# BASICLU User Guide

## Version 2.1

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## 1 Algorithm

BASICLU implements a right-looking LU factorization with dynamic Markowitz search and columnwise threshold pivoting. After a column modification to the matrix it applies either a permutation or the Forrest-Tomlin update to maintain a factorized form. It uses the method of Gilbert and Peierls to solve triangular systems with a sparse right-hand side. A more detailed explanation of the method is given in [Technical Report ERGO 17-002, http://www.maths.ed.ac.uk/ERGO/preprints.html].

### 2 Installation

### 2.1 Compiling BASICLU

Compiling BASICLU requires GNUmake and a C compiler that (partly) supports the ANSI C99 standard.

To compile the package type make in the BASICLU directory. This will create a static and a shared library inside lib/. It will also compile a standalone program maxvolume in example/. You can call the latter with the matrices in example/data/.

Compiler and linker flags can be changed in config.mk or can be given to make on the command line. See the documentation in config.mk.

### 2.2 The integer type

BASICLU integer variables are of type lu\_int, which is typedef'ed in basiclu.h. lu\_int must be a signed integer type. The default is int64\_t. It can be changed before compiling the package. Note:

- The BASICLU routines do not check for integer overflow. It is in your responsibility to choose a sufficiently large integer type for your problems.
- It is required that all integer values arising in the computation can be stored in double variables and converted back to lu\_int without altering their value.

### 3 Low level C interface

The low level C interface consists of routines which do not allocate memory. Memory must be provided by the user and reallocated on request. To use the low level C interface, user code must include basiclu.h. Defined constants start with BASICLU\_ and function names start with basiclu.

Memory must be provided in form of four lu\_int arrays and four double arrays:

- istore, xstore are arrays whose size depends only on the matrix dimension (see basiclu\_initialize for their required length). xstore is used to input parameters to the routines and to return information to the user. The indices of xstore which the user may access have defined names, e.g. xstore[BASICLU\_STATUS] holds the status code. istore need not be accessed by the user.
- Li, Lx, Ui, Ux, Wi, Wx are arrays whose required size is not known in advance. Their size must be given by the user as parameters (see below) and BASICLU will request reallocation if the size is insufficient. These arrays need not be accessed by the user.

### 3.1 basiclu\_initialize

```
lu_int basiclu_initialize
    lu_int m,
    lu_int istore[],
    double xstore[]
);
Purpose:
    Initialize istore, xstore to a BASICLU instance. Set parameters to defaults
    and reset counters. The initialization fixes the dimension of matrices
    which can be processed by this instance.
    This routine must be called once before passing istore, xstore to any other
    basiclu_ routine.
Return:
    BASICLU_OK
        m, istore, xstore were valid arguments. Only in this case are istore,
        xstore initialized.
    BASICLU_ERROR_argument_missing
        istore or xstore is NULL.
    BASICLU_ERROR_invalid_argument
        m is less than or equal to zero.
Arguments:
    lu_int m
        The dimension of matrices which can be processed. m > 0.
    lu_int istore[]
    double xstore[]
        Fixed size arrays. These must be allocated by the user as follows:
          length of istore: BASICLU_SIZE_ISTORE_1 + BASICLU_SIZE_ISTORE_M * m
          length of xstore: BASICLU_SIZE_XSTORE_1 + BASICLU_SIZE_XSTORE_M * m
Info:
    After initialization, the following entries of xstore are maintained
    throughout by all basiclu_ routines:
    xstore[BASICLU_DIM] Matrix dimension (constant).
    xstore[BASICLU_NUPDATE] Number of updates since last factorization. This is
                            the sum of Forrest-Tomlin updates and permutation
                            updates.
    xstore[BASICLU_NFORREST] Number of Forrest-Tomlin updates since last
                             factorization. The upper limit on Forrest-Tomlin
                             updates before refactorization is m, but that is
                             far too much for performance reasons and numerical
                             stability.
    xstore[BASICLU_NFACTORIZE] Number of factorizations since initialization.
```

xstore[BASICLU\_NUPDATE\_TOTAL] Number of updates since initialization.

 ${\tt xstore} \hbox{\tt [BASICLU\_NFORREST\_TOTAL]} \hbox{\tt Number of Forrest-Tomlin updates since initialization.}$ 

 ${\tt xstore} \hbox{\tt [BASICLU\_UNZ]} \hbox{\tt Number of nonzeros in U excluding diagonal elements} \\ \hbox{\tt (changed by updates).}$ 

xstore[BASICLU\_MIN\_PIVOT]

xstore[BASICLU\_TIME\_FACTORIZE] Wall clock time for last factorization.

 $\verb|xstore[BASICLU_TIME_UPDATE|| Wall clock time for all calls to basiclu\_update \\ since last factorization.$ 

xstore[BASICLU\_TIME\_FACTORIZE\_TOTAL]
xstore[BASICLU\_TIME\_SOLVE\_TOTAL]
xstore[BASICLU\_TIME\_UPDATE\_TOTAL] An

xstore[BASICLU\_LFLOPS]
xstore[BASICLU\_UFLOPS]

xstore[BASICLU\_RFLOPS] Number of flops for operations with L, U and update ETA vectors in calls to basiclu\_solve\_sparse and basiclu\_solve\_for\_update since last factorization.

