User's Guide for ParU, an unsymmetric multifrontal multithreaded sparse LU factorization package

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Abstract

ParU is an implementation of the multifrontal sparse LU factorization method. Parallelism is exploited both in the BLAS and across different frontal matrices using OpenMP tasking, a shared-memory programming model for modern multicore architectures. The package is written in C++ and real sparse matrices are supported.

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1 Introduction

The algorithms used in ParU are discussed in a companion paper. FIXME: cite our ACM TOMS submission, and include it the Doc folder. This document gives detailed information on the installation and use of ParU. ParU is a parallel sparse direct solver that uses OpenMP tasking for parallelism. ParU calls UMFPACK for the symbolic analysis phase, after that, some symbolic analysis is done by ParU itself, and then the numeric phase starts. The numeric computation is a task parallel phase using OpenMP, and each task calls parallel BLAS; i.e. nested parallelism. The performance of BLAS has a heavy impact on the performance of ParU. Moreover, the way parallel BLAS can be called in a nested environment can also be very important for ParU's performance.

2 Using ParU in C and C++

ParU relies on CHOLMOD for its basic sparse matrix data structure, a compressed sparse column format. CHOLMOD provides interfaces to the AMD, COLAMD, and METIS ordering methods and many other functions. ParU also relies on UMFPACK for its symbolic analysis.

2.1 Installing the C/C++ library on any system

All of SuiteSparse can be built by cmake with a single top-level CMakeLists.txt file. In addition, each package (including ParU) has its own CMakeLists.txt file to build that package individually. This is the simplest method for building ParU and its dependent pacakages on all systems.

2.2 Installing the C/C++ library on Linux/Unix

In Linux/MacOs, type make at the command line in either the SuiteSparse directory (which compiles all of SuiteSparse) or in the SuiteSparse/ParU directory (which just compiles ParU). ParU will be compiled; you can type make demos to run a set of simple demos.

The use of make is optional. The top-level ParU/Makefile is a simple wrapper that uses cmake to do the actual build.

To fully test the coverage of the lines ParU, go to the Tcov directory and type make. This test requires Linux.

To install the shared library (by default, into /usr/local/lib and /usr/local/include), do make install. To uninstall, do make uninstall. For more options, see the ParU/README.md file.

2.3 C/C++ Example

Below is a simple C++ program that illustrates the use of ParU. The program reads in a problem from stdin in MatrixMarket format [3], solves it, and prints the norm of A and the residual. Some error testing code is omitted to simplify the program, but a robust

user application should check the return values from ParU. The full program can be found in ParU/Demo/paru_simple.cpp. Note that ParU supports only real double-precision matrices. Refer to the CHOLMOD User guide for the CHOLMOD methods used below.

```
#include <iostream>
#include <iomanip>
#include <ios>
#include <cmath>
#include "ParU.h"
int main(int argc, char **argv)
{
   cholmod_common Common, *cc;
   cholmod_sparse *A = NULL;
   ParU_Symbolic Sym = NULL;
   ParU_Numeric Num = NULL;
   ParU_Control Control = NULL;
   double *b = NULL, *x = NULL;
   //~~~~Reading the input matrix
   // start CHOLMOD
   cc = &Common;
   int mtype;
   cholmod_l_start(cc);
   A = (cholmod_sparse *)cholmod_l_read_matrix(stdin, 1, &mtype, cc);
   ParU_Info info;
   ParU_Analyze(A, &Sym, Control);
   int64_t n, anz;
   ParU_Get (Sym, Num, PARU_GET_N, &n, Control));
   ParU_Get (Sym, Num, PARU_GET_ANZ, &anz, Control));
   std::cout << "Input matrix is " << n << "x" << n <<
      " nnz = " << anz << std::endl;</pre>
   ParU_Factorize(A, Sym, &Num, Control);
   std::cout << "ParU: factorization was successful." << std::endl;</pre>
   b = (double *)malloc(n * sizeof(double));
   x = (double *)malloc(n * sizeof(double));
   for (int64_t i = 0; i < n; ++i) b[i] = i + 1;
   ParU_Solve(Sym, Num, b, x, Control));
   double resid, anorm, xnorm, rcond;
   ParU_Residual(A, x, b, resid, anorm, xnorm, Control));
```

```
ParU_Get (Sym, Num, PARU_GET_RCOND_ESTIMATE, &rcond, Control);
   double rresid = (anorm == 0 || xnorm == 0 ) ? 0 : (resid/(anorm*xnorm));
   std::cout << std::scientific << std::setprecision(2)</pre>
       << "Relative residual is |" << rresid << "| anorm is " << anorm
       << ", xnorm is " << xnorm << " and rcond is " << rcond << "."
       << std::endl;
   free(b);
   free(x);
   ParU_FreeNumeric(&Num, Control);
   ParU_FreeSymbolic(&Sym, Control);
   ParU_FreeControl(&Control);
   cholmod_l_free_sparse(&A, cc);
   cholmod_l_finish(cc);
   return (info);
}
  A simple demo for the C interface is shown next. You can see the complete demo in
ParU/Demo/paru_simplec.c.
#include "ParU.h"
int main(int argc, char **argv)
   cholmod_common Common, *cc = NULL;
   cholmod_sparse *A = NULL;
   ParU_C_Symbolic Sym = NULL;
   ParU_C_Numeric Num = NULL;
   ParU_C_Control Control = NULL;
   double *b = NULL, *x = NULL;
   //~~~~Reading the input matrix
   // start CHOLMOD
   cc = &Common;
   int mtype;
   cholmod_l_start(cc);
   // read in the sparse matrix A from stdin
   A = (cholmod_sparse *)cholmod_l_read_matrix(stdin, 1, &mtype, cc);
   ParU_C_Analyze(A, &Sym, Control);
   int64_t n, anz;
   ParU_C_Get_INT64 (Sym, Num, PARU_GET_N, &n, Control);
   ParU_C_Get_INT64 (Sym, Num, PARU_GET_ANZ, &anz, Control);
   printf("Input matrix is %" PRId64 "x%" PRId64 " nnz = %" PRId64 " \n",
```

```
n, n, anz);
   ParU_C_Factorize(A, Sym, &Num, Control);
   b = (double *)malloc(n * sizeof(double));
   x = (double *)malloc(n * sizeof(double));
   for (int64_t i = 0; i < n; ++i) b[i] = i + 1;
   ParU_C_Solve_Axb(Sym, Num, b, x, Control);
   double resid, anorm, xnorm;
   ParU_C_Residual_bAx(A, x, b, &resid, &anorm, &xnorm, Control);
   double rresid = (anorm == 0 || xnorm == 0 ) ? 0 : (resid/(anorm*xnorm));
   double rcond:
   ParU_C_Get_FP64(Sym, Num, PARU_GET_RCOND_ESTIMATE, &rcond, Control);
   printf("Relative residual is |%.2e|, anorm is %.2e, xnorm is %.2e, "
      " and roond is \%.2e.\n",
      rresid, anorm, xnorm, rcond);
   if (b != NULL) free(b);
   if (x != NULL) free(x);
   ParU_C_FreeNumeric(&Num, Control);
   ParU_C_FreeSymbolic(&Sym, Control);
   ParU_C_FreeControl(&Control);
   cholmod_l_free_sparse(&A, cc);
   cholmod_l_finish(cc);
   return (info);
}
```

