linalg 1.2.2

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# 1 Main Page

## 1.1 Introduction

LINALG is a linear algebra library that provides a user-friendly interface to several BLAS and LAPACK routines.

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Version

1.2.2

# 2 Modules Index

## 2.1 Modules List

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4.1.1 Detailed Description	
lapack	
Purpose	
Provides interfaces to various LAPACK routines.	

linalg\_c\_binding

4.2 linalg\_c\_binding Module Reference

#### **Functions/Subroutines**

subroutine mtx\_mult\_c (transa, transb, m, n, k, alpha, a, lda, b, ldb, beta, c)

Performs the matrix operation: C = alpha \* op(A) \* op(B) + beta \* C.

• subroutine cmtx\_mult\_c (transa, transb, m, n, k, alpha, a, lda, b, ldb, beta, c)

Performs the matrix operation: C = alpha \* op(A) \* op(B) + beta \* C.

• subroutine diag\_mtx\_mult\_left\_c (m, n, k, alpha, a, b, beta, c)

Computes the matirx operation: C = alpha \* A \* B + beta \* C, where A is a diagonal amtrix.

• subroutine disg mtx mult right c (m, n, k, alpha, a, b, beta, c)

Comptues the matrix operation: C = alpha \* A \* B + beta \* C, where B is a diagonal matrix.

• subroutine diag\_mtx\_mult\_cmplx\_left\_c (m, n, k, alpha, a, b, beta, c)

Computes the matirx operation: C = alpha \* A \* B + beta \* C, where A is a diagonal amtrix.

subroutine diag\_mtx\_mult\_cmplx\_right\_c (m, n, k, alpha, a, b, beta, c)

Comptues the matrix operation: C = alpha \* A \* B + beta \* C, where B is a diagonal matrix.

• subroutine diag\_cmtx\_mult\_left\_c (m, n, k, alpha, a, b, beta, c)

Computes the matirx operation: C = alpha \* A \* B + beta \* C, where A is a diagonal amtrix.

• subroutine diag\_cmtx\_mult\_right\_c (m, n, k, alpha, a, b, beta, c)

Comptues the matrix operation: C = alpha \* A \* B + beta \* C, where B is a diagonal matrix.

• subroutine rank1\_update\_c (m, n, alpha, x, y, a)

Performs the rank-1 update to matrix A such that: A = alpha \* X \* Y \* \* T + A, where A is an M-by-N matrix, alpha is a scalar, X is an M-element array, and N is an N-element array.

pure real(dp) function trace c (m, n, x)

Computes the trace of a matrix (the sum of the main diagonal elements).

• integer(i32) function mtx rank c (m, n, a, err)

Computes the rank of a matrix.

real(dp) function det\_c (n, a, err)

Computes the determinant of a square matrix.

• subroutine swap\_c (n, x, y)

Swaps the contents of two arrays.

- subroutine **tri\_mtx\_mult\_c** (upper, n, alpha, a, beta, b, err)
- subroutine lu\_factor\_c (m, n, a, ipvt, err)

Computes the LU factorization of an M-by-N matrix.

• subroutine form\_lu\_c (n, lu, ipvt, u, p)

Extracts the L, U, and P matrices from the output of the lu\_factor routine.

• subroutine qr\_factor\_c (m, n, a, tau, err)

Computes the QR factorization of an M-by-N matrix without pivoting.

• subroutine qr\_factor\_pivot\_c (m, n, a, tau, jpvt, err)

Computes the QR factorization of an M-by-N matrix with column pivoting such that A\*P=Q\*R.

• subroutine form\_qr\_c (m, n, r, tau, q, err)

Forms the full M-by-M orthogonal matrix Q from the elementary reflectors returned by the base QR factorization algorithm.

• subroutine form\_qr\_pivot\_c (m, n, r, tau, pvt, q, p, err)

Forms the full M-by-M orthogonal matrix Q from the elementary reflectors returned by the base QR factorization algorithm.

• subroutine mult\_qr\_c (trans, m, n, q, tau, c, err)

Multiplies a general matrix by the orthogonal matrix Q from a QR factorization such that: C = op(Q) \* C.

• subroutine qr\_rank1\_update\_c (m, n, q, r, u, v, err)

Computes the rank 1 update to an M-by-N QR factored matrix A  $(M \ge N)$  where A = Q \* R, and A1 = A + U \* V \* T such that A1 = Q1 \* R1.

• subroutine cholesky factor c (n, a, upper, err)

Computes the Cholesky factorization of a symmetric, positive definite matrix.

subroutine cholesky\_rank1\_update\_c (n, r, u, err)

Computes the rank 1 update to a Cholesky factored matrix (upper triangular).

subroutine cholesky\_rank1\_downdate\_c (n, r, u, err)

Computes the rank 1 downdate to a Cholesky factored matrix (upper triangular).

• subroutine rz factor c (m, n, a, tau, err)

Factors an upper trapezoidal matrix by means of orthogonal transformations such that  $A = R * Z = (R \ 0) * Z$ . Z is an orthogonal matrix of dimension N-by-N, and R is an M-by-M upper triangular matrix.

• subroutine mult\_rz\_c (trans, m, n, I, a, tau, c, err)

Multiplies a general matrix by the orthogonal matrix Z from an RZ factorization such that: C = op(Z) \* C.

• subroutine svd\_c (m, n, a, s, u, vt, err)

Computes the singular value decomposition of a matrix A. The SVD is defined as: A = U \* S \* V \* \* T, where U is an M-by-M orthogonal matrix, S is an M-by-N diagonal matrix, and V is an N-by-N orthogonal matrix.

subroutine solve\_tri\_mtx\_c (upper, trans, nounit, n, nrhs, alpha, a, b)

Solves one of the matrix equations: op(A) \* X = alpha \* B, where A is a triangular matrix.

• subroutine solve\_lu\_c (n, nrhs, a, ipvt, b)

Solves a system of LU-factored equations.

• subroutine solve\_qr\_c (m, n, nrhs, a, tau, b, err)

Solves a system of M QR-factored equations of N unknowns where M >= N.

• subroutine solve qr pivot c (m, n, nrhs, a, tau, jpvt, b, err)

Solves a system of M QR-factored equations of N unknowns where the QR factorization made use of column pivoting.

• subroutine solve\_cholesky\_c (upper, n, nrhs, a, b)

Solves a system of Cholesky factored equations.

• subroutine mtx inverse c (n, a, err)

Computes the inverse of a square matrix.

• subroutine mtx\_pinverse\_c (m, n, a, ainv, err)

Computes the Moore-Penrose pseudo-inverse of a M-by-N matrix using the singular value decomposition of the matrix.

• subroutine solve\_least\_squares\_c (m, n, nrhs, a, b, err)

Solves the overdetermined or underdetermined system (A\*X = B) of M equations of N unknowns using a QR or LQ factorization of the matrix A. Notice, it is assumed that matrix A has full rank.

subroutine eigen\_symm\_c (n, vecs, a, vals, err)

Computes the eigenvalues, and optionally the eigenvectors of a real, symmetric matrix.

• subroutine eigen\_asymm\_c (n, a, vals, vecs, err)

Computes the eigenvalues, and the right eigenvectors of a square matrix.

• subroutine eigen\_gen\_c (n, a, b, alpha, beta, vecs, err)

Computes the eigenvalues, and optionally the right eigenvectors of a square matrix assuming the structure of the eigenvalue problem is A\*X = lambda\*B\*X.