### 3.2 basiclu\_factorize

```
lu_int basiclu_factorize
    lu_int istore[],
    double xstore[],
    lu_int Li[],
    double Lx[],
    lu_int Ui[],
    double Ux[],
    lu_int Wi[],
    double Wx[],
    const lu_int Bbegin[],
    const lu_int Bend[],
    const lu_int Bi[],
    const double Bx[],
    lu_int cOntinue
);
Purpose:
    Factorize the matrix \boldsymbol{B} into its LU factors. Choose pivot elements by a
    Markowitz criterion subject to columnwise threshold pivoting (the pivot may
    not be smaller than a factor of the largest entry in its column).
Return:
    BASICLU_ERROR_invalid_store if istore, xstore do not hold a BASICLU
    instance. In this case xstore[BASICLU_STATUS] is not set.
    Otherwise return the status code. See xstore[BASICLU_STATUS] below.
Arguments:
    lu_int istore[]
    double xstore[]
        BASICLU instance. The instance determines the dimension of matrix B
        (stored in xstore[BASICLU_DIM]).
    lu int Li∏
    double Lx[]
    lu_int Ui[]
    double Ux[]
    lu_int Wi[]
    double Wx[]
        Arrays used for workspace during the factorization and to store the
        final factors. They must be allocated by the user and their length
        must be provided as parameters:
            xstore[BASICLU_MEMORYL]: length of Li and Lx
            xstore[BASICLU_MEMORYU]: length of Ui and Ux
            xstore[BASICLU_MEMORYW]: length of Wi and Wx
        When the allocated length is insufficient to complete the factorization,
        basiclu_factorize() returns to the caller for reallocation (see
        xstore[BASICLU_STATUS] below). A successful factorization requires at
        least nnz(B) length for each of the arrays.
    const lu_int Bbegin[]
    const lu_int Bend[]
    const lu_int Bi[]
    const double Bx[]
        Matrix B in packed column form. Bi and Bx are arrays of row indices
```

and nonzero values. Column j of matrix B contains elements

```
Bi[Bbegin[j] .. Bend[j]-1], Bx[Bbegin[j] .. Bend[j]-1].
```

The columns must not contain duplicate row indices. The arrays Bbegin and Bend may overlap, so that it is valid to pass Bp, Bp+1 for a matrix stored in compressed column form (Bp, Bi, Bx).

#### lu\_int cOntinue

zero to start a new factorization; nonzero to continue a factorization after reallocation.

#### Parameters:

#### xstore[BASICLU\_DROP\_TOLERANCE]

Nonzeros which magnitude is less than or equal to the drop tolerance can be removed after each pivot step. They are guaranteed removed at the end of the factorization. Default: 1e-20

#### xstore[BASICLU\_ABS\_PIVOT\_TOLERANCE]

A pivot element must be nonzero and in absolute value must be greater than or equal to xstore[BASICLU\_ABS\_PIVOT\_TOLERANCE]. Default: 1e-14

#### xstore[BASICLU\_REL\_PIVOT\_TOLERANCE]

A pivot element must be (in absolute value) greater than or equal to xstore[BASICLU\_REL\_PIVOT\_TOLERANCE] times the largest entry in its column. A value greater than or equal to 1.0 is treated as 1.0 and enforces partial pivoting. Default: 0.1

#### xstore[BASICLU\_BIAS\_NONZEROS]

When this value is greater than or equal to zero, the pivot choice attempts to keep L sparse, putting entries into U when possible. When this value is less than zero, the pivot choice attempts to keep U sparse, putting entries into L when possible. Default: 1

#### xstore[BASICLU\_MAXN\_SEARCH\_PIVOT]

The Markowitz search is terminated after searching xstore[BASICLU\_MAXN\_SERACH\_PIVOT] rows or columns if a numerically stable pivot element has been found. Default: 3

#### xstore[BASICLU\_SEARCH\_ROWS]

If xstore[BASICLU\_SEARCH\_ROWS] is zero, then the Markowitz search only scans columns. If nonzero, then both columns and rows are searched in increasing order of number of entries. Default: 1

# xstore[BASICLU\_PAD] xstore[BASICLU\_STRETCH]

When a row or column cannot be updated by the pivot operation in place, it is appended to the end of the workspace. For a row or column with nz elements, xstore[BASICLU\_PAD] + nz \* xstore[BASICLU\_STRETCH] elements extra space are added for later fill-in.

## Default: xstore[BASICLU\_PAD] = 4, xstore[BASICLU\_STRETCH] = 0.3

#### xstore[BASICLU\_REMOVE\_COLUMNS]

This parameter is present for compatibility to previous versions but has no effect. If during factorization the maximum entry of a column of the

active submatrix becomes zero or less than xstore[BASICLU\_ABS\_PIVOT\_TOLERANCE], then that column is immediately removed without choosing a pivot.

#### Info:

xstore[BASICLU\_STATUS]: status code.

BASICLU\_OK

The factorization has successfully completed.

BASICLU\_WARNING\_singular\_matrix

The factorization did xstore[BASICLU\_RANK] < xstore[BASICLU\_DIM] pivot steps. The remaining elements in the active submatrix are zero or less than xstore[BASICLU\_ABS\_PIVOT\_TOLERANCE]. The factors have been augmented by unit columns to form a square matrix. See basiclu\_get\_factors() on how to get the indices of linearly dependent columns.