2.4 ParU_Info: return values of each ParU method

All ParU C and C++ routines return an enum of type ParU_Info. The user application should check this return value before continuing.

3 C++ Syntax

3.1 ParU_Version: version of the ParU package

ParU has two mechanisms for informing the user application of its date and version: macros that are #defined in ParU.h, and a ParU_Version function. Both methods are provided since it's possible that the ParU.h header found when a user application was compiled might not match the same version found when the same user application was linked with the compiled ParU library.

ParU_Version returns the version in ver array (major, minor, and update, in that order), and the date in the date array provided by the user application.

3.2 ParU_Control: parameters that control ParU

The ParU_Control structure contains parameters that control various ParU options. The object is created by ParU_InitControl, modified by ParU_Set, and deleted by ParU_FreeControl. Its contents can be queried with ParU_Get.

Any ParU function can be passed a NULL pointer for its Control parameter. In that case, defaults are used. To use non-default parameters, create a Control object and then set its parameters.

There are four variants of ParU_Set for setting control parameters, two for integers (int64_t and int32_t) and two for floating-point (double and float) which are the valid options for type in the signature below.

The ParU_Control_enum parameter defines which parameter to set. For integer parameters:

- PARU_CONTROL_MAX_THREADS: number of OpenMP threads to use. If zero or negative, the value is obtained from omp_get_max_threads.
- PARU_CONTROL_STRATEGY: Ordering and factorization strategy to use.
 - PARU_STRATEGY_AUTO: ParU selects its strategy automatically, based on the symbolic analysis of the input matrix, by selecting whichever strategy that UMF-PACK selects.
 - PARU_STRATEGY_UNSYMMETRIC: During numerical factorization, no preference is given for diagonal entries when looking for pivots.
 - PARU_STRATEGY_SYMMETRIC: During numerical factorization, diagonal entries are given preference when looking for pivots. This strategy works well when the nonzero pattern of the matrix is mostly symmetric, and when the diagonal of the matrix is mostly zero-free.
- PARU_CONTROL_UMFPACK_STRATEGY: The ordering strategy used by UMFPACK. ParU uses UMFPACK for its ordering and symbolic analysis phases. The ParU and UMF-PACK strategies are normally the same, but there are cases where best performance is obtained with different strategies.
 - UMFPACK_STRATEGY_AUTO: UMFPACK selects its strategy automatically, based on the symbolic analysis of the input matrix. Let S be the matrix found by UMFPACK after it removes the row and column *singletons* (defined below). If the singleton removal preserves the diagonal of A, the nonzero pattern of S has a *symmetry* $\sigma \geq 0.3$, and the diagonal of S is at least 90% nonzero, then the symmetric strategy is chosen. Otherwise, the unsymmetric strategy is chosen.
 - The symmetry σ of S is defined as the number of matched off-diagonal entries, divided by the total number of off-diagonal entries. An entry s_{ij} is matched if s_{ji} is also an entry. They need not be numerically equal. An entry is a value in A which is present in the input data structure. All nonzeros are entries, but some entries may be numerically zero.

A row singleton is an entry a_{ij} with a single entry in the *i*th row of the matrix A. A column singleton is an entry a_{ij} with a single entry in the *j*th column of the matrix A. When a singleton a_{ij} is found, row i and column j are removed and the process repeats. In the final pruned matrix, all rows and columns have at least two entries.

- UMFPACK_STRATEGY_UNSYMMETRIC: UMFPACK will order columns of the matrix A'A via COLAMD or METIS.
- UMFPACK_STRATEGY_SYMMETRIC: UMFPACK will order the columns of the matrix A + A' via AMD or METIS.
- PARU_CONTROL_ORDERING:

- PARU_ORDERING_AMD: use AMD on A + A' (symmetric strategy) or COLAMD (unsymmetric strategy), which orders A'A without forming it explicitly.
- PARU_ORDERING_METIS: use METIS on A + A' (symmetric strategy) or A'A (unsymmetric strategy), where A'A is explicitly formed.
- PARU_ORDERING_METIS_GUARD: use METIS, AMD, or COLAMD. Symmetric strategy: always use METIS on A + A'. Unsymmetric strategy: use METIS on A'A, unless A has one or more rows with $3.2\sqrt{n}$ or more entries. In that case, A'A is very costly to form, and COLAMD is used instead of METIS.
- PARU_ORDERING_CHOLMOD: use CHOLMOD (AMD/COLAMD then METIS, see above).
- PARU_ORDERING_BEST: try many orderings and pick the best one found.
- PARU_ORDERING_NONE: natural ordering. The permutations P and Q are identity, unless singletons are removed prior to factorization.
- PARU_CONTROL_RELAXED_AMALGAMATION: threshold for relaxed amalgamation. When constructing its frontal matrices, ParU attempts to ensure that all frontal matrices contain at least this many pivot columns. Values less than zero are treated as the default (32), and values greater than 512 are treated as 512.
- PARU_CONTROL_PANEL_WIDTH: Width of panel for dense factorization of each frontal matrix.
- PARU_CONTROL_DGEMM_TINY: Do not call the BLAS dgemm routine if all dimenions of its dense matrices are small than this threshold.
- PARU_CONTROL_DGEMM_TASKED: When calling dgemm, if any dimension of its matrices are at or above this threshold, then a tasked variant of dgemm is used. For the Intel MKL BLAS library, this is a standard call to dgemm, controlled by mkl_set_num_threads_local. For other BLAS library, ParU makes multiple calls to dgemm using a single thread each.
- PARU_CONTROL_DTRSM_TASKED: When calling dtrsm, if any dimension of its matrices are at or above this threshold, then a tasked variant of dtrsm is used. For the Intel MKL BLAS library, this is a standard call to dtrsm, controlled by mkl_set_num_threads_local. For other BLAS library, ParU makes multiple calls to dtrsm using a single thread each.
- PARU_CONTROL_PRESCALE:
 - PARU_PRESCALE_MAX: each row is scaled by the maximum absolute value in the row.
 - PARU_PRESCALE_SUM: each row is scaled by the sum of absolute values in the row.
 - PARU_PRESCALE_NONE: no scaling is performed.
- PARU_CONTROL_SINGLETONS: If nonzero, singletons are permuted to the front of the matrix before factorization. If zero, singletons are left as-is and not treated specially.

