x$ . TYPE is a pointer to an array of size  $A \rightarrow m^*A \rightarrow n$ , stored in column-oriented format. The value of A(i,j) is  $A \rightarrow x$ . TYPE [p] with  $p = i + j + A \rightarrow m$ .  $A \rightarrow nz$  is ignored; the number of entries in A is  $A \rightarrow m \times A \rightarrow n$ .

A may contain shallow components, A->p, A->i, A->j, and A->x. For example, if A->p\_shallow is true, then a non-NULL A->p is a pointer to a read-only array, and the A->p array is not freed by SPEX\_matrix\_free. If A->p is NULL (for a triplet or dense matrix), then A->p\_shallow has no effect.

To simplify the access the entries in A, SPEX package provides the following macros (Note that the TYPE parameter in the macros is one of: mpz, mpq, mpfr, int64 or fp64):

- SPEX\_1D(A,k,TYPE): used to access the kth entry in SPEX\_matrix A using 1D linear addressing for any matrix kind (CSC, triplet or dense), in any type with TYPE specified corresponding
- SPEX\_2D(A,i,j,TYPE): used to access the (i,j)th entry in a dense SPEX\_matrix A.

The SPEX package has a set of functions to allocate, copy(convert), query and destroy a SPEX matrix, SPEX\_matrix, as shown in the following table.

description	section
allocate a $m$ -by- $n$ SPEX_matrix	2.7.4
destroy a SPEX_matrix and free its al-	2.7.5
located memory	
make a copy of a matrix, into another	2.7.6
kind and/or type	
get the number of entries in a matrix	2.7.7
	allocate a m-by-n SPEX_matrix destroy a SPEX_matrix and free its allocated memory make a copy of a matrix, into another

#### 2.7.4 SPEX\_matrix\_allocate: allocate an m-by-n SPEX\_matrix

```
SPEX_info SPEX_matrix_allocate
   SPEX_matrix *A_handle, // matrix to allocate
    SPEX_kind kind, // CSC, triplet, or dense
   SPEX_type type,
                           // mpz, mpq, mpfr, int64, or double (fp64)
                           // # of rows
    int64_t m,
    int64_t n,
                           // # of columns
                           // max # of entries
    int64_t nzmax,
                           // if true, matrix is shallow. A->p, A->i,
    bool shallow,
                           // A->j, A->x are all returned as NULL and must
                           // be set by the caller. All A->*_shallow are
                           // returned as true.
    bool init,
                           // If true, and the data types are mpz, mpq, or
                           // mpfr, the entries are initialized (using the
                           // appropriate SPEX_mp*_init function). If
                            // false, the mpz, mpq, and mpfr arrays are
                            // allocated but not initialized.
    const SPEX_options option
);
```

SPEX\_matrix\_allocate allocates memory space for a m-by-n SPEX\_matrix whose kind (CSC, triplet or dense) and data type (mpz, mpq, mpfr, int64 or fp64) is specified. If shallow is true, all components (A->p, A->i, A->j, A->x) are returned as

NULL, and their shallow flags are all true. The pointers A->p, A->i, A->j, and/or A->x can then be assigned from arrays in the calling application.

If shallow is false, the appropriate individual arrays are allocated (via SPEX\_calloc). The second boolean parameter is used if the entries are mpz\_t, mpq\_t, or mpfr\_t. Specifically, if init is true, the individual entries within A->x.TYPE are initialized using the appropriate SPEX\_mp\*\_init) function. Otherwise, if init is false, the A->x.TYPE array is allocated (via SPEX\_calloc) and left that way. They are not otherwise initialized, and attempting to access the values of these uninitialized entries will lead to undefined behavior. Returns SPEX\_PANIC if SPEX has not been initialized.

#### 2.7.5 SPEX\_matrix\_free: free a SPEX\_matrix

```
SPEX_info SPEX_matrix_free
(
     SPEX_matrix *A_handle, // matrix to free
     const SPEX_options option
);
```

SPEX\_matrix\_free frees the SPEX\_matrix A. Note that the input of the function is the pointer the SPEX\_matrix structure. This is because this function internally sets the pointer of a SPEX\_matrix to be NULL to prevent potential segmentation fault that could be caused by double free. If default settings are desired, option can be input as NULL.

# 2.7.6 SPEX\_matrix\_copy: make a copy of a SPEX\_matrix with a potentially different matrix-format and data-type

SPEX\_matrix\_copy creates a SPEX\_matrix C which is a modified copy of a SPEX\_matrix A. This function can convert between any pair of the 15 kinds of matrices, so the new matrix C can be of any type or kind different than A. On input C must be non-NULL,

and the value of \*C is ignored; it is overwritten, output with the matrix C, which is a copy of A of kind kind and type type.

The input matrix is assumed to be valid. It can be checked first with SPEX\_matrix\_check (Section 2.7.8), if desired. Results are undefined for an invalid input matrix A. Returns SPEX\_PANIC if SPEX has not been initialized.

### 2.7.7 SPEX\_matrix\_nnz: get the number of entries in a SPEX\_matrix

SPEX\_matrix\_nnz returns an integer, nnz, which is equal to the number of entries in a SPEX\_matrix A. For details regarding how the number of entries is obtained for different kinds of matrices, refer to Section 2.7. For any matrix with invalid dimension(s), nnz is returned as -1. If default settings are desired, option can be input as NULL. Returns SPEX\_PANIC if the SPEX working environment has not been initialized (e.g. via SPEX\_initialize).

## 2.7.8 SPEX\_matrix\_check: check and optionally print a SPEX\_matrix

SPEX\_matrix\_check checks the validity of a SPEX\_matrix A in any of the 15 different matrix types (CSC, triplet, dense) × (mpz, mpq, mpfr, int64, fp64). The print level can be changed via option->print\_level (refer to Section 2.6 for more details). If default settings are desired, option can be input as NULL. Returns SPEX\_PANIC if SPEX has not been initialized.

