



**CULA Reference Manual**

**[www.culatools.com](http://www.culatools.com)**

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# CONTENTS

<b>1</b>	<b>Introduction</b>	<b>1</b>
1.1	Attributions . . . . .	1
<b>2</b>	<b>Framework Functions</b>	<b>2</b>
2.1	culaInitialize . . . . .	2
2.2	culaShutdown . . . . .	2
2.3	culaGetLastStatus . . . . .	2
2.4	culaGetStatusString . . . . .	2
2.5	culaGetErrorInfo . . . . .	3
2.6	culaFreeBuffers . . . . .	3
2.7	culaGetDeviceCount . . . . .	3
2.8	culaSelectDevice . . . . .	3
2.9	culaGetExecutingDevice . . . . .	4
2.10	culaGetDeviceInfo . . . . .	4
2.11	culaGetOptimalPitch . . . . .	4
2.12	culaDeviceMalloc . . . . .	4
2.13	culaDeviceFree . . . . .	5
<b>3</b>	<b>Linear Algebra Routines</b>	<b>6</b>
3.1	Data Types . . . . .	6
3.2	Host Interface Compared To Device Interface . . . . .	6
3.3	Note on Leading Dimensions . . . . .	6
3.4	BDSQR . . . . .	7
3.5	GEBRD . . . . .	9
3.6	GEEV . . . . .	12
3.7	GEHRD . . . . .	15
3.8	GELQF . . . . .	17
3.9	GELS . . . . .	18
3.10	GEQLF . . . . .	20
3.11	GEQRF . . . . .	22
3.12	GEQRS . . . . .	23
3.13	GERQF . . . . .	25
3.14	GESV . . . . .	27
3.15	GESV (Iteratively Refined) . . . . .	28
3.16	GESVD . . . . .	31
3.17	GETRF . . . . .	33
3.18	GETRI . . . . .	35
3.19	GETRS . . . . .	36
3.20	GGLSE . . . . .	38

3.21	GGRQF	40
3.22	ORGBR/UNGBR	43
3.23	ORGHR/UNGHR	44
3.24	ORGLQ/UNGLQ	46
3.25	ORGQL/UNGQL	47
3.26	ORGQR/UNGQR	49
3.27	ORGRQ/UNGRQ	50
3.28	ORMLQ/UNMLQ	52
3.29	ORMQL/UNMQL	54
3.30	ORMQR/UNMQR	56
3.31	ORMRQ/UNMRQ	58
3.32	POSV	61
3.33	POTRF	62
3.34	POTRS	64
3.35	STEBZ	65
3.36	STEQR	68
3.37	SYEV/HEEV	70
3.38	SYEVX/HEEVX	71
3.39	SYRDB/HERDB	74
3.40	SYTRD/HETRD	77
3.41	TRTRI	77
3.42	TRTRS	78
<b>4</b>	<b>Differences Between CULA and LAPACK</b>	<b>81</b>
4.1	No Workspace Parameters	81
<b>5</b>	<b>Common Errors</b>	<b>82</b>
5.1	Pivot Arrays	82
5.2	Padding With Zeros	82

# INTRODUCTION

This guide documents CULA's Programming Interface. CULA™ is an implementation of the Linear Algebra PACK-age (LAPACK) interface for *CUDA*™-enabled NVIDIA® graphics processing units (GPUs). It is a companion document to the CULA Programmer's Guide.

This guide is split into the following sections:

- *Framework Functions* - These section documents functions are used in initializing CULA, shutting it down, and querying information about errors.
- *Linear Algebra Routines* - This section documents the Linear Algebra functions that CULA provides
- *Differences Between CULA and LAPACK* - This section lists some of the ways in which CULA differs from LAPACK.
- *Common Errors* - This section lists some of the common errors that apply to usage of several functions.

## 1.1 Attributions

This work has been made possible by the NASA Small Business Innovation Research (SBIR) program. We recognize NVIDIA for their support.

CULA is built on *NVIDIA CUDA 3.1* and *NVIDIA CUBLAS*.

CULA uses the Intel® Math Kernel Library (MKL) internally. For more information, please see the MKL product page at <http://www.intel.com/software/products/mkl>.

The original version of LAPACK from which CULA implements a similar interface can be obtained at <http://www.netlib.org/lapack>. Much of this Reference Manual is based upon the documentation released with netlib.

# FRAMEWORK FUNCTIONS

This section documents the functions that are used in initializing CULA, shutting it down, and querying information about errors.

## 2.1 culaInitialize

### Description

Initializes CULA Must be called before using any other function. Some functions have an exception to this rule: `culaGetDeviceCount`, `culaSelectDevice`

### Returns

`culaNoError` on a successful initialization or the `culaStatus` enum that specifies an error

## 2.2 culaShutdown

### Description

Shuts down CULA Must be called to deallocate CULA internal data

## 2.3 culaGetLastStatus

### Description

Returns the last status code returned from a CULA function

### Returns

The last CULA status code

## 2.4 culaGetStatusString

### Description

Associates a `culaStatus` enum with a readable error string

### Parameters

- **e** - A `culaStatus` error code

**Returns**

A string that corresponds with the specified `culaStatus` enum

## 2.5 `culaGetErrorInfo`

**Description**

This function is used to provide extended functionality that LAPACK's `info` parameter typically provides

**Returns**

Extended information about the last error or zero if it is unavailable

## 2.6 `culaFreeBuffers`

**Description**

Releases any memory buffers stored internally by CULA

## 2.7 `culaGetDeviceCount`

**Description**

Reports the number of GPU devices Can be called before `culaInitialize`

**Parameters**

- **num** - Pointer to receive the number of devices

**Returns**

`culaNoError` on success, `culaArgumentError` on invalid pointer

## 2.8 `culaSelectDevice`

**Description**

Selects a device with which CULA will operate To bind without error, this function must be called before `culaInitialize`

**Parameters**

- **dev** - Specifies the device id of the GPU device

**Returns**

`culaNoError` on success, `culaArgumentError` on an invalid device id, `culaRuntimeError` if the running thread has already been bound to a GPU device

## 2.9 culaGetExecutingDevice

### Description

Reports the id of the GPU device executing CULA

### Parameters

- **dev** - Pointer to receive the GPU device number

### Returns

culaNoError on success, culaArgumentError on invalid pointer

## 2.10 culaGetDeviceInfo

### Description

Prints information to a buffer about a specified device

### Parameters

- **dev** - CUDA device id to print information about
- **buf** - Pointer to a buffer into which information will be printed
- **bufsize** - The size of buf, printed information will not exceed bufsize

### Returns

culaNoError on success, culaArgumentError on invalid buf pointer, invalid device id, or invalid bufsize

## 2.11 culaGetOptimalPitch

### Description

Calculates a pitch that is optimal for CULA when using the device interface

### Parameters

- **pitch** - The optimal pitch for the specified matrix in elements (where  $*pitch \geq \text{rows}$ )
- **rows** - The number of rows of the matrix
- **cols** - The number of columns of the matrix
- **esize** - The size in bytes of the desired element

### Returns

culaNoError on successful allocation, culaInsufficientMemory on failure

## 2.12 culaDeviceMalloc

### Description

Allocates memory on the device in a pitch that is optimal for CULA

### Parameters

- **mem** - Pointer to which a newly allocated buffer will be assigned
- **pitch** - The pitch of the allocation in elements (where  $*pitch \geq \text{rows}$ )
- **rows** - The number of rows of the matrix
- **cols** - The number of columns of the matrix
- **esize** - The size in bytes of the desired element

**Returns**

culaNoError on successful allocation, culaInsufficientMemory on failure

## 2.13 culaDeviceFree

**Description**

Frees memory that has been allocated with culaDeviceMalloc

**Parameters**

- **mem** - Pointer to a buffer that is to be freed

**Returns**

culaNoError on successful free, culaArgumentError on failure

# LINEAR ALGEBRA ROUTINES

This section documents the Linear Algebra functions that CULA provides. For each function, a high-level description of that function is given, followed by a listing of each of the function’s parameters. Where applicable, differences from LAPACK will also be listed.

## 3.1 Data Types

CULA provides 4 data types with which you can perform computations, with one function for each data type. Rather than document each routine separately, this guide includes only one reference for each of the functions, and instead documents the differences between each of these functions (if any) in the generic function description.

Most functions only take pointers to one data type that applies to the S, D, C, or Z variant of the function in question. For the majority of functions, these parameters will be denoted as S/D/C/Z. For those functions that have parameters that differ from their variant, the difference will be noted. For example, for a ‘C/Z’ function that has real (non-complex) parameters, these parameters will be denoted as S/D (although others may be denoted as S/D/C/Z). For an ‘S’ function that has complex parameters, these parameters will be denoted as (C/Z).

Symbol	Host Interface Type	Device Interface Type
S	culaFloat	culaDeviceFloat
D	culaDouble	culaDeviceDouble
C	culaFloatComplex	culaDeviceFloatComplex
Z	culaDoubleComplex	culaDeviceDoubleComplex

## 3.2 Host Interface Compared To Device Interface

For Host interface functions, all matrices/vectors are submitted as pointers to *host* data. For the Device interface, all matrices/vectors are submitted as pointers to GPU data, as allocated by either the *CUDA* toolkit or via *culaDeviceMalloc* (available in CULA premium). All Device interface routines have the word *Device* as part of the function name; all other functions are Host interface.

There are some pointer arguments for which this not the case; these will often be output scalar arguments rather than matrices or vectors. These are denoted as “(type) Pointer, always host” etc.

## 3.3 Note on Leading Dimensions

All LAPACK matrices are specified as a pointer and a “leading dimension” parameter. The leading dimension describes the *allocated* size of the matrix, which may be equal to or larger than the actual matrix height. Thus if a matrix input is described as size “(LDA,N)” it simply means that the *storage* for the matrix is at least *LDA x N* in size. The

section of that array that contains valid data will be described by other parameters, often  $M$  and  $N$ . There will typically be a note differentiating between these.

## 3.4 BDSQR

### CULA Routines

The BDSQR functionality is implemented by the following CULA routines:

- Host Memory
  - `culaSbdsqr`
  - `culaDbdsqr`
  - `culaCbdsqr`
  - `culaZbdsqr`
  - `culaBdsqr` (C++ style, type overloaded)
- Device Memory
  - `culaDeviceSbdsqr`
  - `culaDeviceDbdsqr`
  - `culaDeviceCbdsqr`
  - `culaDeviceZbdsqr`
  - `culaDeviceBdsqr` (C++ style, type overloaded)

### Description

BDSQR computes the singular values and, optionally, the right and/or left singular vectors from the singular value decomposition (SVD) of a real  $N$ -by- $N$  (upper or lower) bidiagonal matrix  $B$  using the implicit zero-shift QR algorithm. The SVD of  $B$  has the form

$$B = Q * S * P^T$$

where  $S$  is the diagonal matrix of singular values,  $Q$  is an orthogonal matrix of left singular vectors, and  $P$  is an orthogonal matrix of right singular vectors. If left singular vectors are requested, this subroutine actually returns  $U*Q$  instead of  $Q$ , and, if right singular vectors are requested, this subroutine returns  $P^T * VT$  instead of  $P^T$ , for given real input matrices  $U$  and  $VT$ . When  $U$  and  $VT$  are the orthogonal/unitary matrices that reduce a general matrix  $A$  to bidiagonal form:  $A = U * B * VT$ , as computed by *GEBRD*, then

$$A = (U * Q) * S * (P^T * VT)$$

is the SVD of  $A$ . Optionally, the subroutine may also compute  $Q^T * C$  for a given real input matrix  $C$ .

See “Computing Small Singular Values of Bidiagonal Matrices With Guaranteed High Relative Accuracy,” by J. Demmel and W. Kahan, LAPACK Working Note #3 (or SIAM J. Sci. Statist. Comput. vol. 11, no. 5, pp. 873-912, Sept 1990) and “Accurate singular values and differential qd algorithms,” by B. Parlett and V. Fernando, Technical Report CPAM-554, Mathematics Department, University of California at Berkeley, July 1992 for a detailed description of the algorithm.

### Parameters

- **uplo**
  - Type: `char`

- Direction: Input

= 'U': B is upper bidiagonal;  
= 'L': B is lower bidiagonal.

- **n**

- Type: int
- Direction: Input

The order of the matrix B.  $N \geq 0$ .

- **ncvt**

- Type: int
- Direction: Input

The number of columns of the matrix VT.  $NCVT \geq 0$ .

- **nru**

- Type: int
- Direction: Input

The number of rows of the matrix U.  $NRU \geq 0$ .

- **ncc**

- Type: int
- Direction: Input

The number of columns of the matrix C.  $NCC \geq 0$ .  $NCC > 0$  is currently not supported and will return `culaFeatureNotImplemented`.

- **d**

- Type: S/D Pointer
- Direction: Input/Output
- Dimension: (N)

On entry, the n diagonal elements of the bidiagonal matrix B.

On exit, if `culaNoError` is returned, the singular values of B in decreasing order.

- **e**

- Type: S/D Pointer
- Direction: Input/Output
- Dimension: (N-1)

On entry, the N-1 offdiagonal elements of the bidiagonal matrix B.

On exit, if `culaNoError` is returned, E is destroyed; if `culaDataError` is returned, D and E will contain the diagonal and superdiagonal elements of a bidiagonal matrix orthogonally equivalent to the one given as input.

- **vt**

- Type: S/D/C/Z Pointer
- Direction: Input/Output

– Dimension: (LDVT, NCVT)

On entry, an N-by-NCVT matrix VT.

On exit, VT is overwritten by  $P^T * VT$ . Not referenced if NCVT = 0.

- **ldvt**

– Type: int

– Direction: Input

The leading dimension of the array VT. LDVT  $\geq \max(1, N)$  if NCVT > 0; LDVT  $\geq 1$  if NCVT = 0.

- **u**

– Type: S/D/C/Z Pointer

– Direction: Input/Output

– Dimension: (LDU, N)

On entry, an NRU-by-N matrix U.

On exit, U is overwritten by  $U * Q$ .

Not referenced if NRU = 0.

- **ldu**

– Type: int

– Direction: Input

The leading dimension of the array U. LDU  $\geq \max(1, NRU)$ .

- **c**

– Type: S/D/C/Z Pointer

– Direction: Input/Output

– Dimension: (LDC, NCC)

On entry, an N-by-NCC matrix C.

On exit, C is overwritten by  $Q^T * C$ .

Not referenced if NCC = 0.

- **ldc**

– Type: int

– Direction: Input

The leading dimension of the array C. LDC  $\geq \max(1, N)$  if NCC > 0; LDC  $\geq 1$  if NCC = 0.

### Differences from LAPACK

See *No Workspace Parameters* section.

## 3.5 GEBRD

### CULA Routines

The GEBRD functionality is implemented by the following CULA routines:

- Host Memory
  - culaSgebrd
  - culaDgebrd
  - culaCgebrd
  - culaZgebrd
  - culaGebrd (C++ style, type overloaded)
- Device Memory
  - culaDeviceSgebrd
  - culaDeviceDgebrd
  - culaDeviceCgebrd
  - culaDeviceZgebrd
  - culaDeviceGebrd (C++ style, type overloaded)

### Description

GEBRD reduces a general real M-by-N matrix A to upper or lower bidiagonal form B by an orthogonal/unitary transformation:  $Q^T * A * P = B$ .

If  $m \geq n$ , B is upper bidiagonal; if  $m < n$ , B is lower bidiagonal.

### Parameters

- **m**

- Type: int
- Direction: Input

The number of rows in the matrix A.  $M \geq 0$ .

- **n**

- Type: int
- Direction: Input

The number of columns in the matrix A.  $N \geq 0$ .