BASICLU\_ERROR\_argument\_missing

One or more of the pointer/array arguments are NULL.

BASICLU\_ERROR\_invalid\_call

cOntinue is nonzero, but the factorization was not started before.

BASICLU\_ERROR\_invalid\_argument

The matrix is invalid (a column has a negative number of entries, a row index is out of range, or a column has duplicate entries).

BASICLU\_REALLOCATE

Factorization requires more memory in Li,Lx and/or Ui,Ux and/or Wi,Wx. The number of additional elements in each of the array pairs required for the next pivot operation is given by:

```
xstore[BASICLU_ADD_MEMORYL] >= 0
xstore[BASICLU_ADD_MEMORYU] >= 0
xstore[BASICLU_ADD_MEMORYW] >= 0
```

The user must reallocate the arrays for which additional memory is required. It is recommended to reallocate for the requested number of additional elements plus some extra space (e.g. 0.5 times the current array length). The new array lengths must be provided in

```
xstore[BASICLU_MEMORYL]: length of Li and Lx
xstore[BASICLU_MEMORYU]: length of Ui and Ux
xstore[BASICLU_MEMORYW]: length of Wi and Wx
```

basiclu\_factorize() can be called again with cOntinue not equal to zero to continue the factorization.

xstore[BASICLU\_MATRIX\_NZ] number of nonzeros in B

xstore[BASICLU\_RANK] number of pivot steps performed

An estimate for numerical stability of the factorization. xstore[BASICLU\_RESIDUAL\_TEST] is the maximum of the scaled residuals

```
||b-Bx|| / (||b|| + ||B||*||x||)
```

and

```
||c-B'y|| / (||c|| + ||B'||*||y||),
```

where x=B\b and y=B'\c are computed from the LU factors, b and c have components +/-1 that are chosen to make x respectively y large, and ||.|| is the 1-norm. Here B is the input matrix after replacing dependent columns by unit columns.

If xstore[BASICLU\_RESIDUAL\_TEST] > 1e-12, say, the factorization is numerically unstable. (This is independent of the condition number of B.) In this case tightening the relative pivot tolerance and refactorizing is appropriate.

xstore[BASICLU\_CONDEST\_L]
xstore[BASICLU\_CONDEST\_U] Estimated 1-norm condition number of L and U.

### 3.3 basiclu\_get\_factors

```
lu_int basiclu_get_factors
    lu_int istore[],
    double xstore[],
    lu_int Li[],
    double Lx[],
    lu_int Ui[],
    double Ux[],
    lu_int Wi[],
    double Wx[],
    lu_int rowperm[],
    lu_int colperm[],
    lu_int Lcolptr[],
    lu_int Lrowidx[],
    double Lvalue[],
    lu_int Ucolptr[],
    lu_int Urowidx[],
    double Uvalue[]
);
Purpose:
    Extract the row and column permutation and the LU factors. This routine can
    be used only after basiclu_factorize() has completed and before a call to
    basiclu_update(). At that point the factorized form of matrix B is
        B[rowperm, colperm] = L*U,
    where L is unit lower triangular and U is upper triangular. If the
    factorization was singular (rank < m), then columns colperm[rank..m-1]
    of B have been replaced by unit columns with entry 1 in position
    rowperm[rank..m-1].
    basiclu\_get\_factors() is intended when the user needs direct access to the
    matrix factors. It is not required to solve linear systems with the factors
    (see basiclu_solve_dense() and basiclu_solve_sparse() instead).
Return:
    BASICLU_ERROR_invalid_store if istore, xstore do not hold a BASICLU
    instance. In this case xstore[BASICLU_STATUS] is not set.
    Otherwise return the status code. See xstore[BASICLU_STATUS] below.
Arguments:
    lu_int istore[]
    double xstore[]
    lu int Li∏
    double Lx[]
    lu_int Ui[]
    double Ux[]
    lu_int Wi[]
    double Wx[]
        The BASICLU instance after basiclu_factorize() has completed.
    lu_int rowperm[m]
        Returns the row permutation. If the row permutation is not required,
        then NULL can be passed (this is not an error).
    lu_int colperm[m]
```

Returns the column permutation. If the column permutation is not required, then NULL can be passed (this is not an error).

```
lu_int Lcolptr[m+1]
lu_int Lrowidx[m+Lnz]
double Lvalue[m+Lnz], where Lnz = xstore[BASICLU_LNZ]
```

If all three arguments are not NULL, then they are filled with L in compressed column form. The indices in each column are sorted with the unit diagonal element at the front.

If any of the three arguments is NULL, then  $\boldsymbol{L}$  is not returned (this is not an error).

```
lu_int Ucolptr[m+1]
lu_int Urowidx[m+Unz]
double Uvalue[m+Unz], where Unz = xstore[BASICLU_UNZ]
```

If all three arguments are not NULL, then they are filled with U in compressed column form. The indices in each column are sorted with the diagonal element at the end.

If any of the three arguments is NULL, then  ${\tt U}$  is not returned (this is not an error).

#### Info:

xstore[BASICLU\_STATUS]: status code.

BASICLU\_OK

The requested quantities have been returned successfully.

 ${\tt BASICLU\_ERROR\_argument\_missing}$ 

One or more of the mandatory pointer/array arguments are NULL.