### 2.7.9 SPEX\_matrix\_div: Divide dense matrix by scalar

This function divides the matrix x by the scalar scalar. On input, x2\_handle is NULL and x must be SPEX\_DENSE of SPEX\_MPZ type. On success, x2\_handle is returned as SPEX\_DENSE with SPEX\_MPQ entries each of which is equal to x / scalar.

### 2.7.10 SPEX\_matrix\_mul: Multiply dense matrix by scalar

This function divides the matrix x by the scalar scalar. On input, x must be SPEX\_DENSE of SPEX\_MPZ type. On success, x is overwritten by x \* scalar.

## 2.8 SPEX\_lu\_analysis structure

The SPEX\_lu\_analysis data structure is used for storing the column permutation for LU factorization and the estimate of the number of nonzeros that may appear in L and U. This need not be modified or accessed in the user application; it simply needs to be passed in directly to the other functions that take it as in input parameter. A SPEX\_lu\_analysis structure has the following components:

- S->q: The column permutation stored as a dense int64\_t vector of size n+1, where n is the number of columns of the analyzed matrix. Currently this vector is obtained via COLAMD, AMD, or is set to no ordering (i.e., [0, 1, ..., n-1]).
- S->lnz: An int64\_t which is an estimate of the number of nonzeros in L. S->lnz must be in the range of  $[n, n^2]$ . If S->lnz is too small, the program may waste time performing extra memory reallocations. This is set during the symbolic analysis.

• S->unz: An int64\_t which is an estimate of the number of nonzeros in U. S->unz must be in the range of  $[n, n^2]$ . If S->unz is too small, the program may waste time performing extra memory reallocations. This is set during the symbolic analysis.

The SPEX package provides the following functions to create and destroy a SPEX\_lu\_analysis structure:

function/macro name	description	section
SPEX_lu_analyze	create SPEX_lu_analysis structure	2.8.1
SPEX_lu_analysis_free	destroy SPEX_lu_analysis structure	2.8.2

## 2.8.1 SPEX\_lu\_analyze: perform symbolic analysis

SPEX\_lu\_analyze performs the symbolic ordering for any LU factorization in SPEX package. Currently, there are three options: no ordering, COLAMD, or AMD, which are passed in by SPEX\_options \*option. For more details, refer to Section 2.6.

The SPEX\_lu\_analysis \*S is created by calling SPEX\_lu\_analyze(&S, A, option) with SPEX\_matrix A properly initialized as CSC matrix and option be NULL if default ordering (COLAMD) is desired. The value of S is ignored on input. On output, S is a pointer to the newly created symbolic analysis structure and SPEX\_OK is returned upon successful completion, or S = NULL with error status returned if a failure occurred. Returns SPEX\_PANIC if SPEX has not been initialized.

The analysis S is freed by SPEX\_lu\_analysis\_free.

### 2.8.2 SPEX\_lu\_analysis\_free: free SPEX\_lu\_analysis structure

```
SPEX_info SPEX_lu_analysis_free
(
     SPEX_lu_analysis **S, // Structure to be deleted
     const SPEX_options option
);
```

SPEX\_lu\_analysis\_free frees a SPEX\_lu\_analysis structure. Note that the input of the function is the pointer to the pointer of a SPEX\_lu\_analysis structure. This is because this function internally sets the pointer of a SPEX\_lu\_analysis to be NULL to prevent potential segmentation fault that could be caused by double free. If default settings are desired, option can be input as NULL. Returns SPEX\_PANIC if SPEX has not been initialized.

## 2.9 SPEX wrapper functions for GMP and MPFR

SPEX provides a wrapper class for all GMP and MPFR functions used by SPEX. The wrapper class provides error-handling for out-of-memory conditions that are not handled by the GMP and MPFR libraries. These wrapper functions are used inside all SPEX functions, wherever any GMP or MPFR functions are used. These functions may also be called by the end-user application.

Each wrapped function has the same name as its corresponding GMP/MPFR function with the added prefix SPEX\_. For example, the default GMP function mpz\_mul is changed to SPEX\_mpz\_mul. Each SPEX GMP/MPFR function returns SPEX\_OK if successful or the correct error code if not. The following table gives a brief list of each currently covered SPEX GMP/MPFR function. For a detailed description of each function, refer to SPEX/SPEX/SPEX\_Utilities/Source/SPEX\_gmp.c.

If additional GMP and MPFR functions are needed in the end-user application, this wrapper mechanism can be extended to those functions. Below are instructions on how to do this.

Given a GMP function void gmpfunc(TYPEa a, TYPEb b, ...), where TYPEa and TYPEb can be GMP type data (mpz\_t, mpq\_t and mpfr\_t, for example) or non-GMP type data (int, double, for example), and they need not to be the same. A wrapper for a new GMP or MPFR function can be created by following this outline:

```
SPEX_info SPEX_gmpfunc
    TYPEa a,
    TYPEb b,
)
{
    // Start the GMP Wrappter
    // uncomment one of the following:
    // If this function is not modifying any {\ensuremath{\mathsf{GMP}}}/{\ensuremath{\mathsf{MPFR}}} type variable, then use
    //SPEX_GMP_WRAPPER_START;
    // If this function is modifying mpz_t type (say TYPEa = mpz_t), then use
    //SPEX_GMPZ_WRAPPER_START(a) ;
    // If this function is modifying mpq_t type (say TYPEa = mpq_t), then use
    //SPEX_GMPQ_WRAPPER_START(a) ;
    // If this function is modifying mpfr_t type (say TYPEa = mpfr_t), then use
    //SPEX_GMPFR_WRAPPER_START(a) ;
    // Call the GMP function
    gmpfunc(a,b,...);
    //Finish the wrapper and return ok if successful.
    SPEX_GMP_WRAPPER_FINISH;
    return SPEX_OK;
}
```