#### 4.2.1 Detailed Description

## linalg\_c\_binding

#### **Purpose**

Provides a C friendly interface to the LINALG library.

#### 4.2.2 Function/Subroutine Documentation

4.2.2.1 subroutine linalg\_c\_binding::cholesky\_factor\_c ( integer(i32), intent(in), value *n*, real(dp), dimension(n,n), intent(inout) *a*, logical(c bool), intent(in), value *upper*, type(errorhandler), intent(inout) *err* )

Computes the Cholesky factorization of a symmetric, positive definite matrix.

## **Parameters**

in	n	The dimension of the matrix.
in,out	а	On input, the N-by-N matrix to factor. On output, the factored matrix is returned in either
		the upper or lower triangular portion of the matrix, dependent upon the value of upper.
in	upper	An optional input that, if specified, provides control over whether the factorization is
		computed as $A = U**T*U$ (set to true), or as $A = L*L**T$ (set to false). The default
		value is true such that $A = U**T*U$ .
in,out	err	The errorhandler object. If no error handling is desired, simply pass NULL, and errors will be dealt with by the default internal error handler. Possible errors that may be encountered
		are as follows.
		LA_MATRIX_FORMAT_ERROR: Occurs if a is not positive definite.

Definition at line 813 of file linalg\_c\_binding.f90.

4.2.2.2 subroutine linalg\_c\_binding::cholesky\_rank1\_downdate\_c ( integer(i32), intent(in), value *n*, real(dp), dimension(n,n), intent(inout) *r*, real(dp), dimension(n), intent(inout) *u*, type(errorhandler), intent(inout) *err* )

Computes the rank 1 downdate to a Cholesky factored matrix (upper triangular).

#### **Parameters**

in	n	The dimension of the matrix.
in,out	r	On input, the N-by-N upper triangular matrix R. On output, the updated matrix R1.
in,out	и	On input, the N-element update vector U. On output, the rotation sines used to transform R to
		R1.
in,out	err	The errorhandler object. If no error handling is desired, simply pass NULL, and errors will be dealt with by the default internal error handler. Possible errors that may be encountered are as follows.
		<ul> <li>LA_ARRAY_SIZE_ERROR: Occurs if any of the input array sizes are incorrect.</li> </ul>
		<ul> <li>LA_OUT_OF_MEMORY_ERROR: Occurs if local memory must be allocated, and there is insufficient memory available.</li> </ul>
		<ul> <li>LA_MATRIX_FORMAT_ERROR: Occurs if the downdated matrix is not positive definite.</li> </ul>
		<ul> <li>LA_SINGULAR_MATRIX_ERROR: Occurs if r is singular.</li> </ul>

Definition at line 887 of file linalg\_c\_binding.f90.

4.2.2.3 subroutine linalg\_c\_binding::cholesky\_rank1\_update\_c ( integer(i32), intent(in), value *n*, real(dp), dimension(n,n), intent(inout) *r*, real(dp), dimension(n), intent(inout) *u*, type(errorhandler), intent(inout) *err* )

Computes the rank 1 update to a Cholesky factored matrix (upper triangular).

in	n	The dimension of the matrix.
in,out	r	On input, the N-by-N upper triangular matrix R. On output, the updated matrix R1.
in,out	и	On input, the N-element update vector U. On output, the rotation sines used to transform R to
		R1.

## **Parameters**

in,out	err	The errorhandler object. If no error handling is desired, simply pass NULL, and errors will be dealt with by the default internal error handler. Possible errors that may be encountered are as follows.
		<ul> <li>LA_OUT_OF_MEMORY_ERROR: Occurs if local memory must be allocated, and there is insufficient memory available.</li> </ul>

Definition at line 848 of file linalg\_c\_binding.f90.

4.2.2.4 subroutine linalg\_c\_binding::cmtx\_mult\_c ( logical(c\_bool), intent(in), value transa, logical(c\_bool), intent(in), value transb, integer(i32), intent(in), value m, integer(i32), intent(in), value n, integer(i32), intent(in), value k, real(dp), intent(in), value alpha, complex(dp), dimension(lda,\*), intent(in) a, integer(i32), intent(in), value lda, complex(dp), dimension(ldb,\*), intent(in) b, integer(i32), intent(in), value ldb, real(dp), intent(in), value beta, complex(dp), dimension(m,n), intent(inout) c)

Performs the matrix operation: C = alpha \* op(A) \* op(B) + beta \* C.

## **Parameters**

in	transa	Set to true if $op(A) == A**T$ ; else, set to false if $op(A) == A$ .
in	transb	Set to true if $op(B) == B**T$ ; else, set to false if $op(B) == B$ .
in	m	The number of rows in matrix C, and the number of rows in matrix op(A).
in	n	The number of columns in matrix C, and the number of columns in matrix op(B).
in	k	The number of columns in matrix op(A), and the number of rows in the matrix op(B).
in	alpha	The scalar multiplier to matrix A.
in	а	The M-by-K matrix A.
in	lda	The leading dimension of matrix A. If transa is true, this value must be at least MAX(1, K); else, if transa is false, this value must be at least MAX(1, M).
in	b	The K-by-N matrix B.
in	ldb	The leading dimension of matrix B. If transb is true, this value must be at least MAX(1, N); else, if transb is false, this value must be at least MAX(1, K).
in	beta	The scalar multiplier to matrix C.
in,out	С	The M-by-N matrix C.

Definition at line 95 of file linalg\_c\_binding.f90.

4.2.2.5 real(dp) function linalg\_c\_binding::det\_c ( integer(i32), intent(in), value *n*, real(dp), dimension(n,n), intent(inout) *a*, type(errorhandler), intent(inout) *err* )

Computes the determinant of a square matrix.

in	n	The dimension of the matrix.
in,out	а	On input, the N-by-N matrix on which to operate. On output the contents are overwritten by
		the LU factorization of the original matrix.

## **Parameters**

in,out	err	The errorhandler object. If no error handling is desired, simply pass NULL, and errors will be dealt with by the default internal error handler. Possible errors that may be encountered are as follows.
		<ul> <li>LA_ARRAY_SIZE_ERROR: Occurs if the input matrix is not square.</li> </ul>
		<ul> <li>LA_OUT_OF_MEMORY_ERROR: Occurs if local memory must be allocated, and there is insufficient memory available.</li> </ul>

Definition at line 373 of file linalg\_c\_binding.f90.

4.2.2.6 subroutine linalg\_c\_binding::diag\_cmtx\_mult\_left\_c ( integer(i32), intent(in), value *m*, integer(i32), intent(in), value *n*, integer(i32), intent(in), value *k*, real(dp), intent(in), value *alpha*, complex(dp), dimension(min(m, k)), intent(in) *a*, complex(dp), dimension(k, n), intent(in) *b*, real(dp), intent(in), value *beta*, complex(dp), dimension(m, n), intent(inout) *c* )

Computes the matirx operation: C = alpha \* A \* B + beta \* C, where A is a diagonal amtrix.

#### **Parameters**

in	m	The number of rows in matrix C.
in	n	The number of columns in matrix C.
in	k	The number of rows in matrix B.
in	alpha	The scalar multiplier to matrix A.
in	а	A MIN(M,K)-element array containing the diagonal elements of matrix A.
in	b	The K-by-N matrix B.
in	beta	The scalar multiplier to matrix C.
in,out	С	The M-by-N matrix C.

Definition at line 239 of file linalg\_c\_binding.f90.