• PARU_CONTROL_MEM_CHUNK: chunk size for parallel memset and memcpy.

For double parameters:

- PARU_CONTROL_PIVOT_TOLERANCE: Pivot tolerance for off-diagonal pivots, or for all pivots when using the unsymmetric strategy. A pivot is chosen if it is at least as large as 0.1 (default) times the maximum absolute value in its column. This threshold allows for the selection of sparse pivot rows. Standard partial pivoting is used with the tolerance is 1.0.
- PARU_CONTROL_DIAG_PIVOT_TOLERANCE: Pivot tolerance for diagonal pivots when using the symmetric strategy.

Default values of Control parameters are defined below:

```
(0)
#define PARU_DEFAULT_MAX_THREADS
#define PARU_DEFAULT_STRATEGY
                                             PARU_STRATEGY_AUTO
#define PARU_DEFAULT_UMFPACK_STRATEGY
                                             UMFPACK_STRATEGY_AUTO
#define PARU_DEFAULT_ORDERING
                                             PARU_ORDERING_METIS_GUARD
#define PARU_DEFAULT_RELAXED_AMALGAMATION
                                             (32)
#define PARU_DEFAULT_PANEL_WIDTH
                                             (32)
#define PARU_DEFAULT_DGEMM_TINY
                                             (4)
#define PARU_DEFAULT_DGEMM_TASKED
                                             (512)
#define PARU_DEFAULT_DTRSM_TASKED
                                             (4096)
#define PARU_DEFAULT_PRESCALE
                                             PARU_PRESCALE_MAX
#define PARU_DEFAULT_SINGLETONS
                                             (1)
#define PARU_DEFAULT_MEM_CHUNK
                                             (1024*1024)
#define PARU_DEFAULT_PIVOT_TOLERANCE
                                             (0.1)
#define PARU_DEFAULT_DIAG_PIVOT_TOLERANCE
                                             (0.001)
```

Refer to the next section for how to use ParU_Get to query the current settings of parameters in the Control object.

3.3 ParU_Get: get information from a ParU opaque object

The ParU_Get method returns properties from any of the three opaque ParU data structures: the ParU_Control object, the ParU_Symbolic object containing a symbolic analysis, and the ParU_Numeric object containing a numeric factorization.

There are several signatures for ParU_Get depending on which object is being queried. To query the ParU_Control object, the ParU_Control_enum is used. To query the other two objects (ParU_Symbolic and ParU_Numeric), the ParU_Get_enum is used. Both enums are listed below:

```
PARU_CONTROL_RELAXED_AMALGAMATION = 1005, // goal for # pivots in fronts
       PARU_CONTROL_PANEL_WIDTH = 1006,
PARU_CONTROL_DGEMM_TINY = 1007,
PARU_CONTROL_DGEMM_TASKED = 1008,
PARU_CONTROL_DTRSM_TASKED = 1009,
PARU_CONTROL_PRESCALE = 1010,
PARU_CONTROL_SINGLETONS = 1011,
PARU_CONTROL_MEM_CHUNK = 1012,

// chunk size of memset and memcpy
        // double parameters:
       PARU_CONTROL_PIVOT_TOLERANCE = 2001, // pivot tolerance
        PARU_CONTROL_DIAG_PIVOT_TOLERANCE = 2002, // diagonal pivot tolerance
   ParU_Control_enum ;
    typedef enum
        // int64_t scalars:
       // # of rows/columns of A and its factors
        PARU_GET_NCOL_SINGLETONS = 5, // # of column singletons
        PARU_GET_STRATEGY = 6, // strategy used by ParU
        PARU_GET_UMFPACK_STRATEGY = 7, // strategy used by UMFPACK
        PARU_GET_ORDERING = 8, // ordering used by UMFPACK
        // int64_t arrays of size n:
        PARU_GET_P = 101,
                                        // partial pivoting row ordering
        PARU_GET_Q = 102,
                                        // fill-reducing column ordering
        // double scalars:
        PARU_GET_FLOP_COUNT = 201, // flop count for factorization
       PARU_GET_RCOND_ESTIMATE = 202, // rcond estimate
       // double array of size n:
        PARU_GET_ROW_SCALE_FACTORS = 301, // row scaling factors
        // pointer to const string (const char **):
        PARU_GET_BLAS_LIBRARY_NAME = 401, // BLAS library used
        PARU_GET_FRONT_TREE_TASKING = 402, // frontal tree: parallel or sequential
   ParU_Get_enum ;
   Use the following signatures to query the symbolic or numeric factorization, or to query
the library itself:
    ParU_Info ParU_Get
    (
        // input:
       {\tt const\ ParU\_Symbolic\ Sym, } \qquad //\ {\tt symbolic\ analysis\ from\ ParU\_Analyze}
        const ParU_Numeric Num, // numeric factorization from ParU_Factorize
```

```
ParU_Get_enum field, // field to get
   // output:
   int64_t *result,
                          // int64_t result: a scalar or an array
   // control:
   ParU Control Control
);
ParU_Info ParU_Get
   // input:
   const ParU_Symbolic Sym, // symbolic analysis from ParU_Analyze
   ParU_Get_enum field,
   // output:
   double *result,
                     // double result: a scalar or an array
   // control:
   ParU_Control Control
);
ParU_Info ParU_Get
   // input:
   ParU_Get_enum field,
                     // field to get
   // output:
                         // string result
   const char **result,
   // control:
   ParU_Control Control
);
```

For example, to make a copy of the size-n column permutation vector from the Symbolic object:

```
int64_t Q [n] ;
ParU_Get (Sym, Num, PARU_GET_Q, Q, Control) ;
```

Most of the int64_t results can be obtained with a NULL numeric object, with the exception of the row permutation P, and the count of the number of entries in the L and U factors.