Note that, other than SPEX\_mpfr\_fprintf, SPEX\_gmp\_fprintf, SPEX\_gmp\_printf and SPEX\_gmp\_fscanf, all of the wrapped GMP/MPFR functions always return SPEX\_info to the caller. Therefore, for some GMP/MPFR functions that have their own return value. For example, for int mpq\_cmp(const mpq\_t a, const mpq\_t b), the return value becomes a parameter of the wrapped function. In general, a GM-P/MPFR function in the form of TYPEr gmpfunc(TYPEa a, TYPEb b, ...), the wrapped function can be constructed as follows:

```
// Call the GMP function
*r = gmpfunc(a,b,...);

//Finish the wrapper and return ok if successful.
SPEX_GMP_WRAPPER_FINISH;
return SPEX_OK;
}
```

MPFR Function	SPEX_MPFR Function	Description
n = mpfr_asprintf(&buff, fmt,)	n = SPEX_mpfr_asprintf(&buff, fmt,)	Print format to allocated string
mpfr_free_str(buff)	SPEX_mpfr_free_str(buff)	Free string allocated by MPFR
<pre>mpfr_init2(x, size)</pre>	SPEX_mpfr_init2(x, size)	Initialize x with size bits
mpfr_set(x, y, rnd)	SPEX_mpfr_set(x, y, rnd)	x = y
mpfr_set_d(x, y, rnd)	SPEX_mpfr_set_d(x, y, rnd)	x = y (double)
mpfr_set_q(x, y, rnd)	SPEX_mpfr_set_q(x, y, rnd)	$x = y \text{ (mpq_t)}$
mpfr_set_z(x, y, rnd)	SPEX_mpfr_set_z(x, y, rnd)	$x = y \text{ (mpz_t)}$
mpfr_get_z(x, y, rnd)	SPEX_mpfr_get_z(x, y, rnd)	$(mpz\_t) \ x = y$
x = mpfr_get_d(y, rnd)	SPEX_mpfr_get_d(x, y, rnd)	$(\text{double}) \ x = y$
mpfr_mul(x, y, z, rnd)	SPEX_mpfr_mul(x, y, z, rnd)	x = y * z
mpfr_mul_d(x, y, z, rnd)	SPEX_mpfr_mul_d(x, y, z, rnd)	x = y * z
mpfr_div_d(x, y, z, rnd)	SPEX_mpfr_div_d(x, y, z, rnd)	x = y + z x = y/z
mpfr_ui_pow_ui(x, y, z, rnd)	SPEX_mpfr_ui_pow_ui(x, y, z, rnd)	$\begin{array}{ c c c c c c c c c c c c c c c c c c c$
mpfr_log2(x, y, rnd)	SPEX_mpfr_log2(x, y, rnd )	$\begin{array}{c c} x - y \\ x = \log_2(y) \end{array}$
mpfr_free_cache()	SPEX_mpfr_free_cache()	Free cache after log2
GMP Function	SPEX_GMP Function	Description
n = gmp_fscanf(fp, fmt,)	n = SPEX_gmp_fscanf(fp, fmt,)	Read from file fp
mpz_init(x)	SPEX_mpz_init(x)	Initialize x
<pre>mpz_init2(x, size)</pre>	SPEX_mpz_init2(x, size)	Initialize x to size bits
<pre>mpz_set(x, y)</pre>	SPEX_mpz_set(x, y)	$x = y \text{ (mpz_t)}$
<pre>mpz_set_ui(x, y)</pre>	SPEX_mpz_set_ui(x, y)	x = y  (signed int)
<pre>mpz_set_si(x, y)</pre>	<pre>SPEX_mpz_set_si(x, y)</pre>	x = y (unsigned int)
<pre>mpz_set_d(x, y)</pre>	SPEX_mpz_set_d(x, y)	x = y (double)
x = mpz_get_d(y)	SPEX_mpz_get_d(x, y)	x = y (double out)
mpz_set_q(x, y)	SPEX_mpz_set_q(x, y)	$x = y \; (\texttt{mpz\_t})$
mpz_mul(x, y, z)	SPEX_mpz_mul(x, y, z)	x = y * z
mpz_add(x, y, z)	SPEX_mpz_add(x, y, z)	x = y + z
mpz_addmul(x, y, z)	SPEX_mpz_addmul(x, y, z)	x = x + y * z
mpz_submul(x, y, z)	SPEX_mpz_submul(x, y, z)	x = x - y * z
mpz_divexact(x, y, z)	SPEX_mpz_divexact(x, y, z)	x = y/z
gcd = mpz_gcd(x, y)	SPEX_mpz_gcd(gcd, x, y)	gcd = gcd(x, y)
lcm = mpz_lcm(x, y)	SPEX_mpz_lcm(lcm, x, y)	lcm = lcm(x, y)
mpz_abs(x, y)	SPEX_mpz_abs(x, y)	x =  y
$r = mpz_cmp(x, y)$	SPEX_mpz_cmp(r, x, y)	$r = 0$ if $x = y$ , $r \neq 0$ if $x \neq y$
r = mpz_cmpabs(x, y)	SPEX_mpz_cmpabs(r, x, y)	$r = 0$ if $ x  =  y $ , $r \neq 0$ if $ x  \neq  y $
r = mpz_cmp_ui(x, y)	SPEX_mpz_cmp_ui(r, x, y)	$r = 0$ if $x = y$ , $r \neq 0$ if $x \neq y$
sgn = mpz_sgn(x)	SPEX_mpz_sgn(sgn, x)	sgn = 0  if  x = 0
size = mpz_sizeinbase(x, base)	SPEX_mpz_sizeinbase(size, x, base)	size of x in base
mpq_init(x)	SPEX_mpq_init(x)	Initialize x
mpq_set(x, y)	SPEX_mpq_set(x, y)	x = y
mpq_set(x, y) mpq_set_z(x, y)	SPEX_mpq_set(x, y) SPEX_mpq_set_z(x, y)	x - y x = y  (mpz)
	SPEX_mpq_set_2(x, y) SPEX_mpq_set_d(x, y)	x = y  (imp2) $x = y  (double)$
mpq_set_d(x, y)	_ 1 1	x = y  (double) x = y/z  (unsigned int)
mpq_set_ui(x, y, z)	SPEX_mpq_set_ui(x, y, z)	( )
mpq_set_num(x, y)	SPEX_mpq_set_num(x, y)	num(x) = y
mpq_set_den(x, y)	SPEX_mpq_set_den(x, y)	den(x) = y
mpq_get_den(x, y)	SPEX_mpq_get_den(x, y)	x = den(y)
$x = mpq_get_d(y)$	SPEX_mpq_get_d(x, y)	(double) $x = y$
mpq_abs(x, y)	SPEX_mpq_abs(x, y)	x =  y
mpq_add(x, y, z)	SPEX_mpq_add(x, y, z)	x = y + z
mpq_mul(x, y, z)	SPEX_mpq_mul(x, y, z)	x = y * z
mpq_div(x, y, z)	SPEX_mpq_div(x, y, z)	x = y/z
$r = mpq\_cmp(x, y)$	SPEX_mpq_cmp(r, x, y)	$r = 0 \text{ if } x = y, r \neq 0 \text{ if } x \neq y$
r = mpq_cmp_ui(x, n, d)	SPEX_mpq_cmp_ui(r, x, n, d)	$r = 0 \text{ if } x = n/d, r \neq 0 \text{ if } x \neq n/d$
r = mpq_equal(x, y)	<pre>SPEX_mpq_equal(r, x, y)</pre>	$r = 0 \text{ if } x = y, r \neq 0 \text{ if } x \neq y$