4.2.2.7 subroutine linalg\_c\_binding::diag\_cmtx\_mult\_right\_c ( integer(i32), intent(in), value *m*, integer(i32), intent(in), value *k*, real(dp), intent(in), value *alpha*, complex(dp), dimension(m, k), intent(in) *a*, complex(dp), dimension(min(k, n)), intent(in) *b*, real(dp), intent(in), value *beta*, complex(dp), dimension(m, n), intent(inout) *c* )

Comptues the matrix operation: C = alpha \* A \* B + beta \* C, where B is a diagonal matrix.

#### **Parameters**

in	m	The number of rows in matrix C.
in	n	The number of columns in matrix C.
in	k	The number of columns in matrix A.
in	alpha	The scalar multiplier to matrix A.
in	а	The M-by-K matrix A.
in	b	A MIN(K,N)-element array containing the diagonal elements of matrix B.
in	beta	The scalar multiplier to matrix C.
in,out	С	The M-by-N matrix C.

Definition at line 264 of file linalg\_c\_binding.f90.

4.2.2.8 subroutine linalg\_c\_binding::diag\_mtx\_mult\_cmplx\_left\_c ( integer(i32), intent(in), value *m*, integer(i32), intent(in), value *n*, integer(i32), intent(in), value *k*, real(dp), intent(in), value *alpha*, complex(dp), dimension(min(m, k)), intent(in) *a*, real(dp), dimension(k, n), intent(in) *b*, real(dp), intent(in), value *beta*, complex(dp), dimension(m, n), intent(inout) *c* )

Computes the matirx operation: C = alpha \* A \* B + beta \* C, where A is a diagonal amtrix.

#### **Parameters**

in	m	The number of rows in matrix C.
in	n	The number of columns in matrix C.
in	k	The number of rows in matrix B.
in	alpha	The scalar multiplier to matrix A.
in	а	A MIN(M,K)-element array containing the diagonal elements of matrix A.
in	b	The K-by-N matrix B.
in	beta	The scalar multiplier to matrix C.
in, out	С	The M-by-N matrix C.

Definition at line 187 of file linalg\_c\_binding.f90.

4.2.2.9 subroutine linalg\_c\_binding::diag\_mtx\_mult\_cmplx\_right\_c ( integer(i32), intent(in), value *m*, integer(i32), intent(in), value *k*, real(dp), intent(in), value *alpha*, real(dp), dimension(m, k), intent(in) *a*, complex(dp), dimension(min(k, n)), intent(in) *b*, real(dp), intent(in), value *beta*, complex(dp), dimension(m, n), intent(inout) *c* )

Comptues the matrix operation: C = alpha \* A \* B + beta \* C, where B is a diagonal matrix.

## **Parameters**

in	m	The number of rows in matrix C.
in	n	The number of columns in matrix C.
in	k	The number of columns in matrix A.
in	alpha	The scalar multiplier to matrix A.
in	а	The M-by-K matrix A.
in	b	A MIN(K,N)-element array containing the diagonal elements of matrix B.
in	beta	The scalar multiplier to matrix C.
in,out	С	The M-by-N matrix C.

Definition at line 213 of file linalg\_c\_binding.f90.

4.2.2.10 subroutine linalg\_c\_binding::diag\_mtx\_mult\_left\_c ( integer(i32), intent(in), value *m*, integer(i32), intent(in), value *k*, real(dp), intent(in), value *alpha*, real(dp), dimension(min(m,k)), intent(in) *a*, real(dp), dimension(k,n), intent(in) *b*, real(dp), intent(in), value *beta*, real(dp), dimension(m,n), intent(inout) *c* )

Computes the matirx operation: C = alpha \* A \* B + beta \* C, where A is a diagonal amtrix.

in	m	The number of rows in matrix C.
in	n	The number of columns in matrix C.
in	k	The number of rows in matrix B.
in	alpha	The scalar multiplier to matrix A.

## **Parameters**

in	а	A MIN(M,K)-element array containing the diagonal elements of matrix A.
in	b	The K-by-N matrix B.
in	beta	The scalar multiplier to matrix C.
in, out	С	The M-by-N matrix C.

Definition at line 137 of file linalg\_c\_binding.f90.

4.2.2.11 subroutine linalg\_c\_binding::disg\_mtx\_mult\_right\_c ( integer(i32), intent(in), value *m*, integer(i32), intent(in), value *n*, integer(i32), intent(in), value *k*, real(dp), intent(in), value *alpha*, real(dp), dimension(m, k), intent(in) *a*, real(dp), dimension(m, n), intent(inout) *c* )

Comptues the matrix operation: C = alpha \* A \* B + beta \* C, where B is a diagonal matrix.

## **Parameters**

in	m	The number of rows in matrix C.
in	n	The number of columns in matrix C.
in	k	The number of columns in matrix A.
in	alpha	The scalar multiplier to matrix A.
in	а	The M-by-K matrix A.
in	b	A MIN(K,N)-element array containing the diagonal elements of matrix B.
in	beta	The scalar multiplier to matrix C.
in,out	С	The M-by-N matrix C.

Definition at line 162 of file linalg\_c\_binding.f90.

4.2.2.12 subroutine linalg\_c\_binding::eigen\_asymm\_c ( integer(i32), intent(in), value n, real(dp), dimension(n,n), intent(inout) a, complex(dp), dimension(n), intent(out) vals, complex(dp), dimension(n,n), intent(out) vecs, type(errorhandler), intent(inout) err )

Computes the eigenvalues, and the right eigenvectors of a square matrix.

in	n	The dimension of the matrix.
in,out	а	On input, the N-by-N matrix on which to operate. On output, the contents of this matrix are overwritten.
out	vals	An N-element array containing the eigenvalues of the matrix on output. The eigenvalues are not sorted.
out	vecs	An N-by-N matrix containing the right eigenvectors (one per column) on output.
in,out	err	The errorhandler object. If no error handling is desired, simply pass NULL, and errors will be dealt with by the default internal error handler. Possible errors that may be encountered are as follows.
		<ul> <li>LA_OUT_OF_MEMORY_ERROR: Occurs if local memory must be allocated, and there is insufficient memory available.</li> </ul>
		LA_CONVERGENCE_ERROR: Occurs if the algorithm failed to converge.

Definition at line 1371 of file linalg\_c\_binding.f90.

4.2.2.13 subroutine linalg\_c\_binding::eigen\_gen\_c ( integer(i32), intent(in), value *n*, real(dp), dimension(n, n), intent(inout) *a*, real(dp), dimension(n, n), intent(inout) *b*, complex(dp), dimension(n), intent(out) *alpha*, real(dp), dimension(n), intent(out) *beta*, complex(dp), dimension(n,n), intent(out) *vecs*, type(errorhandler), intent(inout) *err* )

Computes the eigenvalues, and optionally the right eigenvectors of a square matrix assuming the structure of the eigenvalue problem is A\*X = lambda\*B\*X.

## **Parameters**

in	n	The dimension of the matrix.
in, out	а	On input, the N-by-N matrix A. On output, the contents of this matrix are overwritten.
in, out	b	On input, the N-by-N matrix B. On output, the contents of this matrix are overwritten.
out	alpha	An N-element array that, on output, contains the numerator of the eigenvalue ration ALPHA / BETA. Computation of this ratio isn't necessarily as trivial as it seems as it is entirely possible, and likely, that ALPHA / BETA can overflow or underflow. With that said, the values in ALPHA will always be less than and usually comparable with the NORM(A).
out	beta	An N-element array that, on output, contains the denominator used to determine the eigenvalues as ALPHA / BETA. The values in this array will always be less than and usually comparable with the NORM(B).
out	vecs	An N-by-N matrix containing the right eigenvectors (one per column) on output.
in,out	err	The errorhandler object. If no error handling is desired, simply pass NULL, and errors will be dealt with by the default internal error handler. Possible errors that may be encountered are as follows.  • LA_OUT_OF_MEMORY_ERROR: Occurs if local memory must be allocated, and
		there is insufficient memory available.  • LA_CONVERGENCE_ERROR: Occurs if the algorithm failed to converge.