All of the double results require both the Sym and Num objects to be valid.

The two string results query the ParU library to report how it was compiled. This signature returns a pointer to a constant string that is owned by the library and must not be modified:

```
char *blas_libary_name, *front_tasking;
ParU_Get (PARU_GET_BLAS_LIBRARY_NAME, &blas_name, Control));
ParU_Get (PARU_GET_FRONT_TREE_TASKING, &front_tasking, Control));
The following two signatures are available for querying contents of the Control object:
ParU_Info ParU_Get
(
    // input
```

```
ParU_Control_enum parameter,
                                    // parameter to get
    // output:
    int64_t *c,
                                    // value of parameter
    // control:
   ParU Control Control
);
ParU_Info ParU_Get
    // input
   ParU_Control_enum parameter,
                                    // parameter to get
    // output:
    double *c,
                                    // value of parameter
    // control:
   ParU_Control Control
);
```

3.4 ParU_Set: set Control parameters

Refer to Section 3.2 for the ParU_Set method.

3.5 ParU_Analyze: symbolic analysis

ParU_Analyze takes as input a sparse matrix in the CHOLMOD data structure, A. The matrix must be square, double precision, not complex, and not held in the CHOLMOD symmetric storage format. Refer to the CHOLMOD documentation for details. On output, the symbolic analysis structure Sym is created, passed in as &Sym. The symbolic analysis can be used for different calls to ParU_Factorize for matrices that have the same sparsity pattern but different numerical values. The symbolic analysis structure must be freed by ParU_FreeSymbolic.

3.6 ParU_Factorize: numerical factorization

```
ParU_Control Control
);
```

ParU_Factorize performs the numerical factorization of its input sparse matrix A. The symbolic analyss Sym must have been created by a prior call to ParU_Analyze with the same matrix A, or one with the same sparsity pattern as the one passed to ParU_Factorize. On output, the &Num structure is created. The numeric factorization structure must be freed by ParU_FreeNumeric.

3.7 ParU_Solve: solve a linear system, Ax = b

ParU_Solve solves a sparse linear system Ax = b for a sparse matrix A and vectors x and b, or matrices X and B. The matrix A must have been factorized by ParU_Factorize, and the Sym and Num structures from that call must be passed to this method.

The method has four overloaded signatures, so that it can handle a single right-hand-side vector or a matrix with multiple right-hand-sides, and it provides the option of overwriting the input right-hand-side(s) with the solution(s).

```
ParU_Info ParU_Solve
                                // solve Ax=b, overwriting b with solution x
(
    // input:
    const ParU_Symbolic Sym,
                                // symbolic analysis from ParU_Analyze
    const ParU_Numeric Num,
                                // numeric factorization from ParU_Factorize
    // input/output:
    double *x,
                                // vector of size n-by-1; right-hand on input,
                                // solution on output
    // control:
   ParU_Control Control
);
                                // solve Ax=b
ParU_Info ParU_Solve
    // input:
    const ParU_Symbolic Sym,
                                // symbolic analysis from ParU_Analyze
    const ParU_Numeric Num,
                                // numeric factorization from ParU_Factorize
                                // vector of size n-by-1
    double *b,
    // output
    double *x,
                                // vector of size n-by-1
    // control:
   ParU_Control Control
);
ParU_Info ParU_Solve
                                // solve AX=B, overwriting B with solution X
    // input
    const ParU_Symbolic Sym,
                                // symbolic analysis from ParU_Analyze
    const ParU_Numeric Num,
                                // numeric factorization from ParU_Factorize
    int64_t nrhs,
                                // # of right-hand sides
    // input/output:
                                // X is n-by-nrhs, where A is n-by-n;
    double *X,
                                // holds B on input, solution X on input
```

```
// control:
   ParU_Control Control
);
ParU_Info ParU_Solve
                                // solve AX=B
    // input
    const ParU_Symbolic Sym,
                                // symbolic analysis from ParU_Analyze
    const ParU_Numeric Num,
                                // numeric factorization from ParU_Factorize
    int64_t nrhs,
                                // # of right-hand sides
                                // n-by-nrhs, in column-major storage
    double *B,
    // output:
                                // n-by-nrhs, in column-major storage
    double *X,
    // control:
   ParU_Control Control
);
```

3.8 ParU_LSolve: solve a linear system, Lx = b

ParU_LSolve solves a lower triangular system, Lx = b with vectors x and b, or LX = B with matrices X and B, using the lower triangular factor computed by ParU_Factorize. No scaling or permutations are used.

```
ParU_Info ParU_LSolve
                                // solve Lx=b
    // input
    const ParU_Symbolic Sym,
                                // symbolic analysis from ParU_Analyze
    const ParU_Numeric Num,
                                // numeric factorization from ParU_Factorize
    // input/output:
    double *x,
                                // n-by-1, in column-major storage;
                                // holds b on input, solution x on input
    // control:
   ParU_Control Control
);
                                // solve LX=B
ParU_Info ParU_LSolve
    // input
    const ParU_Symbolic Sym,
                                // symbolic analysis from ParU_Analyze
    const ParU_Numeric Num,
                                // numeric factorization from ParU_Factorize
                                // # of right-hand-sides (# columns of X)
    int64_t nrhs,
    // input/output:
    double *X,
                                // X is n-by-nrhs, where A is n-by-n;
                                // holds B on input, solution X on input
    // control:
   ParU_Control Control
) ;
```