## 2.10 Additional Useful SPEX Utility Functions

### 2.10.1 SPEX\_cumsum: Cumulative sum of a vector

SPEX\_cumsum computes the cumulative sum of the array c and stores it in the array p. Specifically,  $p_i = \sum_{j=1}^i c_j$ . This is mainly used for matrix copy and some factorizations. On input, p and c must not be NULL and n must be at least 0. On completion, the contents of p are overwritten with the cumulative sum of c and SPEX\_OK is returned.

# 2.10.2 SPEX\_check\_solution: Validate solution vector (for debugging)

Given a solution vector  $\mathbf{x}$ , check the solution of the linear system  $A\mathbf{x} = \mathbf{b}$ . This is done by computing a rational-arthmetic  $A*\mathbf{x} == \mathbf{b}$ . Since all routines in SPEX are gauranteed to be exact, this function is for debugging purposes. On input, A is SPEX\_CSC of SPEX\_MPZ type,  $\mathbf{x}$  is SPEX\_DENSE of SPEX\_MPQ type and  $\mathbf{b}$  is SPEX\_DENSE of SPEX\_MPZ type. On success, SPEX\_OK is returned.

## Chapter 3

## SPEX Left LU

## 3.1 Overview

SPEX Left LU is a software package designed to exactly solve unsymmetric sparse linear systems, Ax = b, where  $A \in \mathbb{Q}^{n \times n}$ ,  $b \in \mathbb{Q}^{n \times r}$ , and  $x \in \mathbb{Q}^{n \times r}$ . This package performs a left-looking, roundoff-error-free (REF) LU factorization PAQ = LDU, where L and U are integer, D is diagonal, and P and Q are row and column permutations, respectively. Note that, in order to solve a linear system, the matrix D is never explicitly computed nor needed; thus this package uses only the matrices L and U. The theory associated with this code is the Sparse Left-looking Integer-Preserving (SLIP) LU factorization [8]. Aside from solving sparse linear systems exactly, one of the key goals of this package is to provide a framework for other solvers to benchmark the reliability and stability of their linear solvers, as our final solution vector x is guaranteed to be exact. SPEX Left LU is written in ANSI C and is accompanied by a MATLAB interface.

For all primary computational routines in Section 3.5.1, the input argument A must be stored in a compressed sparse column (CSC) matrix with entries in  $mpz_t$  type (referred to as CSC  $mpz_t$  matrix henceforth), while b must be stored as a dense  $mpz_t$  matrix (i.e., a dense matrix with entries in  $mpz_t$  type). However, the original data type of entries in the input matrix A and right hand side (RHS) vectors b can be any one of: double, int64\_t,  $mpq_t$ ,  $mpz_t$ , or  $mpfr_t$ , and their format(s) are allowed to be CSC, sparse triplet, or dense. Section 3.6.1 discusses the SPEX\_matrix structure, the allowed matrix formats and types, and how to perform conversions across different formats/types.

The matrices L and U are computed using integer-preserving routines with the arbitrary-sized integer (mpz\_t) data type from the GMP Library [7]. The matrices

L and U are computed in a left-looking fashion: one column at a time via the sparse REF triangular solve detailed in [8]. All divisions performed in the algorithm are guaranteed to be exact (i.e., with zero reminder); therefore, no greatest common divisor algorithms are needed.

The permutation matrices P and Q define the pivot ordering; Q is a given fill-reducing column ordering, and P is determined dynamically during the factorization. For the matrix P, the default option is to use a partial pivoting scheme in which the (non-zero) entry with the smallest magnitude in column k is selected as pivot; where ties are broken in favor of the diagonal entry (and arbitrarily otherwise). In addition to this scheme, the code allows diagonal pivoting, partial pivoting selecting the entry with largest magnitude, or various tolerance-based diagonal pivoting schemes. For the matrix Q, the default ordering is obtained via the Column Approximate Minimum Degree (COLAMD) algorithm [4, 5]. Other approaches include using the Approximate Minimum Degree (AMD) ordering [1, 2], or no ordering (Q = I). Section 2.8.1 discusses how to select the desired column ordering prior to factorization.