Definition at line 1420 of file linalg\_c\_binding.f90.

4.2.2.14 subroutine linalg\_c\_binding::eigen\_symm\_c ( integer(i32), intent(in), value *n*, logical(c\_bool), intent(in), value *vecs*, real(dp), dimension(n,n), intent(inout) *a*, real(dp), dimension(n), intent(out) *vals*, type(errorhandler), intent(inout) *err* )

Computes the eigenvalues, and optionally the eigenvectors of a real, symmetric matrix.

in	n	The dimension of the matrix.
in	vecs	Set to true to compute the eigenvectors as well as the eigenvalues; else, set to false to just
		compute the eigenvalues.
in,out	а	On input, the N-by-N symmetric matrix on which to operate. On output, and if vecs is set
		to true, the matrix will contain the eigenvectors (one per column) corresponding to each
		eigenvalue in vals. If vecs is set to false, the lower triangular portion of the matrix is
		overwritten.
out	vals	An N-element array that will contain the eigenvalues sorted into ascending order.
in,out	err	The errorhandler object. If no error handling is desired, simply pass NULL, and errors will be dealt with by the default internal error handler. Possible errors that may be encountered are as follows.
		<ul> <li>LA_OUT_OF_MEMORY_ERROR: Occurs if local memory must be allocated, and there is insufficient memory available.</li> </ul>
		LA_CONVERGENCE_ERROR: Occurs if the algorithm failed to converge.
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Definition at line 1332 of file linalg\_c\_binding.f90.

4.2.2.15 subroutine linalg\_c\_binding::form\_lu\_c ( integer(i32), intent(in), value *n*, real(dp), dimension(n,n), intent(inout) *lu*, integer(i32), dimension(n), intent(in) *ipvt*, real(dp), dimension(n,n), intent(out) *u*, real(dp), dimension(n,n), intent(out) *p* 

Extracts the L, U, and P matrices from the output of the lu factor routine.

#### **Parameters**

in	n	The dimension of the original matrix.
in,out	lu	On input, the N-by-N matrix as output by lu_factor. On output, the N-by-N lower triangular
		matrix L.
in	ipvt	The N-element pivot array as output by lu_factor.
out	и	An N-by-N matrix where the U matrix will be written.
out	р	An N-by-N matrix where the row permutation matrix will be written.

## Remarks

This routine allows extraction of the actual "L", "U", and "P" matrices of the decomposition. To use these matrices to solve the system A\*X = B, the following approach is used.

- 1. First, solve the linear system: L\*Y = P\*B for Y.
- 2. Second, solve the linear system: U\*X = Y for X.

Notice, as both L and U are triangular in structure, the above equations can be solved by forward and backward substitution.

## See Also

- Wikipedia
- Wolfram MathWorld

Definition at line 520 of file linalg\_c\_binding.f90.

4.2.2.16 subroutine linalg\_c\_binding::form\_qr\_c ( integer(i32), intent(in), value *m*, integer(i32), intent(in), value *n*, real(dp), dimension(m,n), intent(inout) *r*, real(dp), dimension(min(m,n)), intent(in) *tau*, real(dp), dimension(m,m), intent(out) *q*, type(errorhandler), intent(inout) *err* )

Forms the full M-by-M orthogonal matrix Q from the elementary reflectors returned by the base QR factorization algorithm.

in	m	The number of rows in the original matrix.
in	n	The number of columns in the original matrix.
in,out	r	On input, an M-by-N matrix where the elements below the diagonal contain the elementary reflectors generated from the QR factorization. On and above the diagonal, the matrix contains the matrix R. On output, the elements below the diagonal are zeroed such that the remaining matrix is simply the M-by-N matrix R.

## **Parameters**

in	tau	A MIN(M, N)-element array containing the scalar factors of each elementary reflector defined in r.
out	q	An M-by-M matrix where the full orthogonal matrix Q will be written. In the event that $M > N$ , Q may be supplied as M-by-N, and therefore only return the useful submatrix Q1 (Q = [Q1, Q2]) as the factorization can be written as $Q * R = [Q1, Q2] * [R1; 0]$ .
in,out	err	The errorhandler object. If no error handling is desired, simply pass NULL, and errors will be dealt with by the default internal error handler. Possible errors that may be encountered are as follows.
		LA_ARRAY_SIZE_ERROR: Occurs if the scalar factor array is not sized appropriately.
		<ul> <li>LA_OUT_OF_MEMORY_ERROR: Occurs if local memory must be allocated, and there is insufficient memory available.</li> </ul>

Definition at line 642 of file linalg\_c\_binding.f90.

4.2.2.17 subroutine linalg\_c\_binding::form\_qr\_pivot\_c ( integer(i32), intent(in), value *m*, integer(i32), intent(in), value *n*, real(dp), dimension(m,n), intent(inout) *r*, real(dp), dimension(min(m,n)), intent(in) *tau*, integer(i32), dimension(n), intent(in) *pvt*, real(dp), dimension(m,m), intent(out) *q*, real(dp), dimension(n,n), intent(out) *p*, type(errorhandler), intent(inout) *err* )

Forms the full M-by-M orthogonal matrix Q from the elementary reflectors returned by the base QR factorization algorithm.

## **Parameters**

in	m	The number of rows in the original matrix.
in	n	The number of columns in the original matrix.
in,out	r	On input, an M-by-N matrix where the elements below the diagonal contain the elementary reflectors generated from the QR factorization. On and above the diagonal, the matrix contains the matrix R. On output, the elements below the diagonal are zeroed such that the remaining matrix is simply the M-by-N matrix R.
in	tau	A MIN(M, N)-element array containing the scalar factors of each elementary reflector defined in r.
in	pvt	An N-element column pivot array as returned by the QR factorization.
out	q	An M-by-M matrix where the full orthogonal matrix Q will be written. In the event that $M > N$ , Q may be supplied as M-by-N, and therefore only return the useful submatrix Q1 (Q = [Q1, Q2]) as the factorization can be written as Q * R = [Q1, Q2] * [R1; 0].
out	р	An N-by-N matrix where the pivot matrix will be written.
in,out	err	The errorhandler object. If no error handling is desired, simply pass NULL, and errors will be dealt with by the default internal error handler. Possible errors that may be encountered are as follows.  • LA_ARRAY_SIZE_ERROR: Occurs if the scalar factor array is not sized appropriately.  • LA_OUT_OF_MEMORY_ERROR: Occurs if local memory must be allocated, and there is insufficient memory available.

Definition at line 691 of file linalg\_c\_binding.f90.

4.2.2.18 subroutine linalg\_c\_binding::lu\_factor\_c ( integer(i32), intent(in), value *m,* integer(i32), intent(in), value *n,* real(dp), dimension(m,n), intent(inout) *a,* integer(i32), dimension(min(m,n)), intent(out) *ipvt,* type(errorhandler), intent(inout) *err* 

Computes the LU factorization of an M-by-N matrix.