3.9 ParU_USolve: solve a linear system, Ux = b

ParU_USolve solves an upper triangular system, Ux = b with vectors x and b, or UX = B with matrices X and B, using the upper triangular factor computed by ParU_Factorize. No scaling or permutations are used.

```
ParU_Info ParU_USolve
                                // solve Ux=b
    // input
    const ParU_Symbolic Sym,
                                // symbolic analysis from ParU_Analyze
    const ParU_Numeric Num,
                                // numeric factorization from ParU_Factorize
    // input/output
    double *x,
                                // n-by-1, in column-major storage;
                                // holds b on input, solution x on input
    // control:
    ParU_Control Control
);
                                // solve UX=B
ParU_Info ParU_USolve
    // input
    const ParU_Symbolic Sym,
                                // symbolic analysis from ParU_Analyze
    const ParU_Numeric Num,
                                // numeric factorization from ParU_Factorize
                                // # of right-hand-sides (# columns of X)
    int64_t nrhs,
    // input/output:
    double *X,
                                // X is n-by-nrhs, where A is n-by-n;
                                // holds B on input, solution X on input
    // control:
   ParU_Control Control
);
```

3.10 ParU_Perm: permute and scale a dense vector or matrix

ParU_Perm permutes and optionally scales a vector b or matrix B. If the input s is NULL, no scaling is applied. The permutation vector P has size n. If the kth index in the permutation is row i, then i = P[k].

For the vector case, the output is x(k) = b(P(k))/s(P(k)), or x(k) = b(P(k)), or if **s** is NULL, for all k in the range 0 to n-1.

For the matrix case, the output is X(k,j) = B(P(k),j)/s(P(k)) for all rows k and all columns j of X and B. If s is NULL, then the output is X(k,j) = B(P(k),j).

```
ParU_Info ParU_Perm
    // inputs
    const int64_t *P,
                      // permutation vector of size n
    const double *s,
                       // vector of size n (optional)
                       // vector of size n
    const double *b,
    int64_t n,
                       // length of P, s, B, and X
    // output
                       // vector of size n
   double *x,
    // control:
   ParU_Control Control
);
ParU_Info ParU_Perm
    // inputs
    const int64_t *P, // permutation vector of size nrows
```

3.11 ParU_InvPerm: permute and scale a dense vector or matrix

ParU_InvPerm permutes and optionally scales a vector b or matrix B. If the input s is NULL, no scaling is applied. The permutation vector P has size n, and its inverse is implicitly used by this method. If the kth index in the permutation is row i, then i = P[k].

For the vector case, the output is x(P(k)) = b(k)/s(P(k)), or x(P(k)) = b(k), or if **s** is NULL, for all k in the range 0 to n-1.

For the matrix case, the output is X(P(k), j) = B(k, j)/s(P(k)) for all rows k and all columns j of X and B. If s is NULL, then the output is X(P(k), j) = B(k, j).

```
ParU_Info ParU_InvPerm
    // inputs
    const int64_t *P,
                      // permutation vector of size n
                       // vector of size n (optional)
    const double *s,
    const double *b,
                       // vector of size n
    int64_t n,
                       // length of P, s, B, and X
    // output
                       // vector of size n
    double *x,
    // control:
   ParU_Control Control
);
ParU_Info ParU_InvPerm
    // inputs
    const int64_t *P,
                       // permutation vector of size nrows
                        // vector of size nrows (optional)
    const double *s,
    const double *B,
                       // array of size nrows-by-ncols
                       // # of rows of X and B
    int64_t nrows,
    int64_t ncols,
                       // # of columns of X and B
    // output
    double *X,
                       // array of size nrows-by-ncols
    // control:
   ParU_Control Control
);
```

The ParU_LSolve, ParU_USolve, ParU_Perm, and ParU_InvPerm can be used together to solve Ax = b or AX = B. For example, if t is a temporary vector of size n, and A is an n-by-n matrix, calling ParU_Solve to solve Ax = b is identical to the following (ignoring any tests for error conditions):

```
int64_t P [n], Q [n];
double t [n], R [n];
ParU_Get (Sym, Num, PARU_GET_P, P, Control);
ParU_Get (Sym, Num, PARU_GET_Q, Q, Control);
ParU_Get (Sym, Num, PARU_GET_ROW_SCALE_FACTORS, R, Control);
ParU_Perm (P, Rs, b, n, t, Control);
ParU_LSolve (Sym, Num, t, Control);
ParU_USolve (Sym, Num, t, Control);
ParU_InvPerm (Q, NULL, t, n, x, Control);
```

The numeric factorization Num contains the row permutation vector P from partial pivoting, and the row scaling vector R. The symbolic analysis structure Sym contains the fill-reducing column preordering, Q.

3.12 ParU_Residual: compute the residual

The ParU_Residual function computes the relative residual of Ax = b or AX = B, in the 1-norm. It also computes the 1-norm of A and the solution X or x.

```
ParU_Info ParU_Residual
    // inputs:
    cholmod_sparse *A, // an n-by-n sparse matrix
    double *x,
                      // vector of size n, solution to Ax=b
    double *b,
                       // vector of size n
    // output:
    double &resid,
                       // residual: norm1(b-A*x) / (norm1(A) * norm1(x))
                       // 1-norm of A
    double &anorm,
                       // 1-norm of x
    double &xnorm,
    // control:
   ParU_Control Control
);
ParU_Info ParU_Residual
(
    // inputs:
    cholmod_sparse *A, // an n-by-n sparse matrix
                       // array of size n-by-nrhs, solution to AX=B
    double *X,
    double *B,
                       // array of size n-by-nrhs
    int64_t nrhs,
    // output:
    double &resid,
                       // residual: norm1(B-A*X) / (norm1(A) * norm1 (X))
    double &anorm,
                       // 1-norm of A
                       // 1-norm of X
    double &xnorm,
    // control:
   ParU_Control Control
);
```

3.13 ParU_FreeNumeric: free a numeric factorization

```
ParU_Info ParU_FreeNumeric
(
```

3.14 ParU_FreeSymbolic: free a symbolic analysis

3.15 ParU_FreeControl: free a Control object

```
ParU_Info ParU_FreeControl
(
    // input/output:
    ParU_Control *Control_handle // Control object to free
) :
```

4 C Syntax

The C interface is quite similar to the C++ interface. The next sections describe the user-callable C functions, their prototypes, and what they can do.