Once the factorization LDU = PAQ is computed, the solution vector x is computed via the sparse REF forward and backward substitution algorithms [8]. Forward substitution is a variant of the sparse REF triangular solve discussed above. Backward substitution is a typical column-oriented sparse backward substitution. Both of these routines require b to be given as a dense  $mpz_t$  matrix. At the conclusion of the forward and backward substitution routines, the final solution vector(s) x are guaranteed to be exact. The solution x is returned as a dense  $mpq_t$  matrix.

A key advantage of utilizing SPEX Left LU with floating-point output is that the solution is guaranteed to be exact until the final (and only) rational-to-floating point conversion. Note that this final conversion is done in higher precision. Thus, the solution x output in double precision are accurate to machine roundoff (approximately  $10^{-16}$ ). In addition, the returned solution can also be accurate to any user-specified precision by using MPFR output.

## 3.2 Licensing

**Copyright:** The copyright of this software is held by Christopher Lourenco, Jinhao Chen, Erick Moreno-Centeno, and Timothy A. Davis.

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License: This software package is dual licensed under the GNU General Public License version 2 or the GNU Lesser General Public License version 3. Details of this license are in SPEX/License/license.txt. For alternative licenses, please contact the authors.

## 3.3 Installation

Installation of SPEX Left LU requires the make utility in Linux/MacOS, or Cygwin make in Windows. With the proper compiler, typing make under the main directory will compile AMD, COLAMD and SPEX Left LU to the respective SPEX/Lib folder. To further install the libraries onto your computer, simply type make install. Thereafter, to use the code inside of your program, precede your code with #include "SPEX.h".

To run the statement coverage tests, go to the Tcov folder and type make. The last line of output should read:

#### statements not yet tested: 0

If you want to use SPEX Left LU within MATLAB, cd in MATLAB to the folder SPEX/SPEX/MATLAB then type

SPEX\_mex\_install. This compiles the necessary code so that you can use the SPEX\_\* functions within MATLAB. Note that

SPEX\_mex\_install does not add the correct directory to your path; therefore, if you want to use the SPEX\_\* functions in future sessions, type pathtool and save your path for future MATLAB sessions. If you cannot save your path because of file permissions, edit your startup.m by adding addpath commands (for more information on how this is done, please type doc startup and doc addpath).

## 3.4 SPEX\_VERSION: the software package version

SPEX Left LU defines the following strings with #define. Refer to the SPEX.h file for details.

Macro	purpose
SPEX_VERSION	current version of the code (as a string)
SPEX_VERSION_MAJOR	major version of the code
SPEX_VERSION_MINOR	minor version of the code
SPEX_VERSION_SUB	sub version of the code

## 3.5 Factorization and Solve Routines

### 3.5.1 SPEX\_lu\_factorize: perform LU factorization

```
SPEX_info SPEX_lu_factorize
    // output:
    SPEX_matrix *L_handle,
                               // lower triangular matrix
    SPEX_matrix *U_handle,
                               // upper triangular matrix
   SPEX_matrix *rhos_handle, // sequence of pivots
    int64_t **pinv_handle,
                               // inverse row permutation
    // input:
    const SPEX_matrix A,
                               // matrix to be factored
    const SPEX_lu_analysis *S,
                                // column permutation and estimates
                                 // of nnz in L and U
    const SPEX_options option
);
```

SPEX\_lu\_factorize performs the SPEX Left-looking LU factorization. This factorization is done via n (number of rows or columns of the square matrix A) iterations of the sparse REF triangular solve function. The overall factorization is PAQ = LDU. This routine allows the factorization and solve to be split into separate phases. For example codes, refer to either SPEX/SPEX\_LU/Demos/spexlu\_denmo.c or Section 3.6.3.

On input, L, U, rhos, and pinv are undefined and ignored. A must be a CSC mpz matrix. Default settings are used if option is input as NULL.

Upon successful completion, the function returns SPEX\_OK, and L and U are lower and upper triangular matrices, respectively, which are CSC matrices of type mpz. rhos contains the sequence of pivots as an n-by-1 dense vector of type mpz.

After factorizing the matrix, the determinant of A can be obtained from rhos [n-1] and A->scale as follows:

```
mpq_t determinant ;
SPEX_mpq_init (determinant) ;
SPEX_mpq_set_z (determinant, rhos->x.mpz[rhos->n-1]) ;
SPEX_mpq_div (determinant, determinant, A->scale) ;
```

The output array pinv contains the inverse row permutation (that is, the row index in the permuted matrix PA. For the *i*th row in A, pinv[i] gives the row index in PA).

Returns SPEX\_PANIC if SPEX has not been initialized. Otherwise, if another error occurs, L, U, rhos, and pinv are all returned as NULL, and an error code will be returned correspondingly.

## **3.5.2** SPEX\_lu\_solve: solve the linear system Ax = b

```
SPEX_info SPEX_lu_solve
                           // solves the linear system LD^{(-1)}U x = b
    // Output
    SPEX_matrix *X_handle,
                               // rational solution to the system
    // input:
    const SPEX_matrix b,
                               // right hand side vector
                               // Input matrix
    const SPEX_matrix A,
    const SPEX_matrix L,
                               // lower triangular matrix
    const SPEX_matrix U,
                               // upper triangular matrix
    const SPEX_matrix rhos,
                               // sequence of pivots
    const SPEX_lu_analysis *S, // symbolic analysis struct
                                // inverse row permutation
    const int64_t *pinv,
    const SPEX_options option
);
```

SPEX\_lu\_solve obtains the solution of mpq\_t type to the linear system Ax = b upon a successful factorization. This function may be called after a successful return from SPEX\_lu\_factorize, which computes L, U, rhos, and pinv.