- **a**

- Type: S/D/C/Z Pointer
- Direction: Input/Output
- Dimension: (LDA, N)

On entry, the M-by-N general matrix to be reduced.

On exit, if  $m \geq n$ , the diagonal and the first superdiagonal are overwritten with the upper bidiagonal matrix B; the elements below the diagonal, with the array TAUQ, represent the orthogonal/unitary matrix Q as a product of elementary reflectors, and the elements above the first superdiagonal, with the array TAUP, represent the orthogonal/unitary matrix P as a product of elementary reflectors;

On exit, if  $m < n$ , the diagonal and the first subdiagonal are overwritten with the lower bidiagonal matrix B; the elements below the first subdiagonal, with the array TAUQ, represent the orthogonal/unitary matrix Q as a product of elementary reflectors, and the elements above the diagonal, with the array TAUP, represent the orthogonal/unitary matrix P as a product of elementary reflectors. See Further Details.

- **lda**

- Type: int
- Direction: Input

The leading dimension of the array A. LDA  $\geq$  max(1,M).

- **d**

- Type: S/D Pointer
- Direction: Output
- Dimension: (min(M,N))

The diagonal elements of the bidiagonal matrix B: D(i) = A(i,i).

- **e**

- Type: S/D Pointer
- Direction: Output
- Dimension: (min(M,N)-1)

The off-diagonal elements of the bidiagonal matrix B: if  $m \geq n$ , E(i) = A(i,i+1) for  $i = 1, 2, \dots, n-1$ ; if  $m < n$ , E(i) = A(i+1,i) for  $i = 1, 2, \dots, m-1$ .

- **tauq**

- Type: S/D/C/Z Pointer
- Direction: Output
- Dimension: (min(M,N))

The scalar factors of the elementary reflectors which represent the orthogonal/unitary matrix Q. See Further Details.

- **taup**

- Type: S/D/C/Z Pointer
- Direction: Output
- Dimension: (min(M,N))

The scalar factors of the elementary reflectors which represent the orthogonal/unitary matrix P. See Further Details.

### Further Details

The matrices Q and P are represented as products of elementary reflectors:

If  $m \geq n$ ,

$$Q = H(1) H(2) \dots H(n) \text{ and } P = G(1) G(2) \dots G(n-1)$$

Each H(i) and G(i) has the form:

$$H(i) = I - \tau_q * v * v' \text{ and } G(i) = I - \tau_p * u * u'$$

where  $\tau_q$  and  $\tau_p$  are real scalars, and  $v$  and  $u$  are real vectors;  $v(1:i-1) = 0$ ,  $v(i) = 1$ , and  $v(i+1:m)$  is stored on exit in A(i+1:m,i);  $u(1:i) = 0$ ,  $u(i+1) = 1$ , and  $u(i+2:n)$  is stored on exit in A(i,i+2:n);  $\tau_q$  is stored in TAUQ(i) and  $\tau_p$  in TAUP(i).

If  $m < n$ ,

$$Q = H(1) H(2) \dots H(m-1) \text{ and } P = G(1) G(2) \dots G(m)$$

Each  $H(i)$  and  $G(i)$  has the form:

$$H(i) = I - \text{tauq} * v * v' \text{ and } G(i) = I - \text{taup} * u * u'$$

where  $\text{tauq}$  and  $\text{taup}$  are real scalars, and  $v$  and  $u$  are real vectors;  $v(1:i) = 0$ ,  $v(i+1) = 1$ , and  $v(i+2:m)$  is stored on exit in  $A(i+2:m,i)$ ;  $u(1:i-1) = 0$ ,  $u(i) = 1$ , and  $u(i+1:n)$  is stored on exit in  $A(i,i+1:n)$ ;  $\text{tauq}$  is stored in  $\text{TAUQ}(i)$  and  $\text{taup}$  in  $\text{TAUP}(i)$ .

The contents of  $A$  on exit are illustrated by the following examples:

$m = 6$  and  $n = 5$  ( $m > n$ ):

```
( d  e  u1  u1  u1 )
( v1 d  e  u2  u2 )
( v1 v2 d  e  u3 )
( v1 v2 v3 d  e  )
( v1 v2 v3 v4 d  )
( v1 v2 v3 v4 v5 )
```

$m = 5$  and  $n = 6$  ( $m < n$ ):

```
( d  u1  u1  u1  u1  u1 )
( e  d  u2  u2  u2  u2 )
( v1 e  d  u3  u3  u3 )
( v1 v2 e  d  u4  u4 )
( v1 v2 v3 e  d  u5 )
```

where  $d$  and  $e$  denote diagonal and off-diagonal elements of  $B$ ,  $v_i$  denotes an element of the vector defining  $H(i)$ , and  $u_i$  an element of the vector defining  $G(i)$ .

### Differences from LAPACK

See *No Workspace Parameters* section.

## 3.6 GEEV

### CULA Routines

The GEEV functionality is implemented by the following CULA routines:

- Host Memory
  - `culaSgeev`
  - `culaDgeev`
  - `culaCgeev`
  - `culaZgeev`
  - `culaGeev` (C++ style, type overloaded)
- Device Memory
  - `culaDeviceSgeev`
  - `culaDeviceDgeev`
  - `culaDeviceCgeev`
  - `culaDeviceZgeev`
  - `culaDeviceGeev` (C++ style, type overloaded)

### Description

GEEV computes for an  $N$ -by- $N$  real nonsymmetric matrix  $A$ , the eigenvalues and, optionally, the left and/or right eigenvectors.

The right eigenvector  $v(j)$  of  $A$  satisfies

$$A * v(j) = \text{lambda}(j) * v(j)$$

where  $\lambda(j)$  is its eigenvalue.

The left eigenvector  $u(j)$  of  $A$  satisfies

$$u(j)^H * A = \lambda(j) * u(j)^H$$

where  $u(j)^H$  denotes the conjugate transpose of  $u(j)$ .

The computed eigenvectors are normalized to have Euclidean norm equal to 1 and largest component real.

### Parameters

- **jobvl**

- Type: char

- Direction: Input

- = 'N': left eigenvectors of  $A$  are not computed;

- = 'V': left eigenvectors of  $A$  are computed.

- **jobvr**

- Type: char

- Direction: Input

- = 'N': right eigenvectors of  $A$  are not computed;

- = 'V': right eigenvectors of  $A$  are computed.

- **n**

- Type: int

- Direction: Input

- The order of the matrix  $A$ .  $N \geq 0$ .

- **a**

- Type: S/D/C/Z Pointer

- Direction: Input/Output

- Dimension: (LDA, N)

- On entry, the  $N$ -by- $N$  matrix  $A$ .

- On exit,  $A$  has been overwritten.

- **lda**

- Type: int

- Direction: Input

- The leading dimension of the array  $A$ .  $LDA \geq \max(1, N)$ .

- **wr** (Real variants (S/D) only)

- Type: S/D Pointer

- Direction: Output

- Dimension: (N)

- **wi** (Real variants (S/D) only)

- Type: S/D Pointer

- Direction: Output
- Dimension: (N)

WR and WI contain the real and imaginary parts, respectively, of the computed eigenvalues. Complex conjugate pairs of eigenvalues appear consecutively with the eigenvalue having the positive imaginary part first.

- **w** (Complex variants (C/Z) only)

- Type: C/Z Pointer
- Direction: Output
- Dimension: (N)

W contains the computed eigenvalues.

Note: the **wi** and **wr** parameters only appear in the real (non-complex) variants of geev; in the complex variants these are bundled into one **w**.

- **vl**

- Type: S/D/C/Z Pointer
- Direction: Output
- Dimension: (LDVL, N)

If JOBVL = 'V', the left eigenvectors  $u(j)$  are stored one after another in the columns of VL, in the same order as their eigenvalues.

If JOBVL = 'N', VL is not referenced.

For real variants (S/D): If the  $j$ -th eigenvalue is real, then  $u(j) = VL(:,j)$ , the  $j$ -th column of VL. If the  $j$ -th and  $(j+1)$ -st eigenvalues form a complex conjugate pair, then  $u(j) = VL(:,j) + i*VL(:,j+1)$  and  $u(j+1) = VL(:,j) - i*VL(:,j+1)$ .

For complex variants (C/Z):  $u(j) = VL(:,j)$ , the  $j$ -th column of VL.

- **ldvl**

- Type: int
- Direction: Input

The leading dimension of the array VL. LDVL  $\geq$  1; if JOBVL = 'V', LDVL  $\geq$  N.

- **vr**

- Type: S/D/C/Z Pointer
- Direction: Output
- Dimension: (LDVR, N)

If JOBVR = 'V', the right eigenvectors  $v(j)$  are stored one after another in the columns of VR, in the same order as their eigenvalues.

If JOBVR = 'N', VR is not referenced.

If the  $j$ -th eigenvalue is real, then  $v(j) = VR(:,j)$ , the  $j$ -th column of VR. If the  $j$ -th and  $(j+1)$ -st eigenvalues form a complex conjugate pair, then  $v(j) = VR(:,j) + i*VR(:,j+1)$  and  $v(j+1) = VR(:,j) - i*VR(:,j+1)$ .

For complex variants (C/Z):  $v(j) = VR(:,j)$ , the  $j$ -th column of VR.

- **ldvr**

- Type: int
- Direction: Input

The leading dimension of the array VR. LDVR  $\geq$  1; if JOBVR = 'V', LDVR  $\geq$  N.

### Differences from LAPACK

See *No Workspace Parameters* section.

## 3.7 GEHRD

### CULA Routines

The GEHRD functionality is implemented by the following CULA routines:

- Host Memory
  - culaSgehrd
  - culaDgehrd
  - culaCgehrd
  - culaZgehrd
  - culaGehrd (C++ style, type overloaded)
- Device Memory
  - culaDeviceSgehrd
  - culaDeviceDgehrd
  - culaDeviceCgehrd
  - culaDeviceZgehrd
  - culaDeviceGehrd (C++ style, type overloaded)

### Description

GEHRD reduces a real/complex general matrix A to upper Hessenberg form H by an unitary similarity transformation:  $Q' * A * Q = H$ .

### Parameters

- **n**
  - Type: int
  - Direction: Input

The order of the matrix A. N  $\geq$  0.

- **ilo**
  - Type: int
  - Direction: Input
- **ihi**
  - Type: int

- Direction: Input

It is assumed that A is already upper triangular in rows and columns 1:ILO-1 and IHI+1:N. ILO and IHI are normally set by a previous call to GEBAL; otherwise they should be set to 1 and N respectively. See Further Details.  $1 \leq ILO \leq IHI \leq N$ , if  $N > 0$ ;  $ILO=1$  and  $IHI=0$ , if  $N=0$ .

- **a**

- Type: S/D/C/Z Pointer
- Direction: Input/Output
- Dimension: (LDA, N)

On entry, the N-by-N general matrix to be reduced.

On exit, the upper triangle and the first subdiagonal of A are overwritten with the upper Hessenberg matrix H, and the elements below the first subdiagonal, with the array TAU, represent the unitary matrix Q as a product of elementary reflectors. See Further Details.

- **lda**

- Type: int
- Direction: Input

The leading dimension of the array A.  $LDA \geq \max(1, N)$ .

- **tau**

- Type: S/D/C/Z Pointer
- Direction: Output
- Dimension: (N-1)

The scalar factors of the elementary reflectors (see Further Details). Elements 1:ILO-1 and IHI:N-1 of TAU are set to zero.

### Further Details

The matrix Q is represented as a product of (ihi-ilo) elementary reflectors

$$Q = H(ilo) H(ilo+1) \dots H(ihi-1).$$

Each H(i) has the form

$$H(i) = I - \tau * v * v'$$

where tau is a real/complex scalar, and v is a real/complex vector with  $v(1:i) = 0$ ,  $v(i+1) = 1$  and  $v(ihi+1:n) = 0$ ;  $v(i+2:ihi)$  is stored on exit in  $A(i+2:ihi, i)$ , and tau in  $TAU(i)$ .

The contents of A are illustrated by the following example, with  $n = 7$ ,  $ilo = 2$  and  $ihi = 6$ :

on entry,	on exit,
( a a a a a a a )	( a a h h h h a )
( a a a a a a a )	( a h h h h a )
( a a a a a a a )	( h h h h h h )
( a a a a a a a )	( v2 h h h h h )
( a a a a a a a )	( v2 v3 h h h h )
( a a a a a a a )	( v2 v3 v4 h h h )
( a a a a a a a )	( a )

where  $a$  denotes an element of the original matrix  $A$ ,  $h$  denotes a modified element of the upper Hessenberg matrix  $H$ , and  $v_i$  denotes an element of the vector defining  $H(i)$ .

### Differences from LAPACK

See *No Workspace Parameters* section.

## 3.8 GELQF

### CULA Routines

The GELQF functionality is implemented by the following CULA routines:

- Host Memory
  - `culaSgelqf`
  - `culaDgelqf`
  - `culaCgelqf`
  - `culaZgelqf`
  - `culaGelqf` (C++ style, type overloaded)
- Device Memory
  - `culaDeviceSgelqf`
  - `culaDeviceDgelqf`
  - `culaDeviceCgelqf`
  - `culaDeviceZgelqf`
  - `culaDeviceGelqf` (C++ style, type overloaded)

### Description

GELQF computes an LQ factorization of a real M-by-N matrix  $A$ :  $A = L * Q$ .

### Parameters

- **m**
  - Type: `int`
  - Direction: Input

The number of rows of the matrix  $A$ .  $M \geq 0$ .
- **n**
  - Type: `int`
  - Direction: Input

The number of columns of the matrix  $A$ .  $N \geq 0$ .
- **a**
  - Type: S/D/C/Z Pointer
  - Direction: Input/Output

- Dimension: (LDA, N)

On entry, the M-by-N matrix A.

On exit, the elements on and below the diagonal of the array contain the m-by-min(m,n) lower trapezoidal matrix L (L is lower triangular if  $m \leq n$ ); the elements above the diagonal, with the array TAU, represent the orthogonal/unitary matrix Q as a product of elementary reflectors (see Further Details).

- **lda**

- Type: int
- Direction: Input

The leading dimension of the array A.  $LDA \geq \max(1, M)$ .

- **tau**

- Type: S/D/C/Z Pointer
- Direction: Output
- Dimension: (min(M, N))

The scalar factors of the elementary reflectors (see Further Details).

### Further Details

The matrix Q is represented as a product of elementary reflectors

$$Q = H(k) \dots H(2) H(1), \text{ where } k = \min(m, n).$$

Each H(i) has the form

$$H(i) = I - \tau * v * v'$$

where tau is a real scalar, and v is a real vector with  $v(1:i-1) = 0$  and  $v(i) = 1$ ;  $v(i+1:n)$  is stored on exit in  $A(i, i+1:n)$ , and tau in TAU(i).

### Differences from LAPACK

See *No Workspace Parameters* section.

## 3.9 GELS

### CULA Routines

The GELS functionality is implemented by the following CULA routines:

- Host Memory
  - culaSgels
  - culaDgels
  - culaCgels
  - culaZgels
  - culaGels (C++ style, type overloaded)
- Device Memory
  - culaDeviceSgels
  - culaDeviceDgels

- culaDeviceCgels
- culaDeviceZgels
- culaDeviceGels (C++ style, type overloaded)

### Description

GELS solves overdetermined or underdetermined real linear systems involving an M-by-N matrix A, or its transpose, using a QR or LQ factorization of A. It is assumed that A has full rank.

The following options are provided:

1. If TRANS = 'N' and  $m \geq n$ : find the least squares solution of an overdetermined system, i.e., solve the least squares problem minimize  $\|B - A * X\|$ .
2. If TRANS = 'N' and  $m < n$ : find the minimum norm solution of an underdetermined system  $A * X = B$ .
3. If TRANS = 'T' and  $m \geq n$ : find the minimum norm solution of an undetermined system  $A^T * X = B$ .
4. If TRANS = 'T' and  $m < n$ : find the least squares solution of an overdetermined system, i.e., solve the least squares problem minimize  $\|B - A^T * X\|$ .