BASICLU\_ERROR\_invalid\_call

The BASICLU instance does not hold a fresh factorization (either basiclu\_factorize() has not completed or basiclu\_update() has been called in the meanwhile).

### 3.4 basiclu\_solve\_dense

```
lu_int basiclu_solve_dense
    lu_int istore[],
    double xstore[],
    lu_int Li[],
    double Lx[],
    lu_int Ui[],
    double Ux[],
    lu_int Wi[],
    double Wx[],
    const double rhs[],
    double lhs[],
    char trans
);
Purpose:
    Given the factorization computed by basiclu_factorize() or basiclu_update()
    and the dense right-hand side, rhs, solve a linear system for the solution
    lhs.
Return:
    {\tt BASICLU\_ERROR\_invalid\_store} \ \ {\tt if} \ \ {\tt istore}, \ \ {\tt xstore} \ \ {\tt do} \ \ {\tt not} \ \ {\tt hold} \ \ {\tt a} \ \ {\tt BASICLU}
    instance. In this case xstore[BASICLU_STATUS] is not set.
    Otherwise return the status code. See xstore[BASICLU_STATUS] below.
Arguments:
    lu_int istore[]
    double xstore[]
    lu_int Li[]
    double Lx[]
    lu_int Ui[]
    double Ux[]
    lu_int Wi[]
    double Wx[]
        Factorization computed by basiclu_factorize() or basiclu_update().
    const double rhs[m]
        The right-hand side vector.
    double lhs[m]
        Uninitialized on entry. On return lhs holds the solution to the linear
        system.
        lhs and rhs are allowed to overlap. To overwrite rhs with the solution
        pass pointers to the same array.
    char trans
        Defines which system to solve. 't' or 'T' for the transposed system, any
        other character for the forward system.
Info:
    xstore[BASICLU_STATUS]: status code.
        BASICLU_OK
```

The linear system has been successfully solved.

BASICLU\_ERROR\_argument\_missing

One or more of the pointer/array arguments are NULL.

BASICLU\_ERROR\_invalid\_call

The factorization is invalid.

### 3.5 basiclu\_solve\_sparse

```
lu_int basiclu_solve_sparse
    lu_int istore[],
    double xstore[],
    lu_int Li[],
    double Lx[],
    lu_int Ui[],
    double Ux[],
    lu_int Wi[],
    double Wx [],
    lu_int nzrhs,
    const lu_int irhs[],
    const double xrhs[],
    lu_int *p_nzlhs,
    lu_int ilhs[],
    double lhs[],
    char trans
):
Purpose:
    Given the factorization computed by basiclu_factorize() or basiclu_update()
    and the sparse right-hand side, rhs, solve a linear system for the solution
    lhs.
Return:
    BASICLU_ERROR_invalid_store if istore, xstore do not hold a BASICLU
    instance. In this case xstore[BASICLU_STATUS] is not set.
    Otherwise return the status code. See xstore[BASICLU_STATUS] below.
Arguments:
    lu_int istore[]
    double xstore[]
    lu_int Li[]
    double Lx[]
    lu_int Ui[]
    double Ux[]
    lu_int Wi[]
    double Wx[]
        Factorization computed by basiclu_factorize() or basiclu_update().
    lu_int nzrhs
    const lu_int irhs[nzrhs]
    const double xrhs[nzrhs]
        The right-hand side vector in compressed format. irhs[0..nzrhs-1] are
        the indices of nonzeros and xrhs[0..nzrhs-1] the corresponding values.
        irhs must not contain duplicates.
    lu_int *p_nzlhs
    lu_int ilhs[m]
    lu_int lhs[m]
        *p_nzlhs is uninitialized on entry. On return *p_nzlhs holds
        the number of nonzeros in the solution.
        The contents of ilhs is uninitialized on entry. On return
        ilhs[0..*p_nzlhs-1] holds the indices of nonzeros in the solution.
        The contents lhs must be initialized to zero on entry. On return
        the solution is scattered into lhs.
```

#### char trans

Defines which system to solve. 't' or 'T' for the transposed system, any other character for the forward system.

#### Parameters:

#### xstore[BASICLU\_SPARSE\_THRESHOLD]

Defines which method is used for solving a triangular system. A triangular solve can be done either by the two phase method of Gilbert and Peierls ("sparse solve") or by a sequential pass through the vector ("sequential solve").

Solving B\*x=b requires two triangular solves. The first triangular solve is done sparse. The second triangular solve is done sparse if its right-hand side has not more than m \* xstore[BASICLU\_SPARSE\_THRESHOLD] nonzeros. Otherwise the sequential solve is used.

Default: 0.05

#### xstore[BASICLU\_DROP\_TOLERANCE]

Nonzeros which magnitude is less than or equal to the drop tolerance are removed after each triangular solve. Default: 1e-20

#### Info:

xstore[BASICLU\_STATUS]: status code.

BASICLU\_OK

The linear system has been successfully solved.

BASICLU\_ERROR\_argument\_missing

One or more of the pointer/array arguments are NULL.

BASICLU\_ERROR\_invalid\_call

The factorization is invalid.

BASICLU\_ERROR\_invalid\_argument

The right-hand side is invalid (nzrhs < 0 or nzrhs > m or one or more indices out of range).