On input, SPEX\_matrix x is undefined. A, L and U must be CSC mpz\_t matrices while b and rhos must be dense mpz\_t matrices. All matrices must have matched dimensions: the matrices L and U must be square lower and upper triangular matrices the same size as A, and rhos must be a dense n-by-1 vector. The input matrix b must have same number of rows as A. Default settings are used if option is input as NULL.

Upon successful completion, the function returns SPEX\_OK, and x contains the solution of  $mpq_t$  type with dense format to the linear system Ax = b. If desired, option->check can be set to true to enable a post-check of the solution of this function. However, this is intended for debugging only; the SPEX library is guaranteed to return the exact solution. Otherwise (in case of error occurred), the function returns corresponding error code.

This function is primarily for applications that require intermediate results. For additional information, refer to either SPEX/SPEX\_LU/Demos/spexlu\_demo.c or Section 3.6.3. Returns SPEX\_PANIC if SPEX has not been initialized.

#### 3.5.3 SPEX\_lu\_backslash: solve Ax = b

SPEX\_lu\_backslash solves the linear system Ax = b and returns the solution as a dense matrix of mpq\_t, mpfr\_t or double numbers. This function performs symbolic analysis, factorization, and solving all in one line. It can be thought of as an exact version of MATLAB sparse backslash.

On input, SPEX\_matrix x is undefined. type must be one of: SPEX\_MPQ, SPEX\_MPFR or SPEX\_FP64 to specify the data type of the solution entries. A should be a square CSC mpz\_t matrix while b should be a dense mpz\_t matrix. In addition, A->m should be equal to b->m. Default settings are used if option is input as NULL.

Upon successful completion, the function returns SPEX\_OK, and x contains the solution of data type specified by type to the linear system Ax = b. If desired, option->check can be set to true to enable solution checking process in this function. However, this is intended for debugging only; SPEX library is guaranteed to return the exact solution. Otherwise (in case of error occurred), the function returns corresponding error code.

Returns SPEX\_PANIC if SPEX has not been initialized.

For a complete example, refer to SPEX/SPEX\_LU/Demos/example.c, SPEX/SPEX\_LU/Demos/example2.c, or Section 3.6.2.

## 3.6 Using SPEX Left LU in C

Using SPEX Left LU in C has three steps:

- 1. initialize and populate data structures,
- 2. perform symbolic analysis, factorize the matrix A and solve the linear system for each b vector, and

3. free all used memory and finalize.

Step 1 is discussed in Section 3.6.1. For Step 2, performing symbolic analysis and factorizing A and solving the linear Ax = b can be done in one of two ways. If only the solution vector x is required, SPEX Left LU provides a simple interface for this purpose which is discussed in Section 3.6.2. Alternatively, if the L and U factors are required, refer to Section 3.6.3. Finally, step 3 is discussed in Section 3.6.4. For the remainder of this section, n will indicate the dimension of A (that is,  $A \in \mathbb{Z}^{n \times n}$ ) and numRHS will indicate the number of right hand side vectors being solved (that is, if numRHS = r, then  $b \in \mathbb{Z}^{n \times r}$ ).

# 3.6.1 SPEX Left LU initialization and population of data structures

This section discusses how to initialize and populate the global data structures required for SPEX Left LU.

#### Initializing the environment

SPEX is built upon the GNU Multiple Precision Arithmetic (GMP) [7] and GNU Multiple Precision Floating Point Reliable (MPFR) [6] libraries and provides wrappers to all GMP/MPFR functions it uses. This allows SPEX to properly handle memory management failures, which GMP/MPFR does not handle. To enable this mechanism, SPEX requires initialization. The following must be done before using any other SPEX function:

```
SPEX_initialize ( ) ;
// or SPEX_initialize_expert (...); if custom memory functions are desired
```

#### Initializing data structures

SPEX assumes three specific input options for all functions. These are:

- SPEX\_matrix A and SPEX\_matrix b: A contains the input coefficient matrix, while b contains the right hand side vector(s) of the linear system Ax = b.
- SPEX\_lu\_analysis\* S: S contains the column permutation used for A as well as estimates of the number of nonzeros in L and U.

• SPEX\_options option: option contains various control options for the factorization including column ordering used, pivot selection scheme, and others. For a full list of the contents of the SPEX\_options structure, refer to Section 2.6. If default settings are desired, option can be set to NULL.

#### Populating data structures

Of the three data structures discussed in Section 3.6.1, S is constructed during symbolic analysis (Section 2.8.1), and option is an optional parameter for selecting non-default parameters. Refer to Section 2.6 for the contents of option.

SPEX allows the input numerical data for A and b to come in one of 5 types: int64\_t, double, mpfr\_t, mpq\_t, and mpz\_t. Moreover, both A and b can be stored in CSC form, sparse triplet form or dense form. CSC form is discussed in Section 2.1. The triplet form stores the contents of the matrix A in three arrays i, j, and x where the kth nonzero entry is stored as A(i[k], j[k]) = x[k]. SPEX stores its dense matrices in in column-oriented format, that is, the (i, j)th entry in A is A->x. TYPE[p] with p = i + j\*A->m.