Several right hand side vectors b and solution vectors x can be handled in a single call; they are stored as the columns of the M-by-NRHS right hand side matrix B and the N-by-NRHS solution matrix X.

### Parameters

- **trans**

- Type: char
- Direction: Input
- = 'N': the linear system involves A;
- = 'T': the linear system involves  $A^T$ .

- **m**

- Type: int
- Direction: Input
- The number of rows of the matrix A.  $M \geq 0$ .

- **n**

- Type: int
- Direction: Input
- The number of columns of the matrix A.  $N \geq 0$ .

- **nrhs**

- Type: int
- Direction: Input
- The number of right hand sides, i.e., the number of columns of the matrices B and X.  $NRHS \geq 0$ .

- **a**

- Type: S/D/C/Z Pointer
- Direction: Input/Output

- Dimension: (LDA, N)

On entry, the M-by-N matrix A.

On exit, if  $M \geq N$ , A is overwritten by details of its QR factorization as returned by *GEQRF*;

if  $M < N$ , A is overwritten by details of its LQ factorization as returned by *GELQF*.

- **lda**

- Type: int
- Direction: Input

The leading dimension of the array A.  $LDA \geq \max(1, M)$ .

- **b**

- Type: S/D/C/Z Pointer
- Direction: Input/Output
- Dimension: (LDB, NRHS)

On entry, the matrix B of right hand side vectors, stored columnwise; B is M-by-NRHS if TRANS = 'N', or N-by-NRHS if TRANS = 'T'.

On exit, if *culaNoError* is returned, B is overwritten by the solution vectors, stored columnwise:

if TRANS = 'N' and  $m \geq n$ , rows 1 to n of B contain the least squares solution vectors; the residual sum of squares for the solution in each column is given by the sum of squares of elements N+1 to M in that column;

if TRANS = 'N' and  $m < n$ , rows 1 to N of B contain the minimum norm solution vectors;

if TRANS = 'T' and  $m \geq n$ , rows 1 to M of B contain the minimum norm solution vectors;

if TRANS = 'T' and  $m < n$ , rows 1 to M of B contain the least squares solution vectors; the residual sum of squares for the solution in each column is given by the sum of squares of elements M+1 to N in that column.

- **ldb**

- Type: int
- Direction: Input

The leading dimension of the array B.  $LDB \geq \max(1, M, N)$ .

### Differences from LAPACK

See *No Workspace Parameters* section.

## 3.10 GEQLF

### CULA Routines

The GEQLF functionality is implemented by the following CULA routines:

- Host Memory
  - *culaSgeqlf*
  - *culaDgeqlf*
  - *culaCgeqlf*

- culaZgeqlf
- culaGeqlf (C++ style, type overloaded)
- Device Memory
  - culaDeviceSgeqlf
  - culaDeviceDgeqlf
  - culaDeviceCgeqlf
  - culaDeviceZgeqlf
  - culaDeviceGeqlf (C++ style, type overloaded)

### Description

GEQLF computes a QL factorization of a real/complex M-by-N matrix A:  $A = Q * L$ .

### Parameters

- **m**
  - Type: int
  - Direction: Input

The number of rows of the matrix A.  $M \geq 0$ .
- **n**
  - Type: int
  - Direction: Input

The number of columns of the matrix A.  $N \geq 0$ .
- **a**
  - Type: S/D/C/Z Pointer,
  - Direction: Input/Output
  - Dimension: (LDA, N)

On entry, the M-by-N matrix A.

On exit, if  $m \geq n$ , the lower triangle of the subarray  $A(m-n+1:m, 1:n)$  contains the N-by-N lower triangular matrix L; if  $m \leq n$ , the elements on and below the (n-m)-th superdiagonal contain the M-by-N lower trapezoidal matrix L; the remaining elements, with the array TAU, represent the orthogonal/unitary matrix Q as a product of elementary reflectors (see Further Details).
- **lda**
  - Type: int
  - Direction: Input

The leading dimension of the array A.  $LDA \geq \max(1, M)$ .
- **tau**
  - Type: S/D/C/Z Pointer,
  - Direction: Output
  - Dimension: (min(M, N))

The scalar factors of the elementary reflectors (see Further Details).

### Further Details

The matrix  $Q$  is represented as a product of elementary reflectors

$$Q = H(k) \dots H(2) H(1), \text{ where } k = \min(m,n).$$

Each  $H(i)$  has the form

$$H(i) = I - \tau * v * v'$$

where  $\tau$  is a real/complex scalar, and  $v$  is a real/complex vector with  $v(m-k+i+1:m) = 0$  and  $v(m-k+i) = 1$ ;  $v(1:m-k+i-1)$  is stored on exit in  $A(1:m-k+i-1, n-k+i)$ , and  $\tau$  in  $TAU(i)$ .

### Differences from LAPACK

See *No Workspace Parameters* section.

## 3.11 GEQRF

### CULA Routines

The GEQRF functionality is implemented by the following CULA routines:

- Host Memory
  - `culaSgeqrf`
  - `culaDgeqrf`
  - `culaCgeqrf`
  - `culaZgeqrf`
  - `culaGeqrf` (C++ style, type overloaded)
- Device Memory
  - `culaDeviceSgeqrf`
  - `culaDeviceDgeqrf`
  - `culaDeviceCgeqrf`
  - `culaDeviceZgeqrf`
  - `culaDeviceGeqrf` (C++ style, type overloaded)

### Description

GEQRF computes a QR factorization of a real  $M$ -by- $N$  matrix  $A$ :  $A = Q * R$ .

### Parameters

- **m**
  - Type: `int`
  - Direction: Input

The number of rows of the matrix  $A$ .  $M \geq 0$ .
- **n**
  - Type: `int`
  - Direction: Input

The number of columns of the matrix  $A$ .  $N \geq 0$ .

- **a**

- Type: S/D/C/Z Pointer
- Direction: Input/Output
- Dimension: (LDA, N)

On entry, the M-by-N matrix A.

On exit, the elements on and above the diagonal of the array contain the min(M,N)-by-N upper trapezoidal matrix R (R is upper triangular if  $m \geq n$ ); the elements below the diagonal, with the array TAU, represent the orthogonal/unitary matrix Q as a product of min(m,n) elementary reflectors (see Further Details).

- **lda**

- Type: int
- Direction: Input

The leading dimension of the array A.  $LDA \geq \max(1, M)$ .

- **tau**

- Type: S/D/C/Z Pointer
- Direction: Output
- Dimension: (min(M, N))

The scalar factors of the elementary reflectors (see Further Details).

### Further Details

The matrix Q is represented as a product of elementary reflectors

$$Q = H(1) H(2) \dots H(k), \text{ where } k = \min(m, n).$$

Each H(i) has the form

$$H(i) = I - \tau * v * v'$$

where tau is a real scalar, and v is a real vector with  $v(1:i-1) = 0$  and  $v(i) = 1$ ;  $v(i+1:m)$  is stored on exit in  $A(i+1:m, i)$ , and tau in TAU(i).

### Differences from LAPACK

See *No Workspace Parameters* section.

## 3.12 GEQRS

### CULA Routines

The GEQRS functionality is implemented by the following CULA routines:

- Host Memory
  - `culaSgeqrs`
  - `culadgeqrs`
  - `culacgeqrs`
  - `culazgeqrs`
  - `culaGeqrs` (C++ style, type overloaded)

- Device Memory
  - culaDeviceSgeqrs
  - culaDeviceDgeqrs
  - culaDeviceCgeqrs
  - culaDeviceZgeqrs
  - culaDeviceGeqrs (C++ style, type overloaded)

### Description

Solve the least squares problem

$$\min \| A * X - B \|$$

using the QR factorization

$$A = Q * R$$

computed by *GEQRF*.

### Parameters

- **m**

- Type: int
- Direction: Input

The number of rows of the matrix A.  $M \geq 0$ .

- **n**

- Type: int
- Direction: Input

The number of columns of the matrix A.  $M \geq N \geq 0$ .

- **nrhs**

- Type: int
- Direction: Input

The number of columns of B.  $NRHS \geq 0$ .

- **a**

- Type: S/D/C/Z Pointer,
- Direction: Input
- Dimension: (LDA, N)

Details of the QR factorization of the original matrix A as returned by *GEQRF*.

- **lda**

- Type: int
- Direction: Input

The leading dimension of the array A.  $LDA \geq M$ .

- **tau**

- Type: S/D/C/Z Pointer,

- Direction: Input
- Dimension: (N)

Details of the orthogonal matrix Q.

- **b**

- Type: S/D/C/Z Pointer,
- Direction: Input/Output
- Dimension: (LDB, NRHS)

On entry, the M-by-NRHS right hand side matrix B.

On exit, the N-by-NRHS solution matrix X.

- **ldb**

- Type: int
- Direction: Input

The leading dimension of the array B. LDB >= M.

### Differences from LAPACK

See *No Workspace Parameters* section.

## 3.13 GERQF

### CULA Routines

The GERQF functionality is implemented by the following CULA routines:

- Host Memory
  - culaSgerqf
  - culaDgerqf
  - culaCgerqf
  - culaZgerqf
  - culaGerqf (C++ style, type overloaded)
- Device Memory
  - culaDeviceSgerqf
  - culaDeviceDgerqf
  - culaDeviceCgerqf
  - culaDeviceZgerqf
  - culaDeviceGerqf (C++ style, type overloaded)

### Description

GERQF computes an RQ factorization of a real M-by-N matrix A:  $A = R * Q$ .

### Parameters

- **m**

- Type: int
- Direction: Input

The number of rows of the matrix A.  $M \geq 0$ .

- **n**

- Type: int
- Direction: Input

The number of columns of the matrix A.  $N \geq 0$ .

- **a**

- Type: S/D/C/Z Pointer
- Direction: Input/Output
- Dimension: (LDA, N)

On entry, the M-by-N matrix A.

On exit, if  $m \leq n$ , the upper triangle of the subarray  $A(1:m, n-m+1:n)$  contains the M-by-M upper triangular matrix R; if  $m > n$ , the elements on and above the  $(m-n)$ -th subdiagonal contain the M-by-N upper trapezoidal matrix R; the remaining elements, with the array TAU, represent the orthogonal/unitary matrix Q as a product of  $\min(m, n)$  elementary reflectors (see Further Details).

- **lda**

- Type: int
- Direction: Input

The leading dimension of the array A.  $LDA \geq \max(1, M)$ .

- **tau**

- Type: S/D/C/Z Pointer
- Direction: Output
- Dimension: ( $\min(M, N)$ )

The scalar factors of the elementary reflectors (see Further Details).

### Further Details

The matrix Q is represented as a product of elementary reflectors

$$Q = H(1) H(2) \dots H(k), \text{ where } k = \min(m, n).$$

Each  $H(i)$  has the form

$$H(i) = I - \tau * v * v'$$

where  $\tau$  is a real scalar, and  $v$  is a real vector with  $v(n-k+i+1:n) = 0$  and  $v(n-k+i) = 1$ ;  $v(1:n-k+i-1)$  is stored on exit in  $A(m-k+i, 1:n-k+i-1)$ , and  $\tau$  in  $TAU(i)$ .

### Differences from LAPACK

See *No Workspace Parameters* section.

## 3.14 GESV

The GESV functionality is implemented by the following CULA routines:

- Host Memory
  - `culaSgesv`
  - `culaDgesv`
  - `culaCgesv`
  - `culaZgesv`
  - `culaGesv` (C++ style, type overloaded)
- Device Memory
  - `culaDeviceSgesv`
  - `culaDeviceDgesv`
  - `culaDeviceCgesv`
  - `culaDeviceZgesv`
  - `culaDeviceGesv` (C++ style, type overloaded)

### Description

GESV computes the solution to a real system of linear equations

$$A * X = B,$$

where A is an N-by-N matrix and X and B are N-by-NRHS matrices.

The LU decomposition with partial pivoting and row interchanges is used to factor A as

$$A = P * L * U,$$

where P is a permutation matrix, L is unit lower triangular, and U is upper triangular. The factored form of A is then used to solve the system of equations  $A * X = B$ .

### Parameters

- **n**
  - Type: `int`
  - Direction: Input

The number of linear equations, i.e., the order of the matrix A.  $N \geq 0$ .
- **nrhs**
  - Type: `int`
  - Direction: Input

The number of right hand sides, i.e., the number of columns of the matrix B.  $NRHS \geq 0$ .
- **a**
  - Type: S/D/C/Z Pointer
  - Direction: Input/Output

- Dimension: (LDA, N)

On entry, the N-by-N coefficient matrix A.

On exit, the factors L and U from the factorization  $A = P*L*U$ ; the unit diagonal elements of L are not stored.

- **lda**

- Type: int
- Direction: Input

The leading dimension of the array A.  $LDA \geq \max(1, N)$ .

- **ipiv**

- Type: int Pointer
- Direction: Output
- Dimension: (N)

The pivot indices that define the permutation matrix P; row i of the matrix was interchanged with row IPIV(i).

- **b**

- Type: S/D/C/Z Pointer
- Direction: Input/Output
- Dimension: (LDB, NRHS)

On entry, the N-by-NRHS matrix of right hand side matrix B.

On exit, if culaNoError is returned, the N-by-NRHS solution matrix X.

- **ldb**

- Type: int
- Direction: Input

The leading dimension of the array B.  $LDB \geq \max(1, N)$ .

### Further Details

See *Pivot Arrays* section.

## 3.15 GESV (Iteratively Refined)

The GESV (Iteratively Refined) functionality is implemented by the following CULA routines:

- Host Memory
  - culaDsgesv
  - culaZcgesv
  - culaGesv (C++ style, type overloaded)
- Device Memory
  - culaDeviceDsgesv
  - culaDeviceZcgesv

– `culaDeviceGesv` (C++ style, type overloaded)

### Description

GESV computes the solution to a real/complex system of linear equations

$$A * X = B,$$

where A is an N-by-N matrix and X and B are N-by-NRHS matrices.

GESV first attempts to factorize the matrix in single-precision and use this factorization within an iterative refinement procedure to produce a solution with double-precision normwise backward error quality (see below). If the approach fails the method switches to a double-precision factorization and solve.

The iterative refinement process is stopped if

$$\text{ITER} > \text{ITERMAX}$$

or for all the RHS we have:

$$\text{RNRM} < \text{SQRT}(N) * \text{XNRM} * \text{ANRM} * \text{EPS} * \text{BWDMAX}$$

where

- ITER is the number of the current iteration in the iterative refinement process
- RNRM is the infinity-norm of the residual
- XNRM is the infinity-norm of the solution
- ANRM is the infinity-operator-norm of the matrix A
- EPS is the machine epsilon for double precision

The value ITERMAX and BWDMAX are fixed to 30 and 1.0D+00 respectively.

### Parameters

- **n**

- Type: `int`
- Direction: Input

The number of linear equations, i.e., the order of the matrix A.  $N \geq 0$ .

- **nrhs**

- Type: `int`
- Direction: Input

The number of right hand sides, i.e., the number of columns of the matrix B.  $\text{NRHS} \geq 0$ .

- **a**

- Type: `D/Z Pointer`
- Direction: Input or Input/Output
- Dimension: `(LDA, N)`

On entry, the N-by-N coefficient matrix A.

On exit, if iterative refinement has been successfully used (`culaNoError` is returned and `iter > 0`, see description below), then A is unchanged, if double precision factorization has been used (`culaNoError` is returned and `iter < 0`, see description below), then the array A contains the factors L and U from the factorization  $A = P * L * U$ ; the unit diagonal elements of L are not stored.