### 3.6 basiclu\_solve\_for\_update

```
lu_int basiclu_solve_for_update
    lu_int istore[],
    double xstore[],
    lu_int Li[],
    double Lx[],
    lu_int Ui[],
    double Ux[],
    lu_int Wi[],
    double Wx[],
    lu_int nzrhs,
    const lu_int irhs[],
    const double xrhs[],
    lu_int *p_nzlhs,
    lu_int ilhs[],
    double lhs[],
    char trans
):
Purpose:
    Given the factorization computed by basiclu_factorize() or basiclu_update(),
    solve a linear system in preparation to update the factorization.
    When the forward system is solved, then the right-hand side is the column
    to be inserted into the factorized matrix. When the transposed system is
    solved, then the right-hand side is a unit vector with entry 1 in position
    of the column to be replaced in the factorized matrix.
    For BASICLU to prepare the update, it is sufficient to compute only a
    partial solution. If the left-hand side is not requested by the user (see
    below), then only one triangular solve is done. If the left-hand side is
    requested, then a second triangular solve is required.
Return:
    BASICLU_ERROR_invalid_store if istore, xstore do not hold a BASICLU
    instance. In this case xstore[BASICLU_STATUS] is not set.
    Otherwise return the status code. See xstore[BASICLU_STATUS] below.
Arguments:
    lu_int istore[]
    double xstore[]
    lu int Li∏
    double Lx[]
    lu_int Ui[]
    double Ux[]
    lu_int Wi[]
    double Wx[]
        Factorization computed by basiclu_factorize() or basiclu_update().
    const lu_int irhs[nzrhs]
    const double xrhs[nzrhs]
        The right-hand side vector in compressed format.
        When the forward system is solved, irhs[0..nzrhs-1] are the indices of
        nonzeros and xrhs[0..nzrhs-1] the corresponding values. irhs must not
```

contain duplicates.

When the transposed system is solved, the right-hand side is a unit vector with entry 1 in position irhs[0]. nzrhs, xrhs and elements of irhs other than irhs[0] are not accessed. xrhs can be NULL.

```
lu_int *p_nzlhs
lu_int ilhs[m]
lu_int lhs[m]
```

If any of  $p_nzlhs$ , ilhs or lhs is NULL, then the solution to the linear system is not requested. In this case only the update is prepared.

#### Otherwise:

\*p\_nzlhs is uninitialized on entry. On return \*p\_nzlhs holds the number of nonzeros in the solution.

The contents of ilhs is uninitialized on entry. On return ilhs[0..\*p\_nzlhs-1] holds the indices of nonzeros in the solution. The contents of lhs must be initialized to zero on entry. On return the solution is scattered into lhs.

#### char trans

Defines which system to solve. 't' or 'T' for the transposed system, any other character for the forward system.

#### Parameters:

```
xstore[BASICLU_MEMORYL]: length of Li and Lx
xstore[BASICLU_MEMORYU]: length of Ui and Ux
xstore[BASICLU_MEMORYW]: length of Wi and Wx
```

#### xstore[BASICLU\_SPARSE\_THRESHOLD]

Defines which method is used for solving a triangular system. A triangular solve can be done either by the two phase method of Gilbert and Peierls ("sparse solve") or by a sequential pass through the vector ("sequential solve").

When the solution to the linear system is requested, then two triangular systems are solved. The first triangular solve is done sparse. The second triangular solve is done sparse if its right-hand side has not more than m \* xstore[BASICLU\_SPARSE\_THRESHOLD] nonzeros. Otherwise the sequential solve is used.

When the solution to the linear system is not requested, then this parameter has no effect.

```
Default: 0.05
```

### ${\tt xstore} \, [{\tt BASICLU\_DROP\_TOLERANCE}]$

Nonzeros which magnitude is less than or equal to the drop tolerance are removed after each triangular solve. Default: 1e-20

#### Info:

```
xstore[BASICLU_STATUS]: status code.
```

#### BASICLU\_OK

The updated has been successfully prepared and, if requested, the solution to the linear system has been computed.

#### BASICLU\_ERROR\_argument\_missing

One or more of the mandatory pointer/array arguments are NULL.

#### BASICLU\_ERROR\_invalid\_call

The factorization is invalid.

#### BASICLU\_ERROR\_maximum\_updates

There have already been m Forrest-Tomlin updates, see xstore[BASICLU\_NFORREST]. The factorization cannot be updated any more and must be recomputed by basiclu\_factorize(). The solution to the linear system has not been computed.

#### BASICLU\_ERROR\_invalid\_argument

The right-hand side is invalid (forward system: nzrhs < 0 or nzrhs > m or one or more indices out of range; backward system: irhs[0] out of range).

#### BASICLU\_REALLOCATE

The solve was aborted because of insufficient memory in Li,Lx or Ui,Ux to store data for basiclu\_update(). The number of additional elements required is given by

```
xstore[BASICLU_ADD_MEMORYL] >= 0
xstore[BASICLU_ADD_MEMORYU] >= 0
```

The user must reallocate the arrays for which additional memory is required. It is recommended to reallocate for the requested number of additional elements plus some extra space for further updates (e.g. 0.5 times the current array length). The new array lengths must be provided in

```
xstore[BASICLU_MEMORYL]: length of Li and Lx
xstore[BASICLU_MEMORYU]: length of Ui and Ux
```

basiclu\_solve\_for\_update() will start from scratch in the next call.