If the data for matrices are in file format to be read, refer to SPEX/SPEX\_LU/Demo /example2.c on how to read in data and construct A and b. If the data for matrices are already stored in vectors corresponding to CSC form, sparse triplet form or dense form, allocate a shallow SPEX\_matrix and assign vectors accordingly, then use SPEX\_matrix\_copy to get a SPEX\_matrix in the desired kind and type. For more details, refer to SPEX/SPEX/SPEX\_LU/Demo/example.c. In a case when A is available in format other than CSC mpz, and/or b is available in format other than dense mpz, the following code snippet shows how to get A and b in a required format.

```
/* Get the matrix A. Assume that A1 is stored in CSC form
  with mpfr_t entries, while b1 is stored in triplet form
  with mpq_t entries. (for A1 and b1 in any other form,
    the exact same code will work) */

SPEX_matrix A, b;
// A is a copy of the A1. A is a CSC matrix with mpz_t entries
SPEX_matrix_copy(&A, SPEX_CSC, SPEX_MPZ, A1, option);
// b is a copy of the b1. b is a dense matrix with mpz_t entries.
SPEX_matrix_copy(&b, SPEX_DENSE, SPEX_MPZ, b1, option);
```

# 3.6.2 Simple SPEX Left LU routines for solving linear systems

After initializing the necessary data structures, SPEX obtains the solution to Ax = b using the simple interface of SPEX Left LU, SPEX\_lu\_backslash. The SPEX\_lu\_backslash function can return x as double, mpq\_t, or mpfr\_t with an associated precision. See Section 3.5.3 for more details. The following code snippet shows how to get solution as a dense mpq\_t matrix.

```
SPEX_matrix x;
SPEX_type my_type = SPEX_MPQ; // SPEX_MPQ, SPEX_MPFR, SPEX_FP64
SPEX_lu_backslash(&x, my_type, A, b, option);
```

On successful return, this function returns SPEX\_OK (see Section 2.4.2).

## 3.6.3 Expert SPEX Left LU routines

If the L and U factors from the SPEX Left LU factorization of the matrix A are required, the steps performed by SPEX\_lu\_backslash can be done with a sequence of calls to SPEX functions:

- 1. declare L, U, the solution matrix x, and others,
- 2. perform symbolic analysis,
- 3. compute the factorization PAQ = LDU,
- 4. solve the linear system Ax = b, and
- 5. convert the final solution into the final desired form.

These steps are discussed below, along with examples.

#### Declare workspace

Using SPEX in this form requires the intermediate variables be declared, such as L, U, etc. The following code snippet shows the detailed list.

```
// A and b are in required type and ready to use
SPEX_matrix L = NULL;
SPEX_matrix U = NULL;
```

```
SPEX_matrix x = NULL;
SPEX_matrix rhos = NULL;
int64_t *pinv = NULL;
SPEX_lu_analysis* S = NULL;

// option needs no declaration if default setting is desired
// only declare option for further modification on default setting
SPEX_options option = SPEX_create_default_options();
```

#### SPEX Left LU symbolic analysis

The symbolic analysis phase of an LU factorization entails computing the symbolic column ordering and estimating the number of nonzeros in L and U. This is performed by calling the following function:

```
SPEX_lu_analyze (&S, A, option) ;
```

#### Computing the factorization

The matrices L and U, the pivot sequence rhos, and the row permutation pinv are computed via the SPEX\_lu\_factorize function (Section 3.5.1). Upon successful completion, this function returns SPEX\_OK.

#### Solving the linear system

After factorization, the next step is to solve the linear system and store the solution as a dense matrix x with entries of rational number mpq\_t. This solution is done via the SPEX\_lu\_solve function (Section 3.5.2). Upon successful completion, this function returns SPEX\_OK.

In this step, option->check can be set to true to enable the solution check process as discussed in Section 3.5.2. The process can verify that the solution vector x satisfies Ax = b in perfect precision intended for debugging. This step is not needed, since the solution returned is guaranteed to be exact. It appears here simply as debugging tool, and as a verification that SPEX is computing its expected result. This test can fail only if it runs out of memory, or if there is a bug in the code (in which case, please notify the authors). Also, note that this process can be quite time consuming; thus it is not recommended to be used in general.

#### Converting the solution vector to the final desired form

Upon completion of the above routines, the solution to the linear system is in a dense mpq\_t matrix. SPEX allows this to be converted into any form of matrix in the set of (CSC, sparse triplet, dense) × (mpfr\_t, mpq\_t, double) using SPEX\_matrix\_copy. The following code snippet shows how to get solution as a dense double matrix; since this involves a floating-point representation, the solution my\_x will no longer be exact, even though x is the exact solution.

```
SPEX_kind my_kind = SPEX_DENSE;  // SPEX_CSC, SPEX_TRIPLET or SPEX_DENSE
SPEX_type my_type = SPEX_FP64;  // SPEX_MPG, SPEX_MPFR, or SPEX_FP64
SPEX_matrix my_x = NULL;  // New output
// Create copy which is stored as my_kind and my_type:
SPEX_matrix_copy( &my_x, my_kind, my_type, x, option);
```

## 3.6.4 Freeing memory

As described in Section 2.5, SPEX provides a number of functions/macros to free SPEX structures:

- SPEX\_matrix: A SPEX\_matrix A data structure can be freed with a call to SPEX\_matrix\_free(&A, NULL);
- SPEX\_lu\_analysis\*: A SPEX\_lu\_analysis\* S data structure can be freed with a call to SPEX\_lu\_analysis\_free(&S, NULL);
- All others including SPEX\_options: These data structures can be freed with a call to the macro SPEX\_FREE(), for example, SPEX\_FREE(option) for SPEX\_options option.

After all usage of the SPEX routines is finished, SPEX\_finalize() must be called (Section 2.4.5) to finalize usage of the library.

## 3.6.5 Examples

The SPEX/SPEX\_LU/Demo folder contains three sample C codes which utilize SPEX. These files demonstrate the usage of SPEX as follows:

• example.c: This example generates a random dense  $50 \times 50$  matrix and a random dense  $50 \times 1$  right hand side vector b and solves the linear system. In this function, the SPEX\_lu\_backslash function is used; and the output is given as a double matrix.