- **lda**

- Type: int
- Direction: Input

The leading dimension of the array A.  $LDA \geq \max(1, N)$ .

- **ipiv**

- Type: int Pointer
- Direction: Output
- Dimension: (N)

The pivot indices that define the permutation matrix P; row i of the matrix was interchanged with row IPIV(i). Corresponds either to the single precision factorization (if culaNoError is returned and iter > 0) or the double precision factorization (if culaNoError is returned and iter < 0).

- **b**

- Type: D/Z Pointer
- Direction: Input/Output
- Dimension: (LDB, NRHS)

The N-by-NRHS right hand side matrix B.

- **ldb**

- Type: int
- Direction: Input

The leading dimension of the array B.  $LDB \geq \max(1, N)$ .

- **x**

- Type: D/Z Pointer
- Direction: Input/Output
- Dimension: (LDX, NRHS)

If culaNoError is returned, the N-by-NRHS solution matrix X.

- **ldx**

- Type: int
- Direction: Input

The leading dimension of the array X.  $LDX \geq \max(1, N)$ .

- **iter**

- Type: int Pointer
- Direction: Output
- Dimension: (1)

> 0: iterative refinement has been successfully used. Returns the number of iterations

< 0: iterative refinement has failed, double-precision factorization has been performed

Value	Operation
-1	the routine fell back to full precision for implementation- or machine-specific reasons
-2	narrowing the precision induced an overflow, the routine fell back to full precision
-3	failure of single precision GETRF
-31	stop the iterative refinement after the 30th iterations

### Differences from LAPACK

See *No Workspace Parameters* section. See *Pivot Arrays* section.

## 3.16 GESVD

### CULA Routines

The GESVD functionality is implemented by the following CULA routines:

- Host Memory
  - `culaSgesvd`
  - `culaDgesvd`
  - `culaCgesvd`
  - `culaZgesvd`
  - `culaGesvd` (C++ style, type overloaded)
- Device Memory
  - `culaDeviceSgesvd`
  - `culaDeviceDgesvd`
  - `culaDeviceCgesvd`
  - `culaDeviceZgesvd`
  - `culaDeviceGesvd` (C++ style, type overloaded)

### Description

GESVD computes the singular value decomposition (SVD) of a real M-by-N matrix A, optionally computing the left and/or right singular vectors. The SVD is written

$$A = U * \text{SIGMA} * \text{transpose}(V)$$

where SIGMA is an M-by-N matrix which is zero except for its min(m,n) diagonal elements, U is an M-by-M orthogonal/unitary matrix, and V is an N-by-N orthogonal/unitary matrix. The diagonal elements of SIGMA are the singular values of A; they are real and non-negative, and are returned in descending order. The first min(m,n) columns of U and V are the left and right singular vectors of A.

Note that the routine returns  $V^T$ , not V. This  $T$  output of GESVD is notable because other implementations, such as Matlab, return the non-transposed version via syntax like  $[U S V] = \text{svd}(A)$ ; The V matrix then needs to be transposed to reconstruct the original matrix, such as  $U * S * V'$ . LAPACK avoids this by pre-transposing this output, but for those working with both LAPACK and Matlab code, this is a common pitfall.

### Parameters

- **jobu**
  - Type: char

- Direction: Input

Specifies options for computing all or part of the matrix U:

- = 'A': all M columns of U are returned in array U;
- = 'S': the first min(m,n) columns of U (the left singular vectors) are returned in the array U;
- = 'O': the first min(m,n) columns of U (the left singular vectors) are overwritten on the array A;
- = 'N': no columns of U (no left singular vectors) are computed.

- **jobvt**

- Type: char
- Direction: Input

Specifies options for computing all or part of the matrix  $V^T$  :

- = 'A': all N rows of  $V^T$  are returned in the array VT;
- = 'S': the first min(m,n) rows of  $V^T$  (the right singular vectors) are returned in the array VT;
- = 'O': the first min(m,n) rows of  $V^T$  (the right singular vectors) are overwritten on the array A;
- = 'N': no rows of  $V^T$  (no right singular vectors) are computed.

JOBVT and JOBU cannot both be 'O'.

- **m**

- Type: int
- Direction: Input

The number of rows of the input matrix A.  $M \geq 0$ .

- **n**

- Type: int
- Direction: Input

The number of columns of the input matrix A.  $N \geq 0$ .

- **a**

- Type: S/D/C/Z Pointer
- Direction: Input/Output
- Dimension: (LDA, N)

On entry, the M-by-N matrix A.

On exit,

if JOBU = 'O', A is overwritten with the first min(m,n) columns of U (the left singular vectors, stored columnwise);

if JOBVT = 'O', A is overwritten with the first min(m,n) rows of  $V^T$  (the right singular vectors, stored rowwise);

if JOBU != 'O' and JOBVT != 'O', the contents of A are destroyed.

- **lda**

- Type: int

- Direction: Input

The leading dimension of the array A.  $LDA \geq \max(1, M)$ .

- **s**

- Type: S/D Pointer
- Direction: Output
- Dimension:  $(\min(M, N))$

The singular values of A, sorted so that  $S(i) \geq S(i+1)$ .

- **u**

- Type: S/D/C/Z Pointer
- Direction: Output
- Dimension:  $(LDU, UCOL)$

$(LDU, M)$  if  $JOBU = 'A'$  or  $(LDU, \min(M, N))$  if  $JOBU = 'S'$ . If  $JOBU = 'A'$ , U contains the M-by-M orthogonal/unitary matrix U; if  $JOBU = 'S'$ , U contains the first  $\min(m, n)$  columns of U (the left singular vectors, stored columnwise); if  $JOBU = 'N'$  or  $'O'$ , U is not referenced.

- **ldu**

- Type: int
- Direction: Input

The leading dimension of the array U.  $LDU \geq 1$ ; if  $JOBU = 'S'$  or  $'A'$ ,  $LDU \geq M$ .

- **vt**

- Type: S/D/C/Z Pointer
- Direction: Output
- Dimension:  $(LDVT, N)$

If  $JOBVT = 'A'$ , VT contains the N-by-N orthogonal/unitary matrix  $V^T$ ; if  $JOBVT = 'S'$ , VT contains the first  $\min(m, n)$  rows of  $V^T$  (the right singular vectors, stored rowwise); if  $JOBVT = 'N'$  or  $'O'$ , VT is not referenced.

- **ldvt**

- Type: int
- Direction: Input

The leading dimension of the array VT.  $LDVT \geq 1$ ; if  $JOBVT = 'A'$ ,  $LDVT \geq N$ ; if  $JOBVT = 'S'$ ,  $LDVT \geq \min(M, N)$ .

### Differences from LAPACK

See *No Workspace Parameters* section.

## 3.17 GETRF

### CULA Routines

The GETRF functionality is implemented by the following CULA routines:

- Host Memory

- culaSgetrf
- culaDgetrf
- culaCgetrf
- culaZgetrf
- culaGetrf (C++ style, type overloaded)

- **Device Memory**

- culaDeviceSgetrf
- culaDeviceDgetrf
- culaDeviceCgetrf
- culaDeviceZgetrf
- culaDeviceGetrf (C++ style, type overloaded)

### Description

GETRF computes an LU factorization of a general M-by-N matrix A using partial pivoting with row interchanges.

The factorization has the form

$$A = P * L * U$$

where P is a permutation matrix, L is lower triangular with unit diagonal elements (lower trapezoidal if  $m > n$ ), and U is upper triangular (upper trapezoidal if  $m < n$ ).

### Parameters

- **m**

- Type: int
- Direction: Input

The number of rows of the matrix A.  $M \geq 0$ .

- **n**

- Type: int
- Direction: Input

The number of columns of the matrix A.  $N \geq 0$ .

- **a**

- Type: S/D/C/Z Pointer
- Direction: Input/Output
- Dimension: (LDA, N)

On entry, the M-by-N matrix to be factored.

On exit, the factors L and U from the factorization  $A = P*L*U$ ; the unit diagonal elements of L are not stored.

- **lda**

- Type: int
- Direction: Input

The leading dimension of the array A.  $LDA \geq \max(1, M)$ .

- **ipiv**
  - Type: int Pointer
  - Direction: Output
  - Dimension: (min(M,N))

The pivot indices; for  $1 \leq i \leq \min(M,N)$ , row  $i$  of the matrix was interchanged with row  $IPIV(i)$ .

#### Further Details

See *Pivot Arrays* section.

## 3.18 GETRI

### CULA Routines

The GETRI functionality is implemented by the following CULA routines:

- Host Memory
  - culaSgetri
  - culaDgetri
  - culaCgetri
  - culaZgetri
  - culaGetri (C++ style, type overloaded)
- Device Memory
  - culaDeviceSgetri
  - culaDeviceDgetri
  - culaDeviceCgetri
  - culaDeviceZgetri
  - culaDeviceGetri (C++ style, type overloaded)

### Description

GETRI computes the inverse of a matrix using the LU factorization computed by *GETRF*.

This method inverts U and then computes  $\text{inv}(A)$  by solving the system  $\text{inv}(A)*L = \text{inv}(U)$  for  $\text{inv}(A)$ .

If solution to a system of linear equations, please favor the routines *GESV*, *GETRF/GETRS*, or *GELS* instead as they will provide more accurate answers in this case.

### Parameters

- **n**
  - Type: int
  - Direction: Input

The order of the matrix A.  $N \geq 0$ .
- **a**
  - Type: S/D/C/Z Pointer
  - Direction: Input/Output

- Dimension: (LDA, N)

On entry, the factors L and U from the factorization  $A = P*L*U$  as computed by *GETRF*.

On exit, if *culaNoError* is returned, the inverse of the original matrix A.

- **lda**

- Type: int
- Direction: Input

The leading dimension of the array A.  $LDA \geq \max(1, N)$ .

- **ipiv**

- Type: int Pointer
- Direction: Input
- Dimension: (N)

The pivot indices from *GETRF*; for  $1 \leq i \leq N$ , row i of the matrix was interchanged with row *IPIV*(i).

### Further Details

See *Pivot Arrays* section.

### Differences from LAPACK

See *No Workspace Parameters* section.

## 3.19 GETRS

### CULA Routines

The GETRS functionality is implemented by the following CULA routines:

- Host Memory
  - *culaSgetrs*
  - *culaDgetrs*
  - *culaCgetrs*
  - *culaZgetrs*
  - *culaGetrs* (C++ style, type overloaded)
- Device Memory
  - *culaDeviceSgetrs*
  - *culaDeviceDgetrs*
  - *culaDeviceCgetrs*
  - *culaDeviceZgetrs*
  - *culaDeviceGetrs* (C++ style, type overloaded)

### Description

GETRS solves a system of linear equations

$$A * X = B \text{ or } A' * X = B$$

with a general N-by-N matrix A using the LU factorization computed by *GETRF*.

### Parameters

- **trans**

- Type: char
- Direction: Input

Specifies the form of the system of equations: = 'N':  $A * X = B$  (No transpose)

= 'T':  $A' * X = B$  (Transpose)

= 'C':  $A' * X = B$  (Conjugate transpose = Transpose)

- **n**

- Type: int
- Direction: Input

The order of the matrix A.  $N \geq 0$ .

- **nrhs**

- Type: int
- Direction: Input

The number of right hand sides, i.e., the number of columns of the matrix B.  $NRHS \geq 0$ .

- **a**

- Type: S/D/C/Z Pointer
- Direction: Input
- Dimension: (LDA, N)

The factors L and U from the factorization  $A = P * L * U$  as computed by *GETRF*.

- **lda**

- Type: int
- Direction: Input

The leading dimension of the array A.  $LDA \geq \max(1, N)$ .

- **ipiv**

- Type: int Pointer
- Direction: Input
- Dimension: (N)

The pivot indices from *GETRF*; for  $1 \leq i \leq N$ , row i of the matrix was interchanged with row  $IPIV(i)$ .

- **b**

- Type: S/D/C/Z Pointer
- Direction: Input/Output
- Dimension: (LDB, NRHS)

On entry, the right hand side matrix B.

On exit, the solution matrix X.

- **ldb**
  - Type: int
  - Direction: Input

The leading dimension of the array B.  $LDB \geq \max(1,N)$ .

### Further Details

See *Pivot Arrays* section.

## 3.20 GGLSE

### CULA Routines

The GGLSE functionality is implemented by the following CULA routines:

- Host Memory
  - culaSgglse
  - culaDgglse
  - culaCgglse
  - culaZgglse
  - culaGglse (C++ style, type overloaded)
- Device Memory
  - culaDeviceSgglse
  - culaDeviceDgglse
  - culaDeviceCgglse
  - culaDeviceZgglse
  - culaDeviceGglse (C++ style, type overloaded)

### Description

GGLSE solves the linear equality-constrained least squares (LSE) problem:

$$\text{minimize } \|c - A*x\|_2 \text{ subject to } B*x = d$$

where A is an M-by-N matrix, B is a P-by-N matrix, c is a given M-vector, and d is a given P-vector. It is assumed that  $P \leq N \leq M+P$ , and

$$\text{rank}(B) = P \text{ and } \text{rank}(A) = N. \quad ((B))$$

These conditions ensure that the LSE problem has a unique solution, which is obtained using a generalized RQ factorization of the matrices (B, A) given by

$$B = (O \ R)*Q, \quad A = Z*T*Q.$$

### Parameters

- **m**
  - Type: int
  - Direction: Input

The number of rows of the matrix A.  $M \geq 0$ .

- **n**

- Type: int
- Direction: Input

The number of columns of the matrices A and B.  $N \geq 0$ .

- **p**

- Type: int
- Direction: Input

The number of rows of the matrix B.  $0 \leq P \leq N \leq M+P$ .

- **a**

- Type: S/D/C/Z Pointer
- Direction: Input/Output
- Dimension: (LDA, N)

On entry, the M-by-N matrix A.

On exit, the elements on and above the diagonal of the array contain the min(M,N)-by-N upper trapezoidal matrix T.

- **lda**

- Type: int
- Direction: Input

The leading dimension of the array A.  $LDA \geq \max(1, M)$ .

- **b**

- Type: S/D/C/Z Pointer
- Direction: Input/Output
- Dimension: (LDB, N)

On entry, the P-by-N matrix B.

On exit, the upper triangle of the subarray B(1:P, N-P+1:N) contains the P-by-P upper triangular matrix R.

- **ldb**

- Type: int
- Direction: Input

The leading dimension of the array B.  $LDB \geq \max(1, P)$ .

- **c**

- Type: S/D/C/Z Pointer
- Direction: Input/Output
- Dimension: (M)

On entry, C contains the right hand side vector for the least squares part of the LSE problem.

On exit, the residual sum of squares for the solution is given by the sum of squares of elements N-P+1 to M of vector C.

- **d**

- Type: S/D/C/Z Pointer
- Direction: Input/Output
- Dimension: (P)

On entry, D contains the right hand side vector for the constrained equation.

On exit, D is destroyed.

- **x**

- Type: S/D/C/Z Pointer
- Direction: Output
- Dimension: (N)

On exit, X is the solution of the LSE problem.

### Differences from LAPACK

See *No Workspace Parameters* section.