### 3.7 basiclu\_update

#### Purpose:

Update the factorization to replace one column of the factorized matrix. A call to basiclu\_update() must be preceded by calls to basiclu\_solve\_for\_update() to provide the column to be inserted and the index of the column to be replaced.

The column to be inserted is defined as the right-hand side in the last call to basiclu\_solve\_for\_update() in which the forward system was solved.

The index of the column to be replaced is defined by the unit vector in the last call to basiclu\_solve\_for\_update() in which the transposed system was solved.

#### Return:

BASICLU\_ERROR\_invalid\_store if istore, xstore do not hold a BASICLU instance. In this case xstore[BASICLU\_STATUS] is not set.

Otherwise return the status code. See xstore[BASICLU\_STATUS] below.

#### Arguments:

```
lu_int istore[]
double xstore[]
lu_int Li[]
double Lx[]
lu_int Ui[]
double Ux[]
lu_int Wi[]
double Wx[]
```

Factorization computed by basiclu\_factorize() or basiclu\_update().

#### double xtbl

This is an optional argument to monitor numerical stability. xtbl can be either of

- (a) element j0 of the solution to the forward system computed by basiclu\_solve\_for\_update(), where j0 is the column to be replaced;
- (b) the dot product of the incoming column and the solution to the transposed system computed by basiclu\_solve\_for\_update().

In either case xstore[BASICLU\_PIVOT\_ERROR] (see below) has a defined value. If monitoring stability is not desired, xtbl can be any value.

#### Parameters:

```
{\tt xstore[BASICLU\_MEMORYL]: length \ of \ Li \ and \ Lx}
```

```
xstore[BASICLU_MEMORYU]: length of Ui and Ux
xstore[BASICLU_MEMORYW]: length of Wi and Wx
```

#### xstore[BASICLU\_DROP\_TOLERANCE]

Nonzeros which magnitude is less than or equal to the drop tolerance are removed from the row eta matrix. Default: 1e-20

#### Info:

xstore[BASICLU\_STATUS]: status code.

#### BASICLU\_OK

The update has successfully completed.

BASICLU\_ERROR\_argument\_missing

One or more of the pointer/array arguments are NULL.

BASICLU\_ERROR\_invalid\_call

The factorization is invalid or the update was not prepared by two calls to  $basiclu\_solve\_for\_update()$ .

#### BASICLU\_REALLOCATE

Insufficient memory in Wi,Wx. The number of additional elements required is given by

```
xstore[BASICLU_ADD_MEMORYW] > 0
```

The user must reallocate Wi,Wx. It is recommended to reallocate for the requested number of additional elements plus some extra space for further updates (e.g. 0.5 times the current array length). The new array length must be provided in

xstore[BASICLU\_MEMORYW]: length of Wi and Wx

basiclu\_update will start from scratch in the next call.

#### BASICLU\_ERROR\_singular\_update

The updated factorization would be (numerically) singular. No update has been computed and the old factorization is still valid.

#### xstore[BASICLU\_PIVOT\_ERROR]

When xtbl was given (see above), then xstore[BASICLU\_PIVOT\_ERROR] is a measure for numerical stability. It is the difference between two computations of the new pivot element relative to the new pivot element. A value larger than 1e-10 indicates numerical instability and suggests refactorization (and possibly tightening the pivot tolerance).

#### xstore[BASICLU\_MAX\_ETA]

The maximum entry (in absolute value) in the eta vectors from the Forrest-Tomlin update. A large value, say > 1e6, indicates that pivoting on diagonal element was unstable and refactorization might be necessary.

## 4 High level C interface

The high level C interface consists of wrapper functions around the low level interface which do memory allocation. They maintain the arrays used by the low level interface inside a struct basiclu\_object. To use the high level C interface, user code must include basiclu.h. Defined constants start with BASICLU\_ and function names start with basiclu\_obj\_..

## 4.1 basiclu\_object

```
struct basiclu_object
    lu_int *istore;
    double *xstore;
    lu_int *Li, *Vi, *Wi;
    double *Lx, *Ux, *Wx;
    double *lhs;
   lu_int *ilhs;
    lu_int nzlhs;
    double realloc_factor;
};
{\tt A}\xspace variable of type struct basiclu_object must be defined in user code. Its
members are set and maintained by basiclu_obj_* routines. User code should only
access the following members:
    xstore (read/write)
        set parameters and get info values
    lhs, ilhs, nzlhs (read only)
        holds solution after solve_sparse() and solve_for_update()
    realloc_factor (read/write)
        Arrays are reallocated for max(realloc_factor, 1.0) times the
        required size. Default: 1.5
```

## 4.2 basiclu\_obj\_initialize

```
lu_int basiclu_obj_initialize
    struct basiclu_object *obj,
    lu_int m
);
Purpose:
    Initialize a BASICLU object. When m is positive, then *obj is initialized to
    process matrices of dimension m. When m is zero, then *obj is initialized to
    a "null" object, which cannot be used for factorization, but can be passed
    to basiclu_obj_free().
   This routine must be called once before passing obj to any other
    basiclu_obj_ routine. When obj is initialized to a null object, then the
    routine can be called again to reinitialize obj.
Return:
    BASICLU_OK
        *obj successfully initialized.
    BASICLU_ERROR_argument_missing
        obj is NULL.
    BASICLU_ERROR_invalid_argument
        m is negative.
    BASICLU_ERROR_out_of_memory
        insufficient memory to initialize object.
Arguments:
    struct basiclu_object *obj
        Pointer to the object to be initialized.
    lu_int m
        The dimension of matrices which can be processed, or 0.
```