- example2.c: This example reads in a matrix stored in triplet format from the ExampleMats folder. Additionally, it reads in a right hand side vector from this folder and solves the associated linear system via the SPEX\_lu\_backslash function, and, the solution is given as a matrix of rational numbers.
- spexlu\_demo.c: This example reads in a matrix and right hand side vector from a file and solves the linear system Ax = b using the techniques discussed in Section 3.6.3. This file also allows command line arguments (discussed in README.md) and can be used to replicate the results from [8].

## 3.7 Using SPEX Left LU in MATLAB

After following the installation steps discussed in Section 3.3, using the SPEX Left LU factorization within MATLAB can be done via the SPEX\_lu\_backslash.m function. First, this section describes the option struct in Section 3.7.1. The use of the factorization is discussed in Section 3.7.2. The SPEX/SPEX\_LU/MATLAB folder must be in your MATLAB path.

## 3.7.1 Optional parameter settings

The SPEX Left LU MATLAB interface includes an option struct as in optional input parameter that modifies behavior. If this parameter is not provided, default parameter settings are used. The elements of the option struct are listed below. Any fields not present in the struct are treated as their default values.

- option.pivot: This parameter is a string that controls the pivoting scheme used. When selecting a pivot entry in a given column, the factorization method uses one of the following pivoting strategies:
  - 'smallest': smallest pivot,
  - 'diagonal': diagonal pivot if possible, otherwise smallest pivot,
  - 'first': first nonzero pivot in each column,
  - 'tol smallest': (default) diagonal pivot with a tolerance (option.tol) for the smallest pivot,
  - 'tol largest': diagonal pivot with a tolerance (option.tol) for the largest pivot,
  - 'largest': largest pivot.

- option.order: This parameter is a string controls the fill-reducing column preordering used.
  - 'none': no column ordering; factorize A as-is.
  - 'colamd': COLAMD ordering (default)
  - 'amd': AMD ordering

The 'colamd' is recommended for most cases. The 'AMD' ordering is suitable if the nonzero pattern of A is mostly symmetric. In this case, option.pivot = 'diagonal' is a useful option.

- option.tol: This parameter determines the tolerance used if one of the threshold pivoting schemes is chosen. The default value is 1 and this parameter can take any value in the range (0, 1].
- option.solution: a string determining how x is to be returned:
  - 'double': x is converted to a 64-bit floating-point approximate solution.
     This is the default.
  - 'vpa': x is returned as a vpa array with option.digits digits (default is given by the MATLAB digits function). The result may be inexact, if an entry in x cannot be represented in the specified number of digits. To convert this x to double, use x=double(x).
  - 'char': x is returned as a cell array of strings, where x {i} = 'numerator/denominator' and both numerator and denominator are arbitrary-length strings of decimal digits. The result is always exact, although x cannot be directly used in MATLAB for numerical calculations. It can be inspected or analyzed using MATLAB string manipulation. To convert x to vpa, use x=vpa(x). To convert x to double, use x=double(vpa(x)).
- option.digits: the number of decimal digits to use for x, if option.solution is 'vpa'. Must be in range 2 to 2<sup>29</sup>.
- option.print: display the inputs and outputs (0: nothing (default), 1: just errors, 2: terse, 3: all).

#### 3.7.2 SPEX\_lu\_backslash.m

The SPEX\_lu\_backslash.m function solves the linear system Ax = b where  $A \in \mathbb{R}^{n \times n}$ ,  $x \in \mathbb{R}^{n \times m}$  and  $b \in \mathbb{R}^{n \times m}$ . The final solution vector(s) obtained via this function are exact prior to their conversion to double precision.

The SPEX Left LU function expects as input a sparse matrix A and dense set of right hand side vectors b. Optionally, option struct can be passed in. Currently, there are 2 ways to use this function outlined below:

- $x = SPEX_lu_backslash(A,b)$  returns the solution to Ax = b using default settings. The solution vectors are more accurate than the solution obtained via  $x = A \setminus b$ . The solution x is returned as a MATLAB double matrix.
- $x = SPEX_lu_backslash(A,b,option)$  returns the solution to Ax = b using non-default settings from the option struct.

If the result x is held as a MATLAB double matrix, in conventional floating-point representation (double), it is guaranteed to be exact only if the exact solution can be held in double without modification.

The solution x may also be returned as a MATLAB vpa array, or as a cell array of strings; See Section 3.7.1 for details.

## Bibliography

- [1] P. R. AMESTOY, T. A. DAVIS, AND I. S. DUFF, An approximate minimum degree ordering algorithm, SIAM Journal on Matrix Analysis and Applications, 17 (1996), pp. 886–905.
- [2] —, Algorithm 837: AMD, an approximate minimum degree ordering algorithm, ACM Transactions on Mathematical Software (TOMS), 30 (2004), pp. 381–388.
- [3] T. Davis, SuiteSparse, 2020. http://faculty.cse.tamu.edu/davis/suitesparse.html.
- [4] T. A. Davis, J. R. Gilbert, S. I. Larimore, and E. G. Ng, Algorithm 836: COLAMD, a column approximate minimum degree ordering algorithm, ACM Transactions on Mathematical Software (TOMS), 30 (2004), pp. 377–380.
- [5] —, A column approximate minimum degree ordering algorithm, ACM Transactions on Mathematical Software (TOMS), 30 (2004), pp. 353–376.
- [6] L. Fousse, G. Hanrot, V. Lefèvre, P. Pélissier, and P. Zimmermann, MPFR: a multiple-precision binary floating-point library with correct rounding, ACM Transactions on Mathematical Software (TOMS), 33 (2007), p. 13.
- [7] T. Granlund et al., GNU MP 6.0 Multiple Precision Arithmetic Library, Samurai Media Limited, 2015.
- [8] C. Lourenco, A. R. Escobedo, E. Moreno-Centeno, and T. A. Davis, Exact solution of sparse linear systems via left-looking roundoff-error-free LU factorization in time proportional to arithmetic work, SIAM Journal on Matrix Analysis and Applications, 40 (2019), pp. 609–638.