#### **Parameters**

in	m	The number of rows in the matrix.
in	n	The number of columns in the matrix.
in,out	а	On input, the M-by-N matrix on which to operate. On output, the LU factored matrix in the form [L\U] where the unit diagonal elements of L are not stored.
out	ipvt	An MIN(M, N)-element array used to track row-pivot operations. The array stored pivot information such that row I is interchanged with row IPVT(I).
in,out	err	The errorhandler object. If no error handling is desired, simply pass NULL, and errors will be dealt with by the default internal error handler. Possible errors that may be encountered are as follows.  • LA_ARRAY_SIZE_ERROR: Occurs if the pivot array is not sized appropriately.  • LA_SINGULAR_MATRIX_ERROR: Occurs as a warning if a is found to be singular.

Definition at line 474 of file linalg\_c\_binding.f90.

4.2.2.19 subroutine linalg\_c\_binding::mtx\_inverse\_c ( integer(i32), intent(in), value *n*, real(dp), dimension(n,n), intent(inout) *a*, type(errorhandler), intent(inout) *err* )

Computes the inverse of a square matrix.

## **Parameters**

n	The dimension of the matrix.
а	On input, the N-by-N matrix to invert. On output, the inverted matrix.
err	The errorhandler object. If no error handling is desired, simply pass NULL, and errors will be dealt with by the default internal error handler. Possible errors that may be encountered are as follows.
	<ul> <li>LA_OUT_OF_MEMORY_ERROR: Occurs if local memory must be allocated, and there is insufficient memory available.</li> <li>LA_SINGULAR_MATRIX_ERROR: Occurs if the input matrix is singular.</li> </ul>
	а

Definition at line 1213 of file linalg c binding.f90.

4.2.2.20 subroutine linalg\_c\_binding::mtx\_mult\_c ( logical(c\_bool), intent(in), value transa, logical(c\_bool), intent(in), value transb, integer(i32), intent(in), value m, integer(i32), intent(in), value n, integer(i32), intent(in), value k, real(dp), intent(in), value alpha, real(dp), dimension(lda,\*), intent(in) a, integer(i32), intent(in), value lda, real(dp), dimension(ldb,\*), intent(in) b, integer(i32), intent(in), value ldb, real(dp), intent(in), value beta, real(dp), dimension(m,n), intent(inout) c)

Performs the matrix operation: C = alpha \* op(A) \* op(B) + beta \* C.

## **Parameters**

in	transa	Set to true if $op(A) == A**T$ ; else, set to false if $op(A) == A$ .
in	transb	Set to true if $op(B) == B**T$ ; else, set to false if $op(B) == B$ .
in	m	The number of rows in matrix C, and the number of rows in matrix op(A).
in	n	The number of columns in matrix C, and the number of columns in matrix op(B).
in	k	The number of columns in matrix op(A), and the number of rows in the matrix op(B).
in	alpha	The scalar multiplier to matrix A.
in	а	The M-by-K matrix A.
in	lda	The leading dimension of matrix A. If transa is true, this value must be at least MAX(1, K); else, if transa is false, this value must be at least MAX(1, M).
in	b	The K-by-N matrix B.
in	ldb	The leading dimension of matrix B. If transb is true, this value must be at least MAX(1, N); else, if transb is false, this value must be at least MAX(1, K).
in	beta	The scalar multiplier to matrix C.
in,out	С	The M-by-N matrix C.

Definition at line 46 of file linalg\_c\_binding.f90.

4.2.2.21 subroutine linalg\_c\_binding::mtx\_pinverse\_c ( integer(i32), intent(in), value *m*, integer(i32), intent(in), value *n*, real(dp), dimension(m,n), intent(inout) *a*, real(dp), dimension(n,m), intent(out) *ainv*, type(errorhandler), intent(inout) *err* )

Computes the Moore-Penrose pseudo-inverse of a M-by-N matrix using the singular value decomposition of the matrix.

## **Parameters**

in	т	The number of rows in the matrix to invert.
in	n	The number of columns in the matrix to invert.
in,out	а	On input, the M-by-N matrix to invert. The matrix is overwritten on output.
out	ainv	The N-by-M matrix where the pseudo-inverse of a will be written.
in,out	err	The errorhandler object. If no error handling is desired, simply pass NULL, and errors will be dealt with by the default internal error handler. Possible errors that may be encountered are as follows.
		<ul> <li>LA_OUT_OF_MEMORY_ERROR: Occurs if local memory must be allocated, and there is insufficient memory available.</li> </ul>
		<ul> <li>LA_CONVERGENCE_ERROR: Occurs as a warning if the QR iteration process could not converge to a zero value.</li> </ul>

Definition at line 1250 of file linalg\_c\_binding.f90.

4.2.2.22 integer(i32) function linalg\_c\_binding::mtx\_rank\_c ( integer(i32), intent(in), value *m*, integer(i32), intent(in), value *n*, real(dp), dimension(m,n), intent(inout) *a*, type(errorhandler), intent(inout) *err* )

Computes the rank of a matrix.

in	m	The number of rows in the matrix.
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## **Parameters**

in	n	The number of columns in the matrix.
in,out	а	On input, the M-by-N matrix of interest. On output, the contents of the matrix are overwritten.
in,out	err	The errorhandler object. If no error handling is desired, simply pass NULL, and errors will be dealt with by the default internal error handler. Possible errors that may be encountered are as follows.
		<ul> <li>LA_ARRAY_SIZE_ERROR: Occurs if any of the input arrays are not sized appropriately.</li> </ul>
		<ul> <li>LA_OUT_OF_MEMORY_ERROR: Occurs if local memory must be allocated, and there is insufficient memory available.</li> </ul>
		<ul> <li>LA_CONVERGENCE_ERROR: Occurs as a warning if the QR iteration process could not converge to a zero value.</li> </ul>

Definition at line 340 of file linalg\_c\_binding.f90.

4.2.2.23 subroutine linalg\_c\_binding::mult\_qr\_c ( logical(c\_bool), intent(in), value *trans*, integer(i32), intent(in), value *m*, integer(i32), intent(in), value *n*, real(dp), dimension(m,m), intent(inout) *q*, real(dp), dimension(min(m,n)), intent(in) *tau*, real(dp), dimension(m,n), intent(inout) *c*, type(errorhandler), intent(inout) *err* )

Multiplies a general matrix by the orthogonal matrix Q from a QR factorization such that: C = op(Q) \* C.

## **Parameters**

in	trans	Set to true to apply Q**T; else, set to false.
in	m	The number of rows in the matrix c.
in	n	The number of columns in the matrix $c$ .
in	q	On input, an M-by-M matrix containing the elementary reflectors output from the QR factorization. Notice, the contents of this matrix are restored on exit. that the remaining matrix is simply the M-by-N matrix R.
in	tau	A MIN(M,N)-element array containing the scalar factors of each elementary reflector defined in a.
in,out	С	On input, the M-by-N matrix C. On output, the product of the orthogonal matrix Q and the original matrix C.
in,out	err	<ul> <li>The errorhandler object. If no error handling is desired, simply pass NULL, and errors will be dealt with by the default internal error handler. Possible errors that may be encountered are as follows.</li> <li>LA_ARRAY_SIZE_ERROR: Occurs if the scalar factor array is not sized appropriately.</li> <li>LA_OUT_OF_MEMORY_ERROR: Occurs if local memory must be allocated, and</li> </ul>
		there is insufficient memory available.