4.1 ParU_C_Version: version of the ParU package

ParU_Info ParU_C_Version (int ver [3], char date [128]) ;

4.2 ParU_C_Control: parameters that control ParU

Any C ParU function can be passed a NULL pointer for its Control parameter. In that case, defaults are used. To use non-default parameters, create a Control object and then set its parameters. The object is freed by ParU_C_FreeControl.

The ParU_C_Control structure contains parameters that control various ParU options. The object is created by ParU_C_InitControl, modified by ParU_C_Set, and deleted by ParU_C_FreeControl. Its contents can be queried with ParU_C_Get.

Any ParU function can be passed a NULL pointer for its Control parameter. In that case, defaults are used. To use non-default parameters, create a Control object and then set its parameters.

```
ParU_Info ParU_C_InitControl
(
    ParU_C_Control *Control_C_handle // Control object to create
);
```

```
ParU_Info ParU_C_FreeControl
(
    ParU_C_Control *Control_handle_C // Control object to free
);
```

4.3 ParU_C_Get_*: get information from a ParU opaque object

The ParU_C_Get_* methods retrieve scalars or arrays from the C versions of the Control, Symbolic, or Numeric objects. See Section 3.3 for details.

```
ParU_Info ParU_C_Get_INT64
   // input:
   const ParU_C_Symbolic Sym_C, // symbolic analysis from ParU_C_Analyze
   const ParU_C_Numeric Num_C, // numeric factorization from ParU_C_Factorize
   ParU_Get_enum field,
                             // field to get
   // output:
   int64_t *result,
                             // int64_t result: a scalar or an array
   // control:
   ParU_C_Control Control_C
);
ParU_Info ParU_C_Get_FP64
   // input:
   const ParU_C_Symbolic Sym_C, // symbolic analysis from ParU_C_Analyze
   const ParU_C_Numeric Num_C, // numeric factorization from ParU_C_Factorize
   ParU_Get_enum field,
                             // field to get
   // output:
                     // double result: a scalar or an array
   double *result,
   // control:
   ParU_C_Control Control_C
);
ParU_Info ParU_C_Get_CONSTCHAR
   // input:
   // output:
   const char **result,
                             // string result
   // control:
   ParU_C_Control Control_C
);
```

4.4 ParU_C_Set_*: set Control parameters

The ParU_C_Set_* methods set parameters in the C version of the Control object. See Section 3.2 for details.

```
ParU_Info ParU_C_Set_INT64
(
    // input
```

```
ParU_Control_enum parameter,
                                    // parameter to set
    int64_t c,
                                    // value to set it to
    // control:
   ParU_C_Control Control_C
);
ParU_Info ParU_C_Set_FP64
    // input
   ParU_Control_enum parameter,
                                    // parameter to set
    double c.
                                    // value to set it to
    // control:
   ParU_C_Control Control_C
);
```

4.5 ParU_C_Analyze: symbolic analysis

ParU_C_Analyze performs the symbolic analysis of a sparse matrix, based solely on its nonzero pattern. ParU_C_Analyze is called once and can be used for different ParU_C_Factorize calls for the matrices that have the same pattern but different numerical values. The symbolic analysis structure must be freed by ParU_C_FreeSymbolic.

```
ParU_Info ParU_C_Analyze
(
    // input:
    cholmod_sparse *A, // input matrix to analyze of size n-by-n
    // output:
    ParU_C_Symbolic *Sym_handle_C, // output, symbolic analysis
    // control:
    ParU_C_Control Control_C
);
```

4.6 ParU C Factorize: numeric factorization

ParU_C_Factorize computes the numeric factorization. The ParU_C_Symbolic structure computed in ParU_C_Analyze is an input to this routine. The numeric factorization structure must be freed by ParU_C_FreeNumeric.

4.7 ParU_C_Solve_A*: solve a linear system, Ax = b

The ParU_C_Solve_Axx, ParU_C_Solve_Axb, ParU_C_Solve_AXX and ParU_C_Solve_AXB methods solve a sparse linear system Ax = b for a sparse matrix A and vectors x and b, or matrices X and B. The matrix A must have been factorized by ParU_Factorize, and the Sym and Num structures from that call must be passed to this method.

```
ParU_Info ParU_C_Solve_Axx
                                // solve Ax=b, overwriting b with solution x
(
    // input:
    const ParU_C_Symbolic Sym_C, // symbolic analysis from ParU_C_Analyze
    const ParU_C_Numeric Num_C, // numeric factorization from ParU_C_Factorize
    // input/output:
    double *x,
                           // vector of size n-by-1; right-hand on input,
                           // solution on output
    // control:
   ParU_C_Control Control_C
);
ParU_Info ParU_C_Solve_Axb
                                // solve Ax=b
   // input:
    const ParU_C_Symbolic Sym_C, // symbolic analysis from ParU_C_Analyze
    const ParU_C_Numeric Num_C, // numeric factorization from ParU_C_Factorize
                           // vector of size n-by-1
    double *b,
    // output
   double *x,
                         // vector of size n-by-1
   // control:
   ParU_C_Control Control_C
);
ParU_Info ParU_C_Solve_AXX
                               // solve AX=B, overwriting B with solution X
(
    const ParU_C_Symbolic Sym_C, // symbolic analysis from ParU_C_Analyze
    const ParU_C_Numeric Num_C, // numeric factorization from ParU_C_Factorize
    int64_t nrhs,
    // input/output:
    double *X,
                           // array of size n-by-nrhs in column-major storage,
                           // right-hand-side on input, solution on output.
   // control:
   ParU_C_Control Control_C
);
                                // solve AX=B, overwriting B with solution X
ParU_Info ParU_C_Solve_AXB
    // input
    const ParU_C_Symbolic Sym_C, // symbolic analysis from ParU_C_Analyze
    const ParU_C_Numeric Num_C, // numeric factorization from ParU_C_Factorize
    int64_t nrhs,
    double *B,
                           // array of size n-by-nrhs in column-major storage
    // output:
   double *X,
                           // array of size n-by-nrhs in column-major storage
   // control:
   ParU_C_Control Control_C
);
```