## $4.3 \quad basiclu\_obj\_get\_dim$

```
lu_int basiclu_obj_get_dim
(
    struct basiclu_object *obj
);
Purpose:
```

Returns the dimension for which the object was initialized or 0 when obj is  $_{\mbox{\scriptsize NIIII}\,\mbox{\scriptsize I}}$ 

## 4.4 basiclu\_obj\_factorize

```
lu_int basiclu_obj_factorize
    struct basiclu_object *obj,
   const lu_int *Bbegin,
   const lu_int *Bend,
   const lu_int *Bi,
    const double *Bx
);
Purpose:
    Call basiclu_factorize() on a BASICLU object.
Return:
    BASICLU_ERROR_invalid_object
        obj is NULL or initialized to a null object.
    BASICLU_ERROR_out_of_memory
        reallocation failed because of insufficient memory.
    Other return codes are passed through from basiclu_factorize().
Arguments:
    struct basiclu_object *obj
        Pointer to an initialized BASICLU object.
    The other arguments are passed through to basiclu\_factorize().
```

## 4.5 basiclu\_obj\_get\_factors

```
lu_int basiclu_obj_get_factors
    struct basiclu_object *obj,
   lu_int rowperm[],
   lu_int colperm[],
   lu_int Lcolptr[],
   lu_int Lrowidx[],
   double Lvalue[],
   lu_int Ucolptr[],
   lu_int Urowidx[],
   double Uvalue[]
);
Purpose:
   Call basiclu_get_factors() on a BASICLU object.
Return:
    BASICLU_ERROR_invalid_object
        obj is NULL or initialized to a null object.
    Other return codes are passed through from basiclu_get_factors().
Arguments:
    struct basiclu_object *obj
        Pointer to an initialized BASICLU object.
    The other arguments are passed through to basiclu\_get\_factors().
```

## 4.6 basiclu\_obj\_solve\_dense

```
lu_int basiclu_obj_solve_dense
    struct basiclu_object *obj,
   const double rhs[],
   double lhs[],
    char trans
);
Purpose:
   Call basiclu_solve_dense() on a BASICLU object.
Return:
   BASICLU_ERROR_invalid_object
        obj is NULL or initialized to a null object.
    Other return codes are passed through from basiclu_solve_dense().
Arguments:
    struct basiclu_object *obj
        Pointer to an initialized BASICLU object.
    The other arguments are passed through to basiclu\_solve\_dense().
```

## 4.7 basiclu\_obj\_solve\_sparse

```
lu_int basiclu_obj_solve_sparse
    struct basiclu_object *obj,
    lu_int nzrhs,
    const lu_int irhs[],
    const double xrhs[],
    char trans
);
Purpose:
    Call basiclu_solve_sparse() on a BASICLU object. On success, the solution
    is provided in obj->lhs and the nonzero pattern is stored in
    obj->ilhs[0..obj->nzlhs-1].
Return:
    {\tt BASICLU\_ERROR\_invalid\_object}
        obj is NULL or initialized to a null object.
    Other return codes are passed through from basiclu_solve_sparse().
Arguments:
    struct basiclu_object *obj
        Pointer to an initialized BASICLU object.
    The other arguments are passed through to basiclu\_solve\_sparse().
```

## 4.8 basiclu\_obj\_solve\_for\_update

```
lu_int basiclu_obj_solve_for_update
    struct basiclu_object *obj,
   lu_int nzrhs,
    const lu_int irhs[],
    const double xrhs[],
    char trans,
   lu_int want_solution
);
Purpose:
    Call basiclu_solve_for_update() on a BASICLU object. On success, if the
    solution was requested, it is provided in obj->lhs and the nonzero pattern
    is stored in obj->ilhs[0..obj->nzlhs-1].
Return:
    BASICLU_ERROR_invalid_object
        obj is NULL or initialized to a null object.
    BASICLU_ERROR_out_of_memory
        reallocation failed because of insufficient memory.
    Other return codes are passed through from basiclu_solve_for_update().
Arguments:
    struct basiclu_object *obj
        Pointer to an initialized BASICLU object.
    lu_int want_solution
        Nonzero to compute the solution to the linear system,
        zero to only prepare the update.
    The other arguments are passed through to basiclu_solve_for_update().
```

## 4.9 basiclu\_obj\_update

```
lu_int basiclu_obj_update
    struct basiclu_object *obj,
    double xtbl
);
Purpose:
    Call basiclu_update() on a BASICLU object.
Return:
    {\tt BASICLU\_ERROR\_invalid\_object}
        obj is NULL or initialized to a null object.
    BASICLU_ERROR_out_of_memory
        reallocation failed because of insufficient memory.
    Other return codes are passed through from basiclu_update().
Arguments:
    struct basiclu_object *obj
        Pointer to an initialized BASICLU object.
    The other arguments are passed through to basiclu_update().
```