Definition at line 736 of file linalg\_c\_binding.f90.

4.2.2.24 subroutine linalg\_c\_binding::mult\_rz\_c ( logical(c\_bool), intent(in), value *trans*, integer(i32), intent(in), value *m*, integer(i32), intent(in), value *n*, integer(i32), intent(in), value *l*, real(dp), dimension(m,m), intent(inout) *a*, real(dp), dimension(m), intent(in) *tau*, real(dp), dimension(m,n), intent(inout) *c*, type(errorhandler), intent(inout) *err* )

Multiplies a general matrix by the orthogonal matrix Z from an RZ factorization such that: C = op(Z) \* C.

## **Parameters**

in	trans	Set to true to apply Z**T; else, set to false.
in	m	The number of rows in the matrix c.
in	n	The number of columns in the matrix c.
in	1	The number of columns in matrix a containing the meaningful part of the Householder vectors (M $>=$ L $>=$ 0).
in,out	а	On input, the M-by-M matrix Z as output by $rz\_factor$ . The matrix is used as in-place storage during execution; however, the contents of the matrix are restored on exit.
in	tau	An M-element array containing the scalar factors of the elementary reflectors found in a.
in,out	С	On input, the M-by-N matrix C. On output, the product of the orthogonal matrix Z and the original matrix C.
in,out	err	The errorhandler object. If no error handling is desired, simply pass NULL, and errors will be dealt with by the default internal error handler. Possible errors that may be encountered are as follows.  • LA_OUT_OF_MEMORY_ERROR: Occurs if local memory must be allocated, and there is insufficient memory available.

Definition at line 968 of file linalg\_c\_binding.f90.

4.2.2.25 subroutine linalg\_c\_binding::qr\_factor\_c ( integer(i32), intent(in), value *m*, integer(i32), intent(in), value *n*, real(dp), dimension(m,n), intent(inout) *a*, real(dp), dimension(min(m,n)), intent(out) *tau*, type(errorhandler), intent(inout) *err* )

Computes the QR factorization of an M-by-N matrix without pivoting.

## **Parameters**

in	m	The number of rows in the matrix.
in	n	The number of columns in the matrix.
in,out	а	On input, the M-by-N matrix to factor. On output, the elements on and above the diagonal contain the MIN(M, N)-by-N upper trapezoidal matrix R (R is upper triangular if $M \ge N$ ). The elements below the diagonal, along with the array tau, represent the orthogonal matrix Q as a product of elementary reflectors.
out	tau	A MIN(M, N)-element array used to store the scalar factors of the elementary reflectors.
in,out	err	The errorhandler object. If no error handling is desired, simply pass NULL, and errors will be dealt with by the default internal error handler. Possible errors that may be encountered are as follows.
		<ul> <li>LA_ARRAY_SIZE_ERROR: Occurs if the scalar factor array is not sized appropriately.</li> </ul>
		<ul> <li>LA_OUT_OF_MEMORY_ERROR: Occurs if local memory must be allocated, and there is insufficient memory available.</li> </ul>

Definition at line 552 of file linalg\_c\_binding.f90.

4.2.2.26 subroutine linalg\_c\_binding::qr\_factor\_pivot\_c ( integer(i32), intent(in), value *m*, integer(i32), intent(in), value *n*, real(dp), dimension(m,n), intent(inout) *a*, real(dp), dimension(min(m,n)), intent(out) *tau*, integer(i32), dimension(n), intent(inout) *jpvt*, type(errorhandler), intent(inout) *err* )

Computes the QR factorization of an M-by-N matrix with column pivoting such that A \* P = Q \* R.

## **Parameters**

in	m	The number of rows in the matrix.
in	n	The number of columns in the matrix.
in,out	а	On input, the M-by-N matrix to factor. On output, the elements on and above the diagonal contain the MIN(M, N)-by-N upper trapezoidal matrix R (R is upper triangular if $M \ge N$ ). The elements below the diagonal, along with the array tau, represent the orthogonal matrix Q as a product of elementary reflectors.
out	tau	A MIN(M, N)-element array used to store the scalar factors of the elementary reflectors.
in,out	jpvt	On input, an N-element array that if $JPVT(I)$ .ne. 0, the I-th column of A is permuted to the front of A $*$ P; if $JPVT(I) = 0$ , the I-th column of A is a free column. On output, if $JPVT(I) = K$ , then the I-th column of A $*$ P was the K-th column of A.
in,out	err	The errorhandler object. If no error handling is desired, simply pass NULL, and errors will be dealt with by the default internal error handler. Possible errors that may be encountered are as follows.  • LA_ARRAY_SIZE_ERROR: Occurs if the scalar factor array is not sized appropriately.  • LA_OUT_OF_MEMORY_ERROR: Occurs if local memory must be allocated, and there is insufficient memory available.

Definition at line 597 of file linalg\_c\_binding.f90.

4.2.2.27 subroutine linalg\_c\_binding::qr\_rank1\_update\_c ( integer(i32), intent(in), value *m*, integer(i32), intent(in), value *n*, real(dp), dimension(m,m), intent(inout) *q*, real(dp), dimension(m,n), intent(inout) *r*, real(dp), dimension(m), intent(inout) *u*, real(dp), dimension(n), intent(inout) *v*, type(errorhandler), intent(inout) *err* )

Computes the rank 1 update to an M-by-N QR factored matrix A (M >= N) where A = Q \* R, and A1 = A + U \* V\*\*T such that A1 = Q1 \* R1.

## **Parameters**

in	m	The number of rows in the original matrix.
in	n	The number of columns in the original matrix.
in,out	q	On input, the original M-by-M orthogonal matrix Q. On output, the updated matrix Q1.
in,out	r	On input, the M-by-N matrix R. On output, the updated matrix R1.
in,out	и	On input, the M-element U update vector. On output, the original content of the array is overwritten.
in,out	V	On input, the N-element V update vector. On output, the original content of the array is overwritten.
in,out	err	The errorhandler object. If no error handling is desired, simply pass NULL, and errors will be dealt with by the default internal error handler. Possible errors that may be encountered are as follows.  • LA_OUT_OF_MEMORY_ERROR: Occurs if local memory must be allocated, and there is insufficient memory available.

Definition at line 777 of file linalg\_c\_binding.f90.

4.2.2.28 subroutine linalg\_c\_binding::rank1\_update\_c ( integer(i32), intent(in), value *m*, integer(i32), intent(in), value *n*, real(dp), intent(in), value *alpha*, real(dp), dimension(m), intent(in) *x*, real(dp), dimension(n), intent(in) *y*, real(dp), dimension(m,n), intent(inout) *a* )

Performs the rank-1 update to matrix A such that: A = alpha \* X \* Y \* \* T + A, where A is an M-by-N matrix, alpha is a scalar, X is an M-element array, and N is an N-element array.

#### **Parameters**

in	m	The number of elements in $\mathbf{x}$ , and the number of rows in matrix $\mathbf{a}$ .
in	n	The number of elements in $y$ , and the number of columns in matrix $a$ .
in	alpha	The scalar multiplier.
in	x	An M-element array.
in	У	An N-element array.
in,out	а	On input, the M-by-N matrix to update. On output, the updated M-by-N matrix.

#### **Notes**

This routine is based upon the BLAS routine DGER.

Definition at line 293 of file linalg c binding.f90.