4.8 ParU_C_Solve_L*: solve a linear system, Lx = b

The ParU_C_Solve_Lxx and ParU_C_Solve_LXX methods solve lower triangular systems, Lx = b with vectors x and b, or LX = B with matrices X and B, using the lower triangular factor computed by ParU_Factorize. No scaling or permutations are used.

```
ParU_Info ParU_C_Solve_Lxx
                                 // solve Lx=b, overwriting b with solution x
    // input:
    const ParU_C_Symbolic Sym_C, // symbolic analysis from ParU_C_Analyze
    const ParU_C_Numeric Num_C, // numeric factorization from ParU_C_Factorize
    // input/output:
    double *x,
                            // vector of size n-by-1; right-hand on input,
                            // solution on output
    // control:
   ParU_C_Control Control_C
);
ParU_Info ParU_C_Solve_LXX
                                // solve LX=B, overwriting B with solution X
   // input
    const ParU_C_Symbolic Sym_C, // symbolic analysis from ParU_C_Analyze
    const ParU_C_Numeric Num_C, // numeric factorization from ParU_C_Factorize
    int64_t nrhs,
    // input/output:
    double *X,
                            // array of size n-by-nrhs in column-major storage,
                            // right-hand-side on input, solution on output.
    // control:
   ParU_C_Control Control_C
);
```

4.9 ParU_C_Solve_U*: solve a linear system, Ux = b

The ParU_C_Solve_Uxx and ParU_C_Solve_UXX methods solve an upper triangular system, Ux = b or UX = B. No scaling or permutation is performed.

```
ParU_Info ParU_C_Solve_Uxx
                                // solve Ux=b, overwriting b with solution x
   // input:
   const ParU_C_Symbolic Sym_C, // symbolic analysis from ParU_C_Analyze
    const ParU_C_Numeric Num_C, // numeric factorization from ParU_C_Factorize
   // input/output:
   double *x,
                           // vector of size n-by-1; right-hand on input,
                           // solution on output
   // control:
   ParU_C_Control Control_C
);
                           // solve UX=B, overwriting B with solution X
ParU_Info ParU_C_Solve_UXX
   const ParU_C_Symbolic Sym_C, // symbolic analysis from ParU_C_Analyze
    const ParU_C_Numeric Num_C, // numeric factorization from ParU_C_Factorize
```

4.10 ParU_C_Perm: permute and scale a dense vector or matrix

ParU_C_Perm and ParU_C_Perm_X permutes and optionally scale a dense vector or matrix. Refer to Section 3.10 for details.

```
ParU_Info ParU_C_Perm
   // inputs
   const int64_t *P,
                    // permutation vector of size n
   const double *s, // vector of size n (optional)
   const double *b, // vector of size n
                     // length of P, s, B, and X
   int64_t n,
   // output
                    // vector of size n
   double *x,
   // control:
   ParU_C_Control Control_C
);
ParU_Info ParU_C_Perm_X
   // inputs
   const int64_t *P, // permutation vector of size nrows
   const double *s, // vector of size nrows (optional)
   const double *B, // array of size nrows-by-ncols
   int64_t ncols,
                    // # of columns of X and B
   // output
   double *X,
                     // array of size nrows-by-ncols
   // control:
   ParU_C_Control Control_C
);
```

4.11 ParU_C_InvPerm: permute and scale a dense vector or matrix

ParU_C_InvPerm and ParU_C_InvPerm_X and permutes and optionally scale a dense vector or matrix. Refer to Section 3.11 for details.

```
// output
                      // vector of size n
   double *x,
    // control
   ParU_C_Control Control_C
);
ParU_Info ParU_C_InvPerm_X
   // inputs
   const int64_t *P,
                      // permutation vector of size nrows
    const double *s,
                      // vector of size nrows (optional)
    const double *B, // array of size nrows-by-ncols
                    // # of rows of X and B
    int64_t nrows,
                      // # of columns of X and B
    int64_t ncols,
   // output
   double *X,
                       // array of size nrows-by-ncols
    // control
   ParU_C_Control Control_C
);
```

4.12 ParU_C_Residual_*: compute the residual

ParU_C_Residual_bAx and ParU_C_Residual_BAX compute the relative residual of Ax = b or AX = B, in the 1-norm, and the 1-norm of A and the solution X or x.

```
ParU_Info ParU_C_Residual_bAx
(
   // inputs:
    cholmod_sparse *A, // an n-by-n sparse matrix
   double *x,
                    // vector of size n
   double *b,
                       // vector of size n
   // output:
                      // residual: norm1(b-A*x) / (norm1(A) * norm1 (x))
   double *residc,
   double *anormc,
                      // 1-norm of A
                       // 1-norm of x
   double *xnormc,
   // control:
   ParU_C_Control Control_C
);
ParU_Info ParU_C_Residual_BAX
    // inputs:
    cholmod_sparse *A, // an n-by-n sparse matrix
   double *X,
                    // array of size n-by-nrhs
   double *B,
                       // array of size n-by-nrhs
    int64_t nrhs,
    // output:
                      // residual: norm1(B-A*X) / (norm1(A) * norm1 (X))
   double *residc,
   double *anormc,
                       // 1-norm of A
   double *xnormc,
                       // 1-norm of X
   // control:
   ParU_C_Control Control_C
);
```

4.13 ParU_C_FreeNumeric: free the numeric factorization

4.14 ParU_C_FreeSymbolic: free the symbolic analysis structure

5 Thread safety of malloc, calloc, realloc, and free

ParU is a C++ library but uses the C memory manager for all of its memory allocations, for compatibility with the other packages in SuiteSparse. It makes limited use of the C++ new and delete, but overrides those functions to use SuiteSparse_malloc and SuiteSparse_free. ParU relies on the memory manager routines defined by the SuiteSparse_config library (SuiteSparse_malloc, SuiteSparse_calloc, SuiteSparse_realloc, and SuiteSparse_free). By default, those routines relies on the C malloc, calloc, realloc, and free methods, respectively. They can be redefined; refer to the documentation of SuiteSparse_config on how to do this.

The malloc, calloc, realloc, and free methods must be thread-safe, since ParU calls those methods from within its parallel tasks. All of their implementations in the standard C libraries that we are aware of are thread-safe. However, if your memory manager routines are not thread-safe, ParU will fail catastrophically.

6 Using ParU in MATLAB

To use ParU in MATLAB, you must first compile the paru mexFunction. In MATLAB, go to the ParU/MATLAB directory and type paru_make. Then add the ParU/MATLAB directory to your MATLAB path for future use.