## 4.10 basiclu\_obj\_free

```
void basiclu_obj_free
(
    struct basiclu_object *obj
);

Purpose:
    Free memory allocated from a BASICLU object. The object must have been initialized before by basiclu_obj_initialize(). Subsequent calls to basiclu_obj_free() will do nothing.

Arguments:
    struct basiclu_object *obj

    Pointer to the object which memory is to be freed. When obj is NULL, then the routine does nothing.
```

### 4.11 basiclu\_obj\_maxvolume

```
lu_int basiclu_obj_maxvolume
(
    struct basiclu_object *obj,
    lu_int ncol,
    const lu_int Ap[],
    const lu_int Ai[],
    const double Ax[],
    lu_int basis[],
    lu_int isbasic[],
    double volumetol,
    lu_int *p_nupdate
);
```

#### Purpose:

Make one pass over the columns of a rectangular (ncol >= nrow) matrix and pivot each nonbasic column into the basis when it increases the volume (i.e. the absolute value of the determinant) of the basis matrix. This is one main loop of the "maximum volume" algorithm described in [1,2].

- [1] C. T. Pan, "On the existence and computation of rank-revealing LU factorizations". Linear Algebra Appl., 316(1-3), pp. 199-222, 2000
- [2] S. A. Goreinov, I. V. Oseledets, D. V. Savostyanov, E. E. Tyrtyshnikov, N. L. Zamarashkin, "How to find a good submatrix". In "Matrix methods: theory, algorithms and applications", pp. 247-256. World Sci. Publ., Hackensack, NJ, 2010.

#### Return:

BASICLU\_ERROR\_invalid\_argument when volumetol is less than 1.0. BASICLU\_ERROR\_out\_of\_memory when memory allocation in this function failed.

The return code from a basiclu\_obj\_\* function called when not BASICLU\_OK. (Note that BASICLU\_WARNING\_singular\_matrix means that the algorithm failed.)

BASICLU\_OK otherwise.

#### Arguments:

```
struct basiclu_object *obj
```

Pointer to an initialized BASICLU object. The dimension of the object specifies the number of rows of the matrix.

```
lu_int ncol
const lu_int Ap[ncol+1]
const lu_int Ai[]
const double Ax[]
```

Matrix A in compressed sparse column format. Column j contains elements

```
Ai[Ap[j] .. Ap[j+1]-1], Ax[Ap[j] .. Ap[j+1]-1].
```

The columns must not contain duplicate row indices. The row indices per column need not be sorted.

#### lu\_int basis[nrow]

On entry holds the column indices of A that form the initial basis. On return holds the updated basis. A basis defines a square nonsingular submatrix of A. If the initial basis is (numerically) singular, then the initial LU factorization will fail and BASICLU\_WARNING\_singular\_matrix is returned.

#### lu\_int isbasic[ncol]

This array must be consistent with basis[] on entry, and is consistent on return. isbasic[j] must be nonzero iff column j appears in the basis.

#### double volumetol

A column is pivoted into the basis when it increases the absolute value of the determinant of the basis matrix by more than a factor volumetol. This parameter must be >= 1.0. In pratcice typical values are 2.0, 10.0 or even 100.0. The closer the tolerances to 1.0, the more basis changes will usually be necessary to find a maximum volume basis for this tolerance (using repeated calls to basiclu\_obj\_maxvolume(), see below).

#### lu\_int \*p\_nupdate

On return \*p\_nupdate holds the number of basis updates performed. When this is zero and BASICLU\_OK is returned, then the volume of the initial basis is locally (within one basis change) maximum up to a factor volumetol. To find such a basis, basiclu\_obj\_maxvolume() must be called repeatedly starting from an arbitrary basis until \*p\_nupdate is zero. This will happen eventually because each basis update strictly increases the volume of the basis matrix. Hence a basis cannot repeat.

p\_nupdate can be NULL, in which case it is not accessed. This is not an error condition. The number of updates performed can be obtained as the increment to obj->xstore[BASICLU\_NUPDATE\_TOTAL] caused by the call to basiclu\_obj\_maxvolume().

## 5 Julia interface

BASICLU can be used from the Julia programming language. To do so, the package must be compiled and the lib/ directory must be added to the shared library load path of your system. Then run Julia and include the basiclu module by

```
include("path/to/BASICLU/Julia/basiclu.jl")
```

The following is an example for a Julia program using BASICLU. See also the documentation of the module functions and Julia/test.jl.

```
include("BASICLU/Julia/basiclu.jl")
m = 1000
this = basiclu.initialize(m)
B = sprand(m,m,5e-3) + I
                                             # get a sparse matrix
err = basiclu.factorize(this, B)
if err != basiclu.BASICLU_OK
 error("factorization failed or singular")
end
                                             # get a right-hand side
rhs = randn(m)
lhs = basiclu.solve(this, rhs, 'N')
res = norm(B*lhs-rhs,Inf)
                                             # compute residual
col = sparsevec([1], [1.0], m)
                                             \# unit vector to be inserted into B
lhs = basiclu.solve4update(this, col, true)
(vmax,j) = findmax(abs.(lhs))
xtbl = lhs[j]
basiclu.solve4update(this, j)
                                             # prepare to replace column j of B
piverr = basiclu.update(this, xtbl)
lhs = basiclu.solve(this, rhs, 'N')
B[:,j] = col
res = norm(B*lhs-rhs,Inf)
```