## 3.21 GGRQF

### CULA Routines

The GGRQF functionality is implemented by the following CULA routines:

- Host Memory
  - culaSggrqf
  - culaDggrqf
  - culaCggrqf
  - culaZggrqf
  - culaGgrqf (C++ style, type overloaded)
- Device Memory
  - culaDeviceSggrqf
  - culaDeviceDggrqf
  - culaDeviceCggrqf
  - culaDeviceZggrqf
  - culaDeviceGgrqf (C++ style, type overloaded)

### Description

GGRQF computes a generalized RQ factorization of an M-by-N matrix A and a P-by-N matrix B:

$$A = R*Q, B = Z*T*Q,$$

where Q is an N-by-N orthogonal/unitary matrix, Z is a P-by-P orthogonal/unitary matrix, and R and T assume one of the forms:

if  $M \leq N$ ,  $R = \begin{pmatrix} 0 & R12 \end{pmatrix} M$ , or if  $M > N$ ,  $R = \begin{pmatrix} R11 \\ & R21 \end{pmatrix} M-N$ ,  $N-M$   $M \begin{pmatrix} R21 \end{pmatrix} N$   $N$

where R12 or R21 is upper triangular, and

if  $P \geq N$ ,  $T = (T_{11}) N$ , or if  $P < N$ ,  $T = (T_{11} T_{12}) P$ ,  $(0) P-N P N-P N$

where  $T_{11}$  is upper triangular.

In particular, if  $B$  is square and nonsingular, the GRQ factorization of  $A$  and  $B$  implicitly gives the RQ factorization of  $A \cdot \text{inv}(B)$ :

$$A \cdot \text{inv}(B) = (R \cdot \text{inv}(T)) \cdot Z'$$

where  $\text{inv}(B)$  denotes the inverse of the matrix  $B$ , and  $Z'$  denotes the transpose of the matrix  $Z$ .

### Parameters

- **m**

- Type: int
- Direction: Input

The number of rows of the matrix  $A$ .  $M \geq 0$ .

- **p**

- Type: int
- Direction: Input

The number of rows of the matrix  $B$ .  $P \geq 0$ .

- **n**

- Type: int
- Direction: Input

The number of columns of the matrices  $A$  and  $B$ .  $N \geq 0$ .

- **a**

- Type: S/D/C/Z Pointer
- Direction: Input/Output
- Dimension: (LDA, N)

On entry, the  $M$ -by- $N$  matrix  $A$ .

On exit, if  $M \leq N$ , the upper triangle of the subarray  $A(1:M, N-M+1:N)$  contains the  $M$ -by- $M$  upper triangular matrix  $R$ ; if  $M > N$ , the elements on and above the  $(M-N)$ -th subdiagonal contain the  $M$ -by- $N$  upper trapezoidal matrix  $R$ ; the remaining elements, with the array  $\text{TAUA}$ , represent the orthogonal/unitary matrix  $Q$  as a product of elementary reflectors (see Further Details).

- **lda**

- Type: int
- Direction: Input

The leading dimension of the array  $A$ .  $LDA \geq \max(1, M)$ .

- **taua**

- Type: S/D/C/Z Pointer
- Direction: Output
- Dimension: (min(M, N))

The scalar factors of the elementary reflectors which represent the orthogonal/unitary matrix  $Q$  (see Further Details).

- **b**

- Type: S/D/C/Z Pointer
- Direction: Input/Output
- Dimension: (LDB, N)

On entry, the P-by-N matrix B.

On exit, the elements on and above the diagonal of the array contain the min(P,N)-by-N upper trapezoidal matrix T (T is upper triangular if  $P \geq N$ ); the elements below the diagonal, with the array TAUB, represent the orthogonal/unitary matrix Z as a product of elementary reflectors (see Further Details).

- **ldb**

- Type: int
- Direction: Input

The leading dimension of the array B.  $LDB \geq \max(1, P)$ .

- **taub**

- Type: S/D/C/Z Pointer
- Direction: Output
- Dimension: (min(P, N))

The scalar factors of the elementary reflectors which represent the orthogonal/unitary matrix Z (see Further Details).

### Further Details

The matrix Q is represented as a product of elementary reflectors

$$Q = H(1) H(2) \dots H(k), \text{ where } k = \min(m, n).$$

Each H(i) has the form

$$H(i) = I - \text{taua} * v * v'$$

where taua is a real scalar, and v is a real vector with  $v(n-k+i+1:n) = 0$  and  $v(n-k+i) = 1$ ;  $v(1:n-k+i-1)$  is stored on exit in  $A(m-k+i, 1:n-k+i-1)$ , and taua in TAUA(i). To form Q explicitly, use LAPACK subroutine ORGRQ. To use Q to update another matrix, use LAPACK subroutine *ORMRQ/UNMRQ*.

The matrix Z is represented as a product of elementary reflectors

$$Z = H(1) H(2) \dots H(k), \text{ where } k = \min(p, n).$$

Each H(i) has the form

$$H(i) = I - \text{taub} * v * v'$$

where taub is a real scalar, and v is a real vector with  $v(1:i-1) = 0$  and  $v(i) = 1$ ;  $v(i+1:p)$  is stored on exit in  $B(i+1:p, i)$ , and taub in TAUB(i). To form Z explicitly, use LAPACK subroutine *ORGQR/UNGQR*. To use Z to update another matrix, use LAPACK subroutine *ORMQR/UNMQR*.

### Differences from LAPACK

See *No Workspace Parameters* section.

## 3.22 ORGBR/UNGBR

### CULA Routines

The ORGBR/UNGBR functionality is implemented by the following CULA routines:

- Host Memory
  - `culaSorgbr`
  - `culaDorgbr`
  - `culaCungbr`
  - `culaZungbr`
  - `culaOrgbr` (C++ style, type overloaded)
  - `culaUngbr` (C++ style, type overloaded)
- Device Memory
  - `culaDeviceSorgbr`
  - `culaDeviceDorgbr`
  - `culaDeviceCungbr`
  - `culaDeviceZungbr`
  - `culaDeviceOrgbr` (C++ style, type overloaded)
  - `culaDeviceUngbr` (C++ style, type overloaded)

### Description

ORGBR/UNGBR generates one of the real/complex orthogonal/unitary matrices  $Q$  or  $P^T$  determined by *GEBRD* when reducing a real matrix  $A$  to bidiagonal form:  $A = Q * B * P^T$ .  $Q$  and  $P^T$  are defined as products of elementary reflectors  $H(i)$  or  $G(i)$  respectively.

If `VECT = 'Q'`,  $A$  is assumed to have been an  $M$ -by- $K$  matrix, and  $Q$  is of order  $M$ : if  $m \geq k$ ,  $Q = H(1) H(2) \dots H(k)$  and ORGBR returns the first  $n$  columns of  $Q$ , where  $m \geq n \geq k$ ; if  $m < k$ ,  $Q = H(1) H(2) \dots H(m-1)$  and ORGBR returns  $Q$  as an  $M$ -by- $M$  matrix.

If `VECT = 'P'`,  $A$  is assumed to have been a  $K$ -by- $N$  matrix, and  $P^T$  is of order  $N$ : if  $k < n$ ,  $P^T = G(k) \dots G(2) G(1)$  and ORGBR returns the first  $m$  rows of  $P^T$ , where  $n \geq m \geq k$ ; if  $k \geq n$ ,  $P^T = G(n-1) \dots G(2) G(1)$  and ORGBR returns  $P^T$  as an  $N$ -by- $N$  matrix.

### Parameters

- `vect`
  - Type: `char`
  - Direction: Input

Specifies whether the matrix  $Q$  or the matrix  $P^T$  is required, as defined in the transformation applied by *GEBRD*:

- = 'Q': generate  $Q$ ;
- = 'P': generate  $P^T$ .

- `m`
  - Type: `int`

- Direction: Input

The number of rows of the matrix Q or P<sup>T</sup> to be returned.  $M \geq 0$ .

- **n**

- Type: int
- Direction: Input

The number of columns of the matrix Q or P<sup>T</sup> to be returned.  $N \geq 0$ . If VECT = 'Q',  $M \geq N \geq \min(M,K)$ ; if VECT = 'P',  $N \geq M \geq \min(N,K)$ .

- **k**

- Type: int
- Direction: Input

If VECT = 'Q', the number of columns in the original M-by-K matrix reduced by *GEBRD*. If VECT = 'P', the number of rows in the original K-by-N matrix reduced by *GEBRD*.  $K \geq 0$ .

- **a**

- Type: S/D/C/Z Pointer
- Direction: Input/Output
- Dimension: (LDA, N)

On entry, the vectors which define the elementary reflectors, as returned by *GEBRD*.

On exit, the M-by-N matrix Q or P<sup>T</sup>.

- **lda**

- Type: int
- Direction: Input

The leading dimension of the array A.  $LDA \geq \max(1,M)$ .

- **tau**

- Type: S/D/C/Z Pointer, dimension
- Direction: Input

( $\min(M,K)$ ) if VECT = 'Q' ( $\min(N,K)$ ) if VECT = 'P'

TAU(i) must contain the scalar factor of the elementary reflector H(i) or G(i), which determines Q or P<sup>T</sup>, as returned by *GEBRD* in its array argument TAUQ or TAUP.

### Differences from LAPACK

See *No Workspace Parameters* section.

## 3.23 ORGHR/UNGHR

### CULA Routines

The ORGHR/UNGHR functionality is implemented by the following CULA routines:

- Host Memory
  - `culaSorghr`

- culaDorghr
- culaCunghr
- culaZunghr
- culaOrghr (C++ style, type overloaded)
- culaUnghr (C++ style, type overloaded)

- **Device Memory**

- culaDeviceSorghr
- culaDeviceDorghr
- culaDeviceCunghr
- culaDeviceZunghr
- culaDeviceOrghr (C++ style, type overloaded)
- culaDeviceUnghr (C++ style, type overloaded)

### Description

ORGHR/UNGHR generate a real/complex orthogonal/unitary matrix Q which is defined as the product of IHI-ILO elementary reflectors of order N, as returned by *GEHRD*:

$$Q = H(i\text{lo}) H(i\text{lo}+1) \dots H(i\text{hi}-1).$$

### Parameters

- **n**

- Type: int
- Direction: Input

The order of the matrix Q.  $N \geq 0$ .

- **ilo**

- Type: int
- Direction: Input

- **ihi**

- Type: int
- Direction: Input

ILO and IHI must have the same values as in the previous call of *GEHRD*. Q is equal to the unit matrix except in the submatrix  $Q(i\text{lo}+1:i\text{hi}, i\text{lo}+1:i\text{hi})$ .  $1 \leq ILO \leq IHI \leq N$ , if  $N > 0$ ;  $ILO=1$  and  $IHI=0$ , if  $N=0$ .

- **a**

- Type: S/D/C/Z Pointer
- Direction: Input/Output
- Dimension: (LDA, N)

On entry, the vectors which define the elementary reflectors, as returned by *GEHRD*.

On exit, the N-by-N unitary matrix Q.

- **lda**

- Type: int
- Direction: Input

The leading dimension of the array A. LDA  $\geq \max(1,N)$ .

- **tau**

- Type: S/D/C/Z Pointer
- Direction: Input
- Dimension: (N-1)

TAU(i) must contain the scalar factor of the elementary reflector H(i), as returned by *GEHRD*.

### Differences from LAPACK

See *No Workspace Parameters* section.

## 3.24 ORGLQ/UNGLQ

### CULA Routines

The ORGLQ/UNGLQ functionality is implemented by the following CULA routines:

- Host Memory
  - culaSorglq
  - culaDorglq
  - culaCunglq
  - culaZunglq
  - culaOrglq (C++ style, type overloaded)
  - culaUnglq (C++ style, type overloaded)
- Device Memory
  - culaDeviceSorglq
  - culaDeviceDorglq
  - culaDeviceCunglq
  - culaDeviceZunglq
  - culaDeviceOrglq (C++ style, type overloaded)
  - culaDeviceUnglq (C++ style, type overloaded)

### Description

ORGLQ/UNGLQ generates an M-by-N real matrix Q with orthonormal rows, which is defined as the first M rows of a product of K elementary reflectors of order N

$$Q = H(k) \dots H(2) H(1)$$

as returned by *GELQF*.

### Parameters

- **m**
  - Type: int

- Direction: Input

The number of rows of the matrix Q.  $M \geq 0$ .

- **n**

- Type: int

- Direction: Input

The number of columns of the matrix Q.  $N \geq M$ .

- **k**

- Type: int

- Direction: Input

The number of elementary reflectors whose product defines the matrix Q.  $M \geq K \geq 0$ .

- **a**

- Type: S/D/C/Z Pointer

- Direction: Input/Output

- Dimension: (LDA, N)

On entry, the i-th row must contain the vector which defines the elementary reflector H(i), for  $i = 1, 2, \dots, k$ , as returned by *GELQF* in the first k rows of its array argument A.

On exit, the M-by-N matrix Q.

- **lda**

- Type: int

- Direction: Input

The first dimension of the array A.  $LDA \geq \max(1, M)$ .

- **tau**

- Type: S/D/C/Z Pointer

- Direction: Input

- Dimension: (K)

TAU(i) must contain the scalar factor of the elementary reflector H(i), as returned by *GELQF*.

### Differences from LAPACK

See *No Workspace Parameters* section.

## 3.25 ORGQL/UNGQL

### CULA Routines

The ORGQL/UNGQL functionality is implemented by the following CULA routines:

- Host Memory

- `culaSorgql`

- `culaDorgql`

- `culaCungql`

- culaZungql
- culaOrgql (C++ style, type overloaded)
- culaUngql (C++ style, type overloaded)

- **Device Memory**

- culaDeviceSorgql
- culaDeviceDorgql
- culaDeviceCungql
- culaDeviceZungql
- culaDeviceOrgql (C++ style, type overloaded)
- culaDeviceUngql (C++ style, type overloaded)

### Description

ORGQL/UNGQL generates an M-by-N real/complex matrix Q with orthonormal columns, which is defined as the last N columns of a product of K elementary reflectors of order M

$$Q = H(k) \dots H(2) H(1)$$

as returned by *GELQF*.

### Parameters

- **m**

- Type: int
- Direction: Input

The number of rows of the matrix Q.  $M \geq 0$ .

- **n**

- Type: int
- Direction: Input

The number of columns of the matrix Q.  $M \geq N \geq 0$ .

- **k**

- Type: int
- Direction: Input

The number of elementary reflectors whose product defines the matrix Q.  $N \geq K \geq 0$ .

- **a**

- Type: S/D/C/Z Pointer,
- Direction: Input/Output
- Dimension: (LDA, N)

On entry, the (n-k+i)-th column must contain the vector which defines the elementary reflector H(i), for  $i = 1, 2, \dots, k$ , as returned by *GELQF* in the last k columns of its array argument A.

On exit, the M-by-N matrix Q.

- **lda**

- Type: int

- Direction: Input

The first dimension of the array A.  $LDA \geq \max(1, M)$ .

- **tau**

- Type: S/D/C/Z Pointer,
- Direction: Input
- Dimension: (K)

TAU(i) must contain the scalar factor of the elementary reflector H(i), as returned by *GELQF*.

### Differences from LAPACK

See *No Workspace Parameters* section.

## 3.26 ORGQR/UNGQR

### CULA Routines

The ORGQR/UNGQR functionality is implemented by the following CULA routines:

- Host Memory
  - culaSorgqr
  - culaDorgqr
  - culaCungqr
  - culaZungqr
  - culaOrgqr (C++ style, type overloaded)
  - culaUngqr (C++ style, type overloaded)
- Device Memory
  - culaDeviceSorgqr
  - culaDeviceDorgqr
  - culaDeviceCungqr
  - culaDeviceZungqr
  - culaDeviceOrgqr (C++ style, type overloaded)
  - culaDeviceUngqr (C++ style, type overloaded)

### Description

ORGQR/UNGQR generates an M-by-N real/complex matrix Q with orthonormal columns, which is defined as the first N columns of a product of K elementary reflectors of order M

$$Q = H(1) H(2) \dots H(k)$$

as returned by *GEQRF*.

### Parameters

- **m**
  - Type: int

- Direction: Input

The number of rows of the matrix Q.  $M \geq 0$ .

- **n**

- Type: int

- Direction: Input

The number of columns of the matrix Q.  $M \geq N \geq 0$ .