For best performance, paru relies on functions unique to the Intel MKL BLAS. An optional input, paru_make(try_intel), is true by default. paru_make detects the BLAS library used by MATLAB and then attempts to use functions unique to the Intel MKL BLAS library (mkl*set_num_threads_local). This may fail when paru is compiled (in which case paru is compiled with try_intel false). If paru fails when it runs, with a link error reporting that an an mkl_* routine is not found, use paru_make(false) to disable the Intel MKL functions.

The basic usage x=paru(A,b) solves the linear system Ax = b, computing x=A b. The matrix A must be sparse, square, non-singular, and real.

Additional options are available to change paru's behavior, and an additional output parameter reports statistics on the algorithm:

```
\verb'[x,stats] = paru (A,b,opts)'
```

opts is a struct containing the following fields. Any field that is not recognized is ignored, and missing fields are treated as their defaults:

- opts.strategy: ordering strategy, as a string (default: 'auto'):
 - 'auto': the strategy is selected automatically.
 - 'symmetric': ordering of A+A', with preference for diagonal pivoting. Works well for matrices with mostly symmetric nonzero pattern.
 - 'unsymmetric': ordering A'*A, with no preference for diagonal pivoting. Works well for matrices with unsymmetric nonzero pattern.
- opts.tol: relative pivot tolerance for off-diagonal entries (default: 0.1). Pivot entries must be 0.1 times the max absolute value in its column.
- opts.diagtol: relative pivot tolerance for diagonal pivot entries when using the symmetric strategy (default: 0.001). A lower tolerance for diagonal entries tends to reduce fill-in.
- opts.ordering: fill-reducing ordering option, as a string (default: 'amd'):
 - 'amd': AMD for the symmetric strategy, COLAMD for unsymmetric.
 - 'cholmod': use CHOLMOD's ordering strategy: try AMD or COLAMD, and then try METIS if the fill-in from AMD/COLAMD is high; then selects the best ordering found.
 - 'metis': METIS on A+A' for symmetric strategy, A'*A for the unsymmetric strategy.
 - 'metis_guard': use the 'metis' ordering unless the matrix has one or more rows with $3.2\sqrt{n}$ entries, in which case use 'amd'.
 - 'none': no fill-reducing ordering.
- opts.prescale: prescaling the input matrix (default 'max').
 - 'none': no prescaling.
 - 'sum': scale each row by the sum of the absolute values of the row. The prescaled matrix is RA where R(i,i) = 1/sum(abs(A(i,:))).

- 'max': scale each row by the sum of the absolute values of the row. The prescaled matrix is RA where $R(i,i) = 1/\max(abs(A(i,:)))$.

stats is an optional output that provides information on the ParU analysis and factorization of the matrix:

- stats.analysis_time: symbolic analysis time in seconds.
- stats.factorization_time: numeric factorization time in seconds.
- stats.solve_time: forward/backward solve time in seconds.
- stats.strategy_used: symmetric or unsymmetric.
- stats.ordering_used: amd(A+A'), colamd(A), metis(A+A'), metis(A'*A), or none.
- stats.flops: flop count for LU factorization.
- stats.lnz: number of entries in L.
- stats.unz: number of entries in U.
- stats.rcond: rough estimate of the recripical of the condition number.
- stats.blas: BLAS library used, as a string.
- stats.front_tree_tasking: a string stating how the paru mexFunction was compiled, whether or not tasking is available for factorizing multiple fronts at the same time ('sequential' or 'parallel'). Parallel tasking is required for best performance, and requires OpenMP tasking, which is available in OpenMP 4.0 and later.

7 Requirements and Availability

ParU requires several Collected Algorithms of the ACM: CHOLMOD [4, 7], AMD [1, 2], COLAMD [5, 6] and UMFPACK [8] for its ordering/analysis phase and for its basic sparse matrix data structure, and the BLAS [9] for dense matrix computations on its frontal matrices. An efficient implementation of the BLAS is strongly recommended, such as the Intel MKL, the AMD ACML, OpenBLAS, FLAME [10]. or vendor-provide BLAS. Note that while ParU uses nested parallelism heavily the right options for the BLAS library must be chosen to get a good performance.

For best performance, the Intel MKL BLAS is required. ParU relies on the mkl_set_num_threads_local to select the number of threads to use for the BLAS calls from each of its own threads, which required nested parallelism.

ParU also relies heavily on OpenMP tasking to factorize multiple frontal matrices at the same time, where each frontal matrix can also be factorized by multiple threads. If tasking is not available, each frontal matrix is factorized one at a time (but still in parallel). For best performance, nested parallelism is required. However, when using the gcc compiler on Windows and Mac, we have found that the OpenMP library can hang. As a result, on those

platforms, nested parallelism is disabled when using gcc. If using gcc, use a recent compiler (version 7.5.0 fails; 12.2.0 works).

You can query ParU at run time to determine which BLAS library it is using, and whether or not it is compiled to use parallel or sequential factorization of its frontal matrix tree. See ParU_Get (Section 3.3) for details.

SuiteSparse uses a slightly modified version of METIS 5.1.0, distributed along with SuiteSparse itself. Its use is optional, however. ParU uses AMD as its default ordering. METIS tends to give orderings that are good for parallelism. However, METIS itself can be slower than AMD. As a result, the symbolic analysis using METIS can be slow, but usually, the factorization is faster. Therefore, depending on your use case, either use METIS, or you can compile and run your code without using METIS. If you are using METIS on an unsymmetric case, UMFPACK must form the Matrix A^TA . This matrix can have many entries it takes a lot of resources to form it. To avoid such conditions, ParU uses the ordering strategy PARU_ORDERING_METIS_GUARD by default. This ordering strategy uses COLAMD instead of METIS in when A^TA is too costly to construct.

This modified version of METIS is built into CHOLMOD itself, with all functions renamed, so it does not conflict with a standard METIS library. The unmodified METIS library can be safely linked with an application that uses the modified METIS inside CHOLMOD, without any linking conflicts.

The use of OpenMP tasking is optional, but without it, only parallelism within the BLAS can be exploited (if available). ParU depends on parallel tasking to factorize multiple fronts at the same time, and performance will suffer if the compiler and BLAS library are not suitable for this method.

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References

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