4.2.2.29 subroutine linalg\_c\_binding::rz\_factor\_c ( integer(i32), intent(in), value *m*, integer(i32), intent(in), value *n*, real(dp), dimension(m,n), intent(inout) *a*, real(dp), dimension(m), intent(out) *tau*, type(errorhandler), intent(inout) *err* )

Factors an upper trapezoidal matrix by means of orthogonal transformations such that  $A = R * Z = (R \ 0) * Z$ . Z is an orthogonal matrix of dimension N-by-N, and R is an M-by-M upper triangular matrix.

#### **Parameters**

in	m	The number of rows in the original matrix.
in	n	The number of columns in the original matrix.
in,out	а	On input, the M-by-N upper trapezoidal matrix to factor. On output, the leading M-by-M upper triangular part of the matrix contains the upper triangular matrix R, and elements N-L+1 to N of the first M rows of A, with the array tau, represent the orthogonal matrix Z as a product of M elementary reflectors.
out	tau	An M-element array used to store the scalar factors of the elementary reflectors.
in,out	err	The errorhandler object. If no error handling is desired, simply pass NULL, and errors will be dealt with by the default internal error handler. Possible errors that may be encountered are as follows.  • LA_OUT_OF_MEMORY_ERROR: Occurs if local memory must be allocated, and there is insufficient memory available.

Definition at line 926 of file linalg\_c\_binding.f90.

4.2.2.30 subroutine linalg\_c\_binding::solve\_cholesky\_c ( logical(c\_bool), intent(in), value *upper*, integer(i32), intent(in), value *n*, integer(i32), intent(in), value *nrhs*, real(dp), dimension(n,n), intent(in) *a*, real(dp), dimension(n,nrhs), intent(inout) *b* )

Solves a system of Cholesky factored equations.

#### **Parameters**

in	upper	Set to true if the original matrix A was factored such that $A = U**T*U$ ; else, set to false if
		the factorization of A was $A = L**T*L$ .
in	n	The dimension of the original matrix a.
in	nrhs	The number of right-hand-side vectors (number of columns in matrix b).
in	а	The N-by-N Cholesky factored matrix.
in,out	b	On input, the N-by-NRHS right-hand-side matrix B. On output, the solution matrix X.

Definition at line 1189 of file linalg\_c\_binding.f90.

4.2.2.31 subroutine linalg\_c\_binding::solve\_least\_squares\_c ( integer(i32), intent(in), value *m*, integer(i32), intent(in), value *n*, integer(i32), intent(in), value *n*, real(dp), dimension(m, n), intent(inout) *a*, real(dp), dimension(max(m,n), nrhs), intent(inout) *b*, type(errorhandler), intent(inout) *err* )

Solves the overdetermined or underdetermined system (A\*X = B) of M equations of N unknowns using a QR or LQ factorization of the matrix A. Notice, it is assumed that matrix A has full rank.

#### **Parameters**

in	т	The number of rows in the original coefficient matrix A.
in	n	The number of columns in the original coefficient matrix A.
in	nrhs	The number of right-hand-side vectors (number of columns in matrix b).
in,out	а	On input, the M-by-N matrix A. On output, the matrix is overwritten by the details of its complete orthogonal factorization.
in,out	b	If $M >= N$ , the M-by-NRHS matrix B. On output, the first N rows contain the N-by-NRHS solution matrix X. If $M < N$ , an N-by-NRHS matrix with the first M rows containing the matrix B. On output, the N-by-NRHS solution matrix X.
in,out	err	The errorhandler object. If no error handling is desired, simply pass NULL, and errors will be dealt with by the default internal error handler. Possible errors that may be encountered are as follows.  • LA OUT OF MEMORY ERROR: Occurs if local memory must be allocated, and
		there is insufficient memory available.

Definition at line 1291 of file linalg c binding.f90.

4.2.2.32 subroutine linalg\_c\_binding::solve\_lu\_c ( integer(i32), intent(in), value *n*, integer(i32), intent(in), value *n*, real(dp), dimension(n,n), intent(in) *a*, integer(i32), dimension(n), intent(in) *ipvt*, real(dp), dimension(n,nrhs), intent(inout) *b* )

Solves a system of LU-factored equations.

in	n	The dimension of the original matrix a.
in	nrhs	The number of right-hand-side vectors (number of columns in matrix b).
in	а	The N-by-N LU factored matrix as output by lu_factor.
in	ipvt	The N-element pivot array as output by lu_factor.
in,out	b	On input, the N-by-NRHS right-hand-side matrix. On output, the N-by-NRHS solution matrix.

Definition at line 1078 of file linalg\_c\_binding.f90.

4.2.2.33 subroutine linalg\_c\_binding::solve\_qr\_c ( integer(i32), intent(in), value *m*, integer(i32), intent(in), value *nrhs*, real(dp), dimension(m,n), intent(inout) *a*, real(dp), dimension(min(m,n)), intent(in) *tau*, real(dp), dimension(m,nrhs), intent(inout) *b*, type(errorhandler), intent(inout) *err* )

Solves a system of M QR-factored equations of N unknowns where  $M \ge N$ .

#### **Parameters**

in	m	The number of rows in the original coefficient matrix A.
in	n	The number of columns in the original coefficient matrix A.
in	nrhs	The number of right-hand-side vectors (number of columns in matrix b).
in	а	On input, the M-by-N QR factored matrix as returned by qr_factor. On output, the contents of this matrix are restored. Notice, M must be greater than or equal to N.
in	tau	A MIN(M, N)-element array containing the scalar factors of the elementary reflectors as returned by qr_factor.
in	b	On input, the M-by-NRHS right-hand-side matrix. On output, the first N columns are overwritten by the solution matrix X.
in,out	err	The errorhandler object. If no error handling is desired, simply pass NULL, and errors will be dealt with by the default internal error handler. Possible errors that may be encountered are as follows.  • LA_OUT_OF_MEMORY_ERROR: Occurs if local memory must be allocated, and there is insufficient memory available.

Definition at line 1111 of file linalg\_c\_binding.f90.

4.2.2.34 subroutine linalg\_c\_binding::solve\_qr\_pivot\_c ( integer(i32), intent(in), value *m*, integer(i32), intent(in), value *nrhs*, real(dp), dimension(m,n), intent(inout) *a*, real(dp), dimension(min(m,n)), intent(inout) *tau*, integer(i32), dimension(n), intent(in) *jpvt*, real(dp), dimension(max(m,n),nrhs), intent(inout) *b*, type(errorhandler), intent(inout) *err* )

Solves a system of M QR-factored equations of N unknowns where the QR factorization made use of column pivoting.

in	m	The number of rows in the original coefficient matrix A.
in	n	The number of columns in the original coefficient matrix A.
in	nrhs	The number of right-hand-side vectors (number of columns in matrix b).
in	а	On input, the M-by-N QR factored matrix as returned by qr_factor. On output, the contents of this matrix are altered.
in	tau	A MIN(M, N)-element array containing the scalar factors of the elementary reflectors as returned by qr_factor.
in	jpvt	An N-element array, as output by qr_factor, used to track the column pivots.
in	b	On input, the MAX(M, N)-by-NRHS matrix where the first M rows contain the right-hand-side matrix B. On output, the first N rows are overwritten by the solution matrix X.

#### **Parameters**

in,out	err	The errorhandler object. If no error handling is desired, simply pass NULL, and errors will be dealt with by the default internal error handler. Possible errors that may be encountered are as follows.
		<ul> <li>LA_ARRAY_SIZE_ERROR: Occurs if any of the input arrays are not sized appropriately.</li> </ul>
		<ul> <li>LA_OUT_OF_MEMORY_ERROR: Occurs if local memory must be allocated, and there is insufficient memory available.</li> </ul>

Definition at line 1156 of file linalg\_c\_binding.f90.