- **k**

- Type: int

- Direction: Input

The number of elementary reflectors whose product defines the matrix Q.  $N \geq K \geq 0$ .

- **a**

- Type: S/D/C/Z Pointer

- Direction: Input/Output

- Dimension: (LDA, N)

On entry, the i-th column must contain the vector which defines the elementary reflector  $H(i)$ , for  $i = 1, 2, \dots, k$ , as returned by *GEQRF* in the first k columns of its array argument A.

On exit, the M-by-N matrix Q.

- **lda**

- Type: int

- Direction: Input

The first dimension of the array A.  $LDA \geq \max(1, M)$ .

- **tau**

- Type: S/D/C/Z Pointer

- Direction: Input

- Dimension: (K)

TAU(i) must contain the scalar factor of the elementary reflector  $H(i)$ , as returned by *GEQRF*.

### Differences from LAPACK

See *No Workspace Parameters* section.

## 3.27 ORGRQ/UNGRQ

### CULA Routines

The ORGRQ/UNGRQ functionality is implemented by the following CULA routines:

- Host Memory

- `culaSorgrq`

- `culaDorgrq`

- `culaCungrq`

- culaZungrq
- culaOrgrq (C++ style, type overloaded)
- culaUngrq (C++ style, type overloaded)

- **Device Memory**

- culaDeviceSorgrq
- culaDeviceDorgrq
- culaDeviceCungrq
- culaDeviceZungrq
- culaDeviceOrgrq (C++ style, type overloaded)
- culaDeviceUngrq (C++ style, type overloaded)

### Description

ORGRQ/UNGRQ generates an M-by-N complex matrix Q with orthonormal rows, which is defined as the last M rows of a product of K elementary reflectors of order N

$$Q = H(1)' H(2)' \dots H(k)'$$

as returned by *GERQF*.

### Parameters

- **M**

- Direction: Input
- Type: int

The number of rows of the matrix Q.  $M \geq 0$ .

- **N**

- Direction: Input
- Type: int

The number of columns of the matrix Q.  $N \geq M$ .

- **K**

- Direction: Input
- Type: int

The number of elementary reflectors whose product defines the matrix Q.  $M \geq K \geq 0$ .

- **A**

- Direction: Input/Output
- Type: S/D/C/Z Pointer,
- Dimension: (LDA, N)

On entry, the (m-k+i)-th row must contain the vector which defines the elementary reflector H(i), for  $i = 1, 2, \dots, k$ , as returned by *GERQF* in the last k rows of its array argument A. On exit, the M-by-N matrix Q.

- **LDA**

- Direction: Input

- Type: int  
The first dimension of the array A. LDA  $\geq$  max(1,M).

- **TAU**

- Direction: Input
- Type: S/D/C/Z Pointer,
- Dimension: (K)

TAU(i) must contain the scalar factor of the elementary reflector H(i), as returned by *GERQF*.

### Differences from LAPACK

See *No Workspace Parameters* section.

## 3.28 ORMLQ/UNMLQ

### CULA Routines

The ORMLQ/UNMLQ functionality is implemented by the following CULA routines:

- Host Memory
  - culaSormlq
  - culaDormlq
  - culaCunmlq
  - culaZunmlq
  - culaOrmlq (C++ style, type overloaded)
  - culaUnmlq (C++ style, type overloaded)
- Device Memory
  - culaDeviceSormlq
  - culaDeviceDormlq
  - culaDeviceCunmlq
  - culaDeviceZunmlq
  - culaDeviceOrmlq (C++ style, type overloaded)
  - culaDeviceUnmlq (C++ style, type overloaded)

### Description

ORMLQ/UNMLQ overwrite the general real/complex M-by-N matrix C with

	SIDE = 'L'	SIDE = 'R'
TRANS = 'N'	$Q * C$	$C * Q$
TRANS = 'T'	$Q^T * C$	$C * Q^T$

where Q is a real/complex orthogonal/unitary matrix defined as the product of k elementary reflectors

$$Q = H(k) \dots H(2) H(1)$$

as returned by *GELQF*. Q is of order M if SIDE = 'L' and of order N if SIDE = 'R'.

### Parameters

- **side**

- Type: char

- Direction: Input

- = 'L': apply Q or  $Q^T$  from the Left;

- = 'R': apply Q or  $Q^T$  from the Right.

- **trans**

- Type: char

- Direction: Input

- = 'N': No transpose, apply Q;

- = 'T': Transpose, apply  $Q^T$ .

- **m**

- Type: int

- Direction: Input

The number of rows of the matrix C.  $M \geq 0$ .

- **n**

- Type: int

- Direction: Input

The number of columns of the matrix C.  $N \geq 0$ .

- **k**

- Type: int

- Direction: Input

The number of elementary reflectors whose product defines the matrix Q. If SIDE = 'L',  $M \geq K \geq 0$ ; if SIDE = 'R',  $N \geq K \geq 0$ .

- **a**

- Type: S/D/C/Z Pointer, dimension

- Direction: Input

(LDA,M) if SIDE = 'L', (LDA,N) if SIDE = 'R'

The i-th row must contain the vector which defines the elementary reflector  $H(i)$ , for  $i = 1, 2, \dots, k$ , as returned by *GELQF* in the first k rows of its array argument A. A is modified by the routine but restored on exit.

- **lda**

- Type: int

- Direction: Input

The leading dimension of the array A.  $LDA \geq \max(1, K)$ .

- **tau**

- Type: S/D/C/Z Pointer

- Direction: Input

- Dimension: (K)

TAU(i) must contain the scalar factor of the elementary reflector H(i), as returned by *GELQF*.

- **c**

- Type: S/D/C/Z Pointer
- Direction: Input/Output
- Dimension: (LDC, N)

On entry, the M-by-N matrix C.

On exit, C is overwritten by  $Q * C$  or  $Q^T * C$  or  $C * Q^T$  or  $C * Q$ .

- **ldc**

- Type: int
- Direction: Input

The leading dimension of the array C.  $LDC \geq \max(1, M)$ .

### Differences from LAPACK

See *No Workspace Parameters* section.

## 3.29 ORMQL/UNMQL

### CULA Routines

The ORMQL/UNMQL functionality is implemented by the following CULA routines:

- Host Memory

- culaSormql
- culaDormql
- culaCunmql
- culaZunmql
- culaOrmql (C++ style, type overloaded)
- culaUnmql (C++ style, type overloaded)

- Device Memory

- culaDeviceSormql
- culaDeviceDormql
- culaDeviceCunmql
- culaDeviceZunmql
- culaDeviceOrmql (C++ style, type overloaded)
- culaDeviceUnmql (C++ style, type overloaded)

### Description

ORMQL/UNMQL overwrites the general real/complex M-by-N matrix C with

	<b>SIDE = 'L'</b>	<b>SIDE = 'R'</b>
TRANS = 'N':	Q * C	C * Q
TRANS = 'C':	Q**H * C	C * Q**H

where Q is a real/complex orthogonal/unitary matrix defined as the product of k elementary reflectors

$$Q = H(k) \dots H(2) H(1)$$

as returned by *GELQF*. Q is of order M if SIDE = 'L' and of order N if SIDE = 'R'.

### Parameters

- **side**

- Type: char
- Direction: Input
- = 'L': apply Q or Q\*\*H from the Left;
- = 'R': apply Q or Q\*\*H from the Right.

- **trans**

- Type: char
- Direction: Input
- = 'N': No transpose, apply Q;
- = 'C': Transpose, apply Q\*\*H.

- **m**

- Type: int
- Direction: Input
- The number of rows of the matrix C.  $M \geq 0$ .

- **n**

- Type: int
- Direction: Input
- The number of columns of the matrix C.  $N \geq 0$ .

- **k**

- Type: int
- Direction: Input
- The number of elementary reflectors whose product defines the matrix Q.
- If SIDE = 'L',  $M \geq K \geq 0$ ;
- if SIDE = 'R',  $N \geq K \geq 0$ .

- **a**

- Type: S/D/C/Z Pointer,
- Direction: Input
- Dimension: (LDA, K)

The  $i$ -th column must contain the vector which defines the elementary reflector  $H(i)$ , for  $i = 1, 2, \dots, k$ , as returned by *GELQF* in the last  $k$  columns of its array argument  $A$ .  $A$  is modified by the routine but restored on exit.

- **lda**

- Type: int
- Direction: Input

The leading dimension of the array  $A$ .

If  $SIDE = 'L'$ ,  $LDA \geq \max(1, M)$ ;

if  $SIDE = 'R'$ ,  $LDA \geq \max(1, N)$ .

- **tau**

- Type: S/D/C/Z Pointer,
- Direction: Input
- Dimension: ( $K$ )

$\tau(i)$  must contain the scalar factor of the elementary reflector  $H(i)$ , as returned by *GELQF*.

- **c**

- Type: S/D/C/Z Pointer,
- Direction: Input/Output
- Dimension: ( $LDC, N$ )

On entry, the  $M$ -by- $N$  matrix  $C$ .

On exit,  $C$  is overwritten by  $Q^*C$  or  $Q^*H^*C$  or  $C^*Q^*H$  or  $C^*Q$ .

- **ldc**

- Type: int
- Direction: Input

The leading dimension of the array  $C$ .  $LDC \geq \max(1, M)$ .

### Differences from LAPACK

See *No Workspace Parameters* section.

## 3.30 ORMQR/UNMQR

### CULA Routines

The ORMQR/UNMQR functionality is implemented by the following CULA routines:

- Host Memory

- `culaSormqr`
- `culaDormqr`
- `culaCormqr`
- `culaZormqr`
- `culaOrmqr` (C++ style, type overloaded)

- culaUnmqr (C++ style, type overloaded)
- Device Memory
  - culaDeviceSormqr
  - culaDeviceDormqr
  - culaDeviceCormqr
  - culaDeviceZormqr
  - culaDeviceOrmqr (C++ style, type overloaded)
  - culaDeviceUnmqr (C++ style, type overloaded)

**Description**

ORMQR/UNMQR overwrites the general real M-by-N matrix C with

	SIDE = 'L'	SIDE = 'R'
TRANS = 'N'	$Q * C$	$C * Q$
TRANS = 'T'	$Q^T * C$	$C * Q^T$

where Q is a real/complex orthogonal/unitary matrix defined as the product of k elementary reflectors

$$Q = H(1) H(2) \dots H(k)$$

as returned by *GEQRF*. Q is of order M if SIDE = 'L' and of order N if SIDE = 'R'.

**Parameters**

- **side**
  - Type: char
  - Direction: Input
  - = 'L': apply Q or  $Q^T$  from the Left;
  - = 'R': apply Q or  $Q^T$  from the Right.
- **trans**
  - Type: char
  - Direction: Input
  - = 'N': No transpose, apply Q;
  - = 'T': Transpose, apply  $Q^T$ .
- **m**
  - Type: int
  - Direction: Input

The number of rows of the matrix C.  $M \geq 0$ .
- **n**
  - Type: int
  - Direction: Input

The number of columns of the matrix C.  $N \geq 0$ .
- **k**
  - Type: int

- Direction: Input

The number of elementary reflectors whose product defines the matrix Q. If SIDE = 'L',  $M \geq K \geq 0$ ; if SIDE = 'R',  $N \geq K \geq 0$ .

- **a**

- Type: S/D/C/Z Pointer
- Direction: Input
- Dimension: (LDA, K)

The i-th column must contain the vector which defines the elementary reflector H(i), for  $i = 1, 2, \dots, k$ , as returned by *GEQRF* in the first k columns of its array argument A. A is modified by the routine but restored on exit.

- **lda**

- Type: int
- Direction: Input

The leading dimension of the array A. If SIDE = 'L',  $LDA \geq \max(1, M)$ ; if SIDE = 'R',  $LDA \geq \max(1, N)$ .

- **tau**

- Type: S/D/C/Z Pointer
- Direction: Input
- Dimension: (K)

TAU(i) must contain the scalar factor of the elementary reflector H(i), as returned by *GEQRF*.

- **c**

- Type: S/D/C/Z Pointer
- Direction: Input/Output
- Dimension: (LDC, N)

On entry, the M-by-N matrix C.

On exit, C is overwritten by  $Q * C$  or  $Q^T * C$  or  $C * Q^T$  or  $C * Q$ .

- **ldc**

- Type: int
- Direction: Input

The leading dimension of the array C.  $LDC \geq \max(1, M)$ .

### Differences from LAPACK

See *No Workspace Parameters* section.

## 3.31 ORMRQ/UNMRQ

### CULA Routines

The ORMRQ/UNMRQ functionality is implemented by the following CULA routines:

- Host Memory

- culaSormrq
- culaDormrq
- culaCormrq
- culaZormrq
- culaOrmrq (C++ style, type overloaded)
- culaUnmrq (C++ style, type overloaded)

- **Device Memory**

- culaDeviceSormrq
- culaDeviceDormrq
- culaDeviceCormrq
- culaDeviceZormrq
- culaDeviceOrmrq (C++ style, type overloaded)
- culaDeviceUnmrq (C++ style, type overloaded)

### Description

ORMRQ/UNMRQ overwrites the general real M-by-N matrix C with

	<b>SIDE = 'L'</b>	<b>SIDE = 'R'</b>
<b>TRANS = 'N'</b>	$Q * C$	$C * Q$
<b>TRANS = 'T'</b>	$Q^T * C$	$C * Q^T$

where Q is a real/complex orthogonal/unitary matrix defined as the product of k elementary reflectors

$$Q = H(1) H(2) \dots H(k)$$

as returned by *GERQF*. Q is of order M if SIDE = 'L' and of order N if SIDE = 'R'.

### Parameters

- **side**

- Type: char
- Direction: Input
- = 'L': apply Q or  $Q^T$  from the Left;
- = 'R': apply Q or  $Q^T$  from the Right.

- **trans**

- Type: char
- Direction: Input
- = 'N': No transpose, apply Q;
- = 'T': Transpose, apply  $Q^T$ .

- **m**

- Type: int
- Direction: Input

The number of rows of the matrix C.  $M \geq 0$ .

- **n**

- Type: int
- Direction: Input

The number of columns of the matrix C.  $N \geq 0$ .

- **k**

- Type: int
- Direction: Input

The number of elementary reflectors whose product defines the matrix Q. If SIDE = 'L',  $M \geq K \geq 0$ ; if SIDE = 'R',  $N \geq K \geq 0$ .

- **a**

- Type: S/D/C/Z Pointer, dimension
- Direction: Input

(LDA,M) if SIDE = 'L', (LDA,N) if SIDE = 'R'

The i-th row must contain the vector which defines the elementary reflector H(i), for  $i = 1, 2, \dots, k$ , as returned by *GERQF* in the last k rows of its array argument A. A is modified by the routine but restored on exit.

- **lda**

- Type: int
- Direction: Input

The leading dimension of the array A.  $LDA \geq \max(1, K)$ .

- **tau**

- Type: S/D/C/Z Pointer
- Direction: Input
- Dimension: (K)

TAU(i) must contain the scalar factor of the elementary reflector H(i), as returned by *GERQF*.

- **c**

- Type: S/D/C/Z Pointer
- Direction: Input/Output
- Dimension: (LDC, N)

On entry, the M-by-N matrix C.

On exit, C is overwritten by  $Q * C$  or  $Q^T * C$  or  $C * Q^T$  or  $C * Q$ .

- **ldc**

- Type: int
- Direction: Input

The leading dimension of the array C.  $LDC \geq \max(1, M)$ .

### Differences from LAPACK

See *No Workspace Parameters* section.

## 3.32 POSV

### CULA Routines

The POSV functionality is implemented by the following CULA routines:

- Host Memory
  - `culaSposv`
  - `culaDposv`
  - `culaCposv`
  - `culaZposv`
  - `culaPosv` (C++ style, type overloaded)
- Device Memory
  - `culaDeviceSposv`
  - `culaDeviceDposv`
  - `culaDeviceCposv`
  - `culaDeviceZposv`
  - `culaDevicePosv` (C++ style, type overloaded)

### Description

POSV computes the solution to a real system of linear equations

$$A * X = B,$$

where A is an N-by-N symmetric positive definite matrix and X and B are N-by-NRHS matrices.

The Cholesky decomposition is used to factor A as

$$A = U^T * U, \text{ if UPLO} = \text{'U'}, \text{ or } A = L * L^T, \text{ if UPLO} = \text{'L'},$$

where U is an upper triangular matrix and L is a lower triangular matrix. The factored form of A is then used to solve the system of equations  $A * X = B$ .

### Parameters

- **uplo**
  - Type: `char`
  - Direction: Input
  - = 'U': Upper triangle of A is stored;
  - = 'L': Lower triangle of A is stored.

- **n**
  - Type: `int`
  - Direction: Input

The number of linear equations, i.e., the order of the matrix A.  $N \geq 0$ .

- **nrhs**
  - Type: `int`

- Direction: Input

The number of right hand sides, i.e., the number of columns of the matrix B. NRHS  $\geq 0$ .

- **a**

- Type: S/D/C/Z Pointer
- Direction: Input/Output
- Dimension: (LDA, N)

On entry, the symmetric matrix A. If UPLO = 'U', the leading N-by-N upper triangular part of A contains the upper triangular part of the matrix A, and the strictly lower triangular part of A is not referenced. If UPLO = 'L', the leading N-by-N lower triangular part of A contains the lower triangular part of the matrix A, and the strictly upper triangular part of A is not referenced.

On exit, if culaNoError is returned, the factor U or L from the Cholesky factorization  $A = U^T * U$  or  $A = L * L^T$ .

- **lda**

- Type: int
- Direction: Input

The leading dimension of the array A. LDA  $\geq \max(1, N)$ .

- **b**

- Type: S/D/C/Z Pointer
- Direction: Input/Output
- Dimension: (LDB, NRHS)

On entry, the N-by-NRHS right hand side matrix B.

On exit, if culaNoError is returned, the N-by-NRHS solution matrix X.

- **ldb**

- Type: int
- Direction: Input

The leading dimension of the array B. LDB  $\geq \max(1, N)$ .

## 3.33 POTRF

### CULA Routines

The POTRF functionality is implemented by the following CULA routines:

- Host Memory
  - culaSpotrf
  - culaDpotrf
  - culaCpotrf
  - culaZpotrf
  - culaPotrf (C++ style, type overloaded)
- Device Memory

- culaDeviceSpotrf
- culaDeviceDpotrf
- culaDeviceCpotrf
- culaDeviceZpotrf
- culaDevicePotrf (C++ style, type overloaded)

### Description

POTRF computes the Cholesky factorization of a real symmetric positive definite matrix A.

The factorization has the form

$$A = U^T * U, \text{ if UPLO = 'U', or } A = L * L^T, \text{ if UPLO = 'L',}$$

where U is an upper triangular matrix and L is lower triangular.

### Parameters

- **uplo**

- Type: char
- Direction: Input
- = 'U': Upper triangle of A is stored;
- = 'L': Lower triangle of A is stored.

- **n**

- Type: int
- Direction: Input

The order of the matrix A.  $N \geq 0$ .

- **a**

- Type: S/D/C/Z Pointer
- Direction: Input/Output
- Dimension: (LDA, N)

On entry, the symmetric matrix A. If UPLO = 'U', the leading N-by-N upper triangular part of A contains the upper triangular part of the matrix A, and the strictly lower triangular part of A is not referenced. If UPLO = 'L', the leading N-by-N lower triangular part of A contains the lower triangular part of the matrix A, and the strictly upper triangular part of A is not referenced.

On exit, if culaNoError is returned, the factor U or L from the Cholesky factorization  $A = U^T * U$  or  $A = L * L^T$ .

- **lda**

- Type: int
- Direction: Input

The leading dimension of the array A.  $LDA \geq \max(1, N)$ .

## 3.34 POTRS

### CULA Routines

The POTRS functionality is implemented by the following CULA routines:

- Host Memory
  - `culaSpotrs`
  - `culaDpotrs`
  - `culaCpotrs`
  - `culaZpotrs`
  - `culaPotrs` (C++ style, type overloaded)
- Device Memory
  - `culaDeviceSpotrs`
  - `culaDeviceDpotrs`
  - `culaDeviceCpotrs`
  - `culaDeviceZpotrs`
  - `culaDevicePotrs` (C++ style, type overloaded)

### Description

POTRS solves a system of linear equations  $A \cdot X = B$  with a symmetric positive definite matrix  $A$  using the Cholesky factorization  $A = U^T \cdot U$  or  $A = L \cdot L^T$  computed by *POTRF*.

### Parameters

- **uplo**
  - Type: `char`
  - Direction: Input

= 'U': Upper triangle of  $A$  is stored;  
= 'L': Lower triangle of  $A$  is stored.

- **n**
  - Type: `int`
  - Direction: Input

The order of the matrix  $A$ .  $N \geq 0$ .

- **nrhs**
  - Type: `int`
  - Direction: Input

The number of right hand sides, i.e., the number of columns of the matrix  $B$ .  $NRHS \geq 0$ .

- **a**
  - Type: S/D/C/Z Pointer
  - Direction: Input

- Dimension: (LDA, N)

The triangular factor U or L from the Cholesky factorization  $A = U^T * U$  or  $A = L * L^T$ , as computed by *POTRF*.

- **lda**

- Type: int
- Direction: Input

The leading dimension of the array A.  $LDA \geq \max(1, N)$ .

- **b**

- Type: S/D/C/Z Pointer
- Direction: Input/Output
- Dimension: (LDB, NRHS)

On entry, the right hand side matrix B.

On exit, the solution matrix X.

- **ldb**

- Type: int
- Direction: Input

The leading dimension of the array B.  $LDB \geq \max(1, N)$ .

## 3.35 STEBZ

### CULA Routines

The STEBZ functionality is implemented by the following CULA routines:

- Host Memory
  - `culaSstebz`
  - `culaDstebz`
  - `culaStebz` (C++ style, type overloaded)
- Device Memory
  - `culaDeviceSstebz`
  - `culaDeviceDstebz`
  - `culaDeviceStebz` (C++ style, type overloaded)

### Description

STEBZ computes the eigenvalues of a symmetric tridiagonal matrix T. The user may ask for all eigenvalues, all eigenvalues in the half-open interval (VL, VU], or the IL-th through IU-th eigenvalues.

To avoid overflow, the matrix must be scaled so that its largest element is no greater than  $\text{overflow}^{**}(1/2) * \text{underflow}^{**}(1/4)$  in absolute value, and for greatest accuracy, it should not be much smaller than that.

See W. Kahan “Accurate Eigenvalues of a Symmetric Tridiagonal Matrix”, Report CS41, Computer Science Dept., Stanford University, July 21, 1966.

Please note that complex versions of this function do not exist.

## Parameters

- **range**

- Type: char
- Direction: Input
- = 'A': ("All") all eigenvalues will be found.
- = 'V': ("Value") all eigenvalues in the half-open interval (VL, VU] will be found.
- = 'I': ("Index") the IL-th through IU-th eigenvalues (of the entire matrix) will be found.

- **order**

- Type: char
- Direction: Input
- = 'B': ("By Block") the eigenvalues will be grouped by split-off block (see IBLOCK, ISPLIT) and ordered from smallest to largest within the block. This code behaves similarly to "E" and will report only one block.
- = 'E': ("Entire matrix") the eigenvalues for the entire matrix will be ordered from smallest to largest.

- **n**

- Type: int
  - Direction: Input
- The order of the tridiagonal matrix T.  $N \geq 0$ .

- **vl**

- Type: S/D Value
- Direction: Input

- **vu**

- Type: S/D Value
- Direction: Input

If RANGE='V', the lower and upper bounds of the interval to be searched for eigenvalues. Eigenvalues less than or equal to VL, or greater than VU, will not be returned.  $VL < VU$ . Not referenced if RANGE = 'A' or 'I'.

- **il**

- Type: int
- Direction: Input

- **iu**

- Type: int
- Direction: Input

If RANGE='I', the indices (in ascending order) of the smallest and largest eigenvalues to be returned.  $1 \leq IL \leq IU \leq N$ , if  $N > 0$ ;  $IL = 1$  and  $IU = 0$  if  $N = 0$ . Not referenced if RANGE = 'A' or 'V'.

- **abstol**

- Type: S/D

- Direction: Input

The absolute tolerance for the eigenvalues. An eigenvalue (or cluster) is considered to be located if it has been determined to lie in an interval whose width is ABSTOL or less. If ABSTOL is less than or equal to zero, then  $ULP * |T|$  will be used, where  $|T|$  means the 1-norm of T.

Eigenvalues will be computed most accurately when ABSTOL is set to twice the underflow threshold, not zero.

- **d**

- Type: S/D Pointer
- Direction: Input
- Dimension: (N)

The N diagonal elements of the tridiagonal matrix T.

- **e**

- Type: S/D Pointer
- Direction: Input
- Dimension: (N-1)

The (N-1) off-diagonal elements of the tridiagonal matrix T. Not referenced if  $N \leq 1$ .

- **m**

- Type: int Pointer, always host
- Direction: Output

The actual number of eigenvalues found.  $0 \leq M \leq N$ .

- **nsplit**

- Type: int Pointer, always host
- Direction: Output

The number of diagonal blocks in the matrix T.  $1 \leq NSPLIT \leq N$ .

- **w**

- Type: S/D Pointer
- Direction: Output
- Dimension: (N)

On exit, the first M elements of W will contain the eigenvalues. (STEBZ may use the remaining N-M elements as workspace.)

- **iblock**

- Type: int Pointer
- Direction: Output
- Dimension: (N)

At each row/column j where  $E(j)$  is zero or small, the matrix T is considered to split into a block diagonal matrix. On exit, if culaNoError is returned, IBLOCK(i) specifies to which block (from 1 to the number of blocks) the eigenvalue W(i) belongs. (STEBZ may use the remaining N-M elements as workspace.)

- **isplit**

- Type: int Pointer
- Direction: Output
- Dimension: (N)

The splitting points, at which T breaks up into submatrices. The first submatrix consists of rows/columns 1 to ISPLIT(1), the second of rows/columns ISPLIT(1)+1 through ISPLIT(2), etc., and the NSPLIT-th consists of rows/columns ISPLIT(NSPLIT-1)+1 through ISPLIT(NSPLIT)=N.

(Only the first NSPLIT elements will actually be used, but since the user cannot know a priori what value NSPLIT will have, N words must be reserved for ISPLIT.)

### Differences from LAPACK

See *No Workspace Parameters* section.

## 3.36 STEQR

### CULA Routines

The STEQR functionality is implemented by the following CULA routines:

- Host Memory

- culaSsteqr
- culaDsteqr
- culaCsteqr
- culaZsteqr
- culaSteqr (C++ style, type overloaded)

- Device Memory

- culaDeviceSsteqr
- culaDeviceDsteqr
- culaDeviceCsteqr
- culaDeviceZsteqr
- culaDeviceSteqr (C++ style, type overloaded)

### Description

STEQR computes all eigenvalues and, optionally, eigenvectors of a symmetric tridiagonal matrix using the implicit QL or QR method. The eigenvectors of a full or band real/complex symmetric/Hermitian matrix can also be found if HETRD or HPTRD or HBTRD has been used to reduce this matrix to tridiagonal form.

### Parameters

- **compz**

- Type: char
- Direction: Input
- = 'N': Compute eigenvalues only.

= 'V': Compute eigenvalues and eigenvectors of the original symmetric/Hermitian matrix. On entry, Z must contain the unitary matrix used to reduce the original matrix to tridiagonal form.

= 'I': Compute eigenvalues and eigenvectors of the tridiagonal matrix. Z is initialized to the identity matrix.

- **n**

- Type: int
- Direction: Input

The order of the matrix.  $N \geq 0$ .

- **d**

- Type: S/D Pointer,
- Direction: Input/Output
- Dimension: (N)

On entry, the diagonal elements of the tridiagonal matrix.

On exit, if `culaNoError` is returned, the eigenvalues in ascending order.

- **e**

- Type: S/D Pointer,
- Direction: Input/Output
- Dimension: (N-1)

On entry, the (n-1) subdiagonal elements of the tridiagonal matrix.

On exit, E has been destroyed.

- **z**

- Type: S/D/C/Z Pointer,
- Direction: Input/Output
- Dimension: (LDZ, N)

On entry, if `COMPZ = 'V'`, then Z contains the unitary matrix used in the reduction to tridiagonal form.

On exit, if `culaNoError` is returned, then if `COMPZ = 'V'`, Z contains the orthonormal eigenvectors of the original symmetric/Hermitian matrix, and if `COMPZ = 'I'`, Z contains the orthonormal eigenvectors of the symmetric tridiagonal matrix. If `COMPZ = 'N'`, then Z is not referenced.

- **ldz**

- Type: int
- Direction: Input

The leading dimension of the array Z.  $LDZ \geq 1$ , and if eigenvectors are desired, then  $LDZ \geq \max(1, N)$ .

### Differences from LAPACK

See *No Workspace Parameters* section.

## 3.37 SYEV/HEEV

### CULA Routines

The SYEV/HEEV functionality is implemented by the following CULA routines:

- Host Memory
  - `culaSsyev`
  - `culaDsyev`
  - `culaCheev`
  - `culaZheev`
  - `culaSyeV` (C++ style, type overloaded)
  - `culaHeeV` (C++ style, type overloaded)
- Device Memory
  - `culaDeviceSsyev`
  - `culaDeviceDsyev`
  - `culaDeviceCheev`
  - `culaDeviceZheev`
  - `culaDeviceSyeV` (C++ style, type overloaded)
  - `culaDeviceHeeV` (C++ style, type overloaded)

### Description

SYEV/HEEV computes all eigenvalues and, optionally, eigenvectors of a real/complex symmetric/Hermitian matrix A.

### Parameters

- **jobz**
  - Type: `char`
  - Direction: Input
  - = 'N': Compute eigenvalues only;
  - = 'V': Compute eigenvalues and eigenvectors.
- **uplo**
  - Type: `char`
  - Direction: Input
  - = 'U': Upper triangle of A is stored;
  - = 'L': Lower triangle of A is stored.
- **n**
  - Type: `int`
  - Direction: Input

The order of the matrix A.  $N \geq 0$ .
- **a**

- Type: S/D/C/Z Pointer
- Direction: Input/Output
- Dimension: (LDA, N)

On entry, the symmetric/Hermitian matrix A. If UPLO = 'U', the leading N-by-N upper triangular part of A contains the upper triangular part of the matrix A. If UPLO = 'L', the leading N-by-N lower triangular part of A contains the lower triangular part of the matrix A.

On exit, if JOBZ = 'V', then if culaNoError is returned, A contains the orthonormal eigenvectors of the matrix A. If JOBZ = 'N', then on exit the lower triangle (if UPLO='L') or the upper triangle (if UPLO='U') of A, including the diagonal, is destroyed.

- **lda**

- Type: int
- Direction: Input

The leading dimension of the array A. LDA  $\geq$  max(1,N).

- **w**

- Type: S/D Pointer
- Direction: Output
- Dimension: (N)

If culaNoError is returned, the eigenvalues in ascending order.

### Differences from LAPACK

See *No Workspace Parameters* section.

## 3.38 SYEVX/HEEVX

### CULA Routines

The SYEVX/HEEVX functionality is implemented by the following CULA routines:

- Host Memory
  - culaSsyevx
  - culaDsyevx
  - culaCheevx
  - culaZheevx
  - culaSyevx (C++ style, type overloaded)
  - culaHeevx (C++ style, type overloaded)
- Device Memory
  - culaDeviceSsyevx
  - culaDeviceDsyevx
  - culaDeviceCheevx
  - culaDeviceZheevx
  - culaDeviceSyevx (C++ style, type overloaded)

- culaDeviceHeevx (C++ style, type overloaded)

## Description

SYEVX/HEEVX computes selected eigenvalues and, optionally, eigenvectors of a real/complex symmetric/Hermitian matrix A. Eigenvalues and eigenvectors can be selected by specifying either a range of values or a range of indices for the desired eigenvalues.

## Parameters

- **jobz**

- Type: char
- Direction: Input
- = 'N': Compute eigenvalues only;
- = 'V': Compute eigenvalues and eigenvectors.

- **range**

- Type: char
- Direction: Input
- = 'A': all eigenvalues will be found.
- = 'V': all eigenvalues in the half-open interval (VL,VU] will be found.
- = 'I': the IL-th through IU-th eigenvalues will be found.

- **uplo**

- Type: char
- Direction: Input
- = 'U': Upper triangle of A is stored;
- = 'L': Lower triangle of A is stored.

- **n**

- Type: int
- Direction: Input

The order of the matrix A.  $N \geq 0$ .

- **a**

- Type: S/D/C/Z Pointer,
- Direction: Input/Output
- Dimension: (LDA, N)

On entry, the symmetric/Hermitian matrix A. If UPLO = 'U', the leading N-by-N upper triangular part of A contains the upper triangular part of the matrix A. If UPLO = 'L', the leading N-by-N lower triangular part of A contains the lower triangular part of the matrix A.

On exit, the lower triangle (if UPLO='L') or the upper triangle (if UPLO='U') of A, including the diagonal, is destroyed.

- **lda**

- Type: int

- Direction: Input

The leading dimension of the array A.  $LDA \geq \max(1,N)$ .

- **vl**

- Type: S/D/C/Z
- Direction: Input

- **vu**

- Type: S/D/C/Z
- Direction: Input

If RANGE='V', the lower and upper bounds of the interval to be searched for eigenvalues.  $VL < VU$ . Not referenced if RANGE = 'A' or 'I'.

- **il**

- Type: int
- Direction: Input

- **iu**

- Type: int
- Direction: Input

If RANGE='I', the indices (in ascending order) of the smallest and largest eigenvalues to be returned.  $1 \leq IL \leq IU \leq N$ , if  $N > 0$ ;  $IL = 1$  and  $IU = 0$  if  $N = 0$ . Not referenced if RANGE = 'A' or 'V'.

- **abstol**

- Type: S/D/C/Z
- Direction: Input

The absolute error tolerance for the eigenvalues. An approximate eigenvalue is accepted as converged when it is determined to lie in an interval [a,b] of width less than or equal to

$$ABSTOL + EPS * \max(|a|, |b|),$$

where EPS is the machine precision. If ABSTOL is less than or equal to zero, then  $EPS * |T|$  will be used in its place, where  $|T|$  is the 1-norm of the tridiagonal matrix obtained by reducing A to tridiagonal form.

Eigenvalues will be computed most accurately when ABSTOL is set to twice the underflow threshold, not zero. If this routine returns with `culaDataError`, indicating that some eigenvectors did not converge, try setting ABSTOL to the recommended value.

See "Computing Small Singular Values of Bidiagonal Matrices with Guaranteed High Relative Accuracy," by Demmel and Kahan, LAPACK Working Note #3.

- **m**

- Type: int Pointer, always host
- Direction: Output

The total number of eigenvalues found.  $0 \leq M \leq N$ . If RANGE = 'A',  $M = N$ , and if RANGE = 'I',  $M = IU - IL + 1$ .

- **w**

- Type: S/D Pointer,

- Direction: Output
- Dimension: (N)

On normal exit, the first M elements contain the selected eigenvalues in ascending order.

- **z**

- Type: S/D/C/Z Pointer,
- Direction: Output
- Dimension: (LDZ, max(1,M))

If JOBZ = 'V', then if culaNoError is returned, the first M columns of Z contain the orthonormal eigenvectors of the matrix A corresponding to the selected eigenvalues, with the i-th column of Z holding the eigenvector associated with W(i).

If an eigenvector fails to converge, then that column of Z contains the latest approximation to the eigenvector, and the index of the eigenvector is returned in IFAIL.

If JOBZ = 'N', then Z is not referenced.

Note: the user must ensure that at least max(1,M) columns are supplied in the array Z; if RANGE = 'V', the exact value of M is not known in advance and an upper bound must be used.

- **ldz**

- Type: int
- Direction: Input

The leading dimension of the array Z. LDZ >= 1, and if JOBZ = 'V', LDZ >= max(1,N).

- **ifail**

- Type: int Pointer
- Direction: Output
- Dimension: (N)

If JOBZ = 'V', then if culaNoError is returned, the first M elements of IFAIL are zero. If culaDataError is returned, then IFAIL contains the indices of the eigenvectors that failed to converge.

If JOBZ = 'N', then IFAIL is not referenced.

### Differences from LAPACK

See *No Workspace Parameters* section.

## 3.39 SYRDB/HERDB

### CULA Routines

The SYRDB/HERDB functionality is implemented by the following CULA routines:

- Host Memory
  - culaSsyldb
  - culaDsyldb
  - culaCherdb
  - culaZherdb

- culaSyrdb (C++ style, type overloaded)
- culaHerdb (C++ style, type overloaded)
- Device Memory
  - culaDeviceSyrdb
  - culaDeviceDsyrd
  - culaDeviceCherdb
  - culaDeviceZherdb
  - culaDeviceSyrdb (C++ style, type overloaded)
  - culaDeviceHerdb (C++ style, type overloaded)

### Description

Given a symmetric/Hermitian N-by-N matrix A, SYRDB/HERDB reduces A to a symmetric tridiagonal form (T) using a series of orthogonal transformations (Q), such that

$$A = Q * T * Q^T.$$

Note: This function should be used in place of SSYTRD, DSYTRD, CHETRD, and ZHETRD when an orthogonal Q is not needed as the performance of these functions does not scale to large matrix sizes.

See “A framework for symmetric band reduction,” by Bischof, Lang, and Sun, ACM Transactions on Mathematical Software (TOMS) archive Volume 26, Issue 4.

### Parameters

- **jobz**

- Type: char
- Direction: Input

Specifies which matrices outputs are contained within the outputs A and Z.

= ‘N’ : Forms the symmetric tridiagonal matrix T. Overwrites A with the banded matrix, B, and the information needed to construct  $Q_B$ .

= ‘V’ : Forms the symmetric tridiagonal matrix T. Overwrites A with Q.

= ‘U’ : Forms the symmetric tridiagonal matrix T. Overwrites A with the banded matrix, B, and the information needed to construct  $Q_B$ . Also, overwrites Z with  $Z*Q$ .

- **uplo**

- Type: char
- Direction: Input

Specifies the triangular region where the symmetric input matrix is defined.

= ‘U’ : defined within the upper triangular part of A

= ‘L’ : defined within the lower triangular part of A

- **n**

- Type: int
- Direction: Input

The order of the matrix A.  $N \geq 0$ .

- **kd**

- Type: int
- Direction: Input

The bandwidth of the banded output matrix, B.  $KD \geq 1$ .

- **a**

- Type: S/D/C/Z Pointer,
- Direction: Input/Output
- Dimension: (LDA, N)

On entry, A is a real/complex symmetric/Hermitian matrix described by UPLO.

On exit, given the job code of 'V', A is overwritten by Q. Given a job code of 'N' or 'U', A is overwritten by B and  $Q_B$  as defined by UPLO and KD.

- **lda**

- Type: int
- Direction: Input

The leading dimension of the array A.  $LDA \geq \max(1, N)$ .

- **d**

- Type: S/D/C/Z Pointer,
- Direction: Output
- Dimension:  $\max(1, N)$

Holds the diagonal elements of the symmetric tridiagonal matrix T.

- **e**

- Type: S/D/C/Z Pointer,
- Direction: Output
- Dimension:  $\max(N-1)$

Holds the off-diagonal elements of the symmetric tridiagonal matrix T.

- **tau**

- Type: S/D/C/Z Pointer,
- Direction: Output
- Dimension:  $\max(1, N-KD-1)$

The scalar factors of the elementary reflectors that form  $Q_B$ .

- **z**

- Type: S/D Pointer,
- Direction: Input/Output
- Dimension: (N-1)

An optional matrix that can be multiplied by Q given a 'U' job code.

= 'U' : contains the product of itself and Q ( $Z*Q$ ).

= 'N', 'V' : not referenced

- **ldz**
  - Type: int
  - Direction: Input

The leading dimension of the array Z. LDZ >= max(1,N).

#### Differences from LAPACK

See *No Workspace Parameters* section.

## 3.40 SYTRD/HETRD

This function is not implemented in CULA. If a tridiagonal reduction is required, please see *SYRDB/HERDB*

## 3.41 TRTRI

### CULA Routines

The TRTRI functionality is implemented by the following CULA routines:

- Host Memory
  - `culaStrtri`
  - `culaDtrtri`
  - `culaCtrtri`
  - `culaZtrtri`
  - `culaTrtri` (C++ style, type overloaded)
- Device Memory
  - `culaDeviceStrtri`
  - `culaDeviceDtrtri`
  - `culaDeviceCtrtri`
  - `culaDeviceZtrtri`
  - `culaDeviceTrtri` (C++ style, type overloaded)

### Description

TRTRI computes the inverse of a real upper or lower triangular matrix A.

### Parameters

- **uplo**
  - Type: char
  - Direction: Input
  - = 'U': A is upper triangular;
  - = 'L': A is lower triangular.
- **diag**
  - Type: char

- Direction: Input
- = 'N': A is non-unit triangular;
- = 'U': A is unit triangular.

- **n**

- Type: int
- Direction: Input

The order of the matrix A.  $N \geq 0$ .

- **a**

- Type: S/D/C/Z Pointer
- Direction: Input/Output
- Dimension: (LDA, N)

On entry, the triangular matrix A. If UPLO = 'U', the leading N-by-N upper triangular part of the array A contains the upper triangular matrix, and the strictly lower triangular part of A is not referenced. If UPLO = 'L', the leading N-by-N lower triangular part of the array A contains the lower triangular matrix, and the strictly upper triangular part of A is not referenced. If DIAG = 'U', the diagonal elements of A are also not referenced and are assumed to be 1.

On exit, the (triangular) inverse of the original matrix, in the same storage format.

- **lda**

- Type: int
- Direction: Input

The leading dimension of the array A.  $LDA \geq \max(1, N)$ .

## 3.42 TRTRS

### CULA Routines

The TRTRS functionality is implemented by the following CULA routines:

- Host Memory
  - culaStrtrs
  - culaDtrtrs
  - culaCtrtrs
  - culaZtrtrs
  - culaTrtrs (C++ style, type overloaded)
- Device Memory
  - culaDeviceStrtrs
  - culaDeviceDtrtrs
  - culaDeviceCtrtrs
  - culaDeviceZtrtrs
  - culaDeviceTrtrs (C++ style, type overloaded)

## Description

TRTRS solves a triangular system of the form

$$A * X = B \text{ or } A^T * X = B,$$

where A is a triangular matrix of order N, and B is an N-by-NRHS matrix. A check is made to verify that A is nonsingular.

## Parameters

- **uplo**

- Type: char
- Direction: Input
- = 'U': A is upper triangular;
- = 'L': A is lower triangular.

- **trans**

- Type: char
  - Direction: Input
- Specifies the form of the system of equations: = 'N':  $A * X = B$  (No transpose)  
= 'T':  $A^T * X = B$  (Transpose)  
= 'C':  $A^H * X = B$  (Conjugate transpose = Transpose)

- **diag**

- Type: char
- Direction: Input
- = 'N': A is non-unit triangular;
- = 'U': A is unit triangular.

- **n**

- Type: int
  - Direction: Input
- The order of the matrix A.  $N \geq 0$ .

- **nrhs**

- Type: int
  - Direction: Input
- The number of right hand sides, i.e., the number of columns of the matrix B.  $NRHS \geq 0$ .

- **a**

- Type: S/D/C/Z Pointer
- Direction: Input
- Dimension: (LDA, N)

The triangular matrix A. If UPLO = 'U', the leading N-by-N upper triangular part of the array A contains the upper triangular matrix, and the strictly lower triangular part of A is not referenced. If UPLO = 'L', the leading N-by-N lower triangular part of the array A contains the lower triangular

matrix, and the strictly upper triangular part of A is not referenced. If `DIAG = 'U'`, the diagonal elements of A are also not referenced and are assumed to be 1.

- **lda**

- Type: `int`
- Direction: Input

The leading dimension of the array A.  $LDA \geq \max(1, N)$ .

- **b**

- Type: S/D/C/Z Pointer
- Direction: Input/Output
- Dimension: (LDB, NRHS)

On entry, the right hand side matrix B.

On exit, if `culaNoError` is returned, the solution matrix X.

- **ldb**

- Type: `int`
- Direction: Input

The leading dimension of the array B.  $LDB \geq \max(1, N)$ .

# DIFFERENCES BETWEEN CULA AND LAPACK

The usage of some CULA functions differ slightly from their LAPACK equivalents, though they perform the same operations. This section details some of the API-wide ways that CULA and LAPACK differ.

## 4.1 No Workspace Parameters

Many LAPACK functions require a workspace for internal operation. For those LAPACK functions that utilize a workspace, workspace sizes are queried by providing a -1 argument to what is typically an *LWORK* parameter. Upon inspecting this parameter, the LAPACK function will determine the workspace required for this particular problem size and will return the value in the *WORK* parameter. LAPACK (and other similar packages) then require the programmer to provide a pointer to memory of sufficient size, which often requires that the programmer allocate new memory.

CULA uses both main and GPU workspace memories, and as such, LAPACK's workspace query is not appropriate, as the LAPACK interface allows for the specification of only one workspace. Instead of providing a more complicated interface that adds parameters for both main and GPU workspace memories, CULA requires neither. Instead, any workspaces that are required are allocated and tracked internally. This organization yields no significant performance loss, and furthermore reduces the number of function calls by removing the need for a workspace query.

**Note:** Any workspaces that have been allocated internally may be cleared by calling `culaFreeBuffers()`.

# COMMON ERRORS

This section lists some of the common errors users make when using CULA and similar LAPACK packages.

## 5.1 Pivot Arrays

This section applies to functions in the LU Family (`getrf`, `gesv`, `getrs`, etc.).

CULA pivot arrays follow LAPACK conventions. These arrays are created for serial evaluation and describe a series of row interchanges. The array `[2 3 3]` states “swap the first row with the second, then the second row with the third, then the third row is unchanged.” For those working with Matlab, note that Matlab follows a different convention, in which the pivot array describes a set of parallel row interchanges. The Matlab array `[2 3 1]` is equivalent to the first example, and states “for the first row, obtain the second row; for the second row obtain the third; and for the third row obtain the first.”

## 5.2 Padding With Zeros

A common GPU usage pattern is to pad matrices to multiples of 8/16/32 elements in order to achieve performance. Routines such as GEMM (matrix-matrix multiply, as found in *CUBLAS*) are data-insensitive to these extra elements if they are zero. CULA routines function differently and in many cases will react poorly if the zeros are included in the computation space; for instance, solving a system in which the coefficient matrix has a full row or column of zeros will result in a `culaDataError` as the matrix is indeed singular. To avoid this problem, please be sure to set the *LDx* parameters to the padded size, but to set the remainder of the inputs that describe sizes (*M*, *N*, etc) to match the size of the *valid* data for the computation (that is: the size before padding.) This will avoid many data errors.