4.2.2.35 subroutine linalg\_c\_binding::solve\_tri\_mtx\_c ( logical(c\_bool), intent(in), value *upper*, logical(c\_bool), intent(in), value *trans*, logical(c\_bool), intent(in), value *nounit*, integer(i32), intent(in), value *n*, integer(i32), intent(in), value *nrhs*, real(dp), intent(in), value *alpha*, real(dp), dimension(n,n), intent(in) *a*, real(dp), dimension(n,nrhs), intent(inout) *b* )

Solves one of the matrix equations: op(A) \* X = alpha \* B, where A is a triangular matrix.

## **Parameters**

in	upper	Set to true if A is an upper triangular matrix; else, set to false if A is a lower triangular matrix.
in	trans	Set to true if $op(A) = A**T$ ; else, set to false if $op(A) = A$ .
in	nounit	Set to true if A is not a unit-diagonal matrix (ones on every diagonal element); else, set to false if A is a unit-diagonal matrix.
in	n	The dimension of the triangular matrix a.
in	nrhs	The number of right-hand-side vectors (number of columns in matrix b).
in	alpha	The scalar multiplier to B.
in	а	N-by-N triangular matrix on which to operate.
in,out	b	On input, the N-by-NRHS right-hand-side. On output, the N-by-NRHS solution.

Definition at line 1055 of file linalg\_c\_binding.f90.

4.2.2.36 subroutine linalg\_c\_binding::svd\_c ( integer(i32), intent(in), value *m*, integer(i32), intent(in), value *n*, real(dp), dimension(m,n), intent(inout) *a*, real(dp), dimension(min(m,n)), intent(out) *s*, real(dp), dimension(m,m), intent(out) *vt*, type(errorhandler), intent(inout) *err* )

Computes the singular value decomposition of a matrix A. The SVD is defined as: A = U \* S \* V \* \* T, where U is an M-by-M orthogonal matrix, S is an M-by-N diagonal matrix, and V is an N-by-N orthogonal matrix.

in	m	The number of rows in the original matrix.
in	n	The number of columns in the original matrix.
in,out	а	On input, the M-by-N matrix to factor. The matrix is overwritten on output. that the remaining matrix is simply the M-by-N matrix R.
out	s	A MIN(M, N)-element array containing the singular values of a sorted in descending order.
out	и	An M-by-M matrix that on output contains the left singular vectors (matrix U in the decomposition: $A = U * S * V * * T$ )

## **Parameters**

out	vt	An N-by-N matrix that on output contains the right singular vectors (matrix $V**T$ in the decomposition: $A = U * S * V**T$ ).
in,out	err	The errorhandler object. If no error handling is desired, simply pass NULL, and errors will be dealt with by the default internal error handler. Possible errors that may be encountered are as follows.
		<ul> <li>LA_ARRAY_SIZE_ERROR: Occurs if the singular value array is not sized appropriately.</li> </ul>
		<ul> <li>LA_OUT_OF_MEMORY_ERROR: Occurs if local memory must be allocated, and there is insufficient memory available.</li> </ul>
		<ul> <li>LA_CONVERGENCE_ERROR: Occurs as a warning if the QR iteration process could not converge to a zero value.</li> </ul>

Definition at line 1015 of file linalg\_c\_binding.f90.

4.2.2.37 subroutine linalg\_c\_binding::swap\_c ( integer(i32), intent(in), value n, real(dp), dimension(n), intent(inout) x, real(dp), dimension(n), intent(inout) y )

Swaps the contents of two arrays.

#### **Parameters**

in	n	The number of elements either array.
in,out	Х	One of the N-element arrays.
in,out	у	The other N-element array.

Definition at line 398 of file linalg\_c\_binding.f90.

4.2.2.38 pure real(dp) function linalg\_c\_binding::trace\_c ( integer(i32), intent(in), value *m*, integer(i32), intent(in), value *n*, real(dp), dimension(m,n), intent(in) *x* )

Computes the trace of a matrix (the sum of the main diagonal elements).

## **Parameters**

in	m	The number of rows in the matrix.
in	n	The number of columns in the matrix.
in	Х	The matrix on which to operate.

## Returns

The trace of  $\boldsymbol{x}$ .

Definition at line 313 of file linalg\_c\_binding.f90.

## 4.3 linalg\_constants Module Reference

## linalg\_constants

#### **Variables**

• integer, parameter dp = real64

Defines a double-precision (64-bit) floating-point type.

• integer, parameter i32 = int32

Defines a 32-bit signed integer type.

• integer, parameter la\_invalid\_input\_error = 101

An error flag denoting an invalid input.

• integer, parameter la\_array\_size\_error = 102

An error flag denoting an improperly sized array.

• integer, parameter la\_singular\_matrix\_error = 103

An error flag denoting a singular matrix.

• integer, parameter la\_matrix\_format\_error = 104

An error flag denoting an issue with the matrix format.

• integer, parameter la\_out\_of\_memory\_error = 105

An error flag denoting that there is insufficient memory available.

• integer, parameter la\_convergence\_error = 106

An error flag denoting a convergence failure.

• integer, parameter la\_invalid\_operation\_error = 107

An error resulting from an invalid operation.

## 4.3.1 Detailed Description

## linalg\_constants

## Purpose

Provides a set of constants and error flags for the library.

## 4.4 linalg\_core Module Reference

## linalg\_core

## **Data Types**

• interface diag\_mtx\_mult

Multiplies a diagonal matrix with another matrix or array.

• interface mtx\_mult

Performs the matrix operation: C = alpha \* op(A) \* op(B) + beta \* C.

#### **Functions/Subroutines**

• subroutine mtx\_mult\_mtx (transa, transb, alpha, a, b, beta, c, err)

Performs the matrix operation: C = alpha \* op(A) \* op(B) + beta \* C.

subroutine mtx\_mult\_vec (trans, alpha, a, b, beta, c, err)

Performs the matrix-vector operation: c = alpha \* op(A) \* b + beta \* c.

• subroutine, public rank1\_update (alpha, x, y, a, err)

Performs the rank-1 update to matrix A such that: A = alpha \* X \* Y \* \* T + A, where A is an M-by-N matrix, alpha is a scalar, X is an M-element array, and N is an N-element array.

• subroutine diag\_mtx\_mult\_mtx (Iside, trans, alpha, a, b, beta, c, err)

Computes the matrix operation: C = alpha \* A \* op(B) + beta \* C, or C = alpha \* op(B) \* A + beta \* C.

• subroutine diag mtx mult mtx2 (Iside, alpha, a, b, err)

Computes the matrix operation: B = alpha \* A \* op(B), or B = alpha \* op(B) \* A.

subroutine diag mtx mult mtx3 (Iside, trans, alpha, a, b, beta, c, err)

Computes the matrix operation: C = alpha \* A \* op(B) + beta \* C, or C = alpha \* op(B) \* A + beta \* C, where A and C are complex-valued.

• subroutine diag\_mtx\_mult\_mtx4 (Iside, trans, alpha, a, b, beta, c, err)

Computes the matrix operation: C = alpha \* A \* op(B) + beta \* C, or C = alpha \* op(B) \* A + beta \* C, where A, B, and C are complex-valued.

pure real(dp) function, public trace (x)

Computes the trace of a matrix (the sum of the main diagonal elements).

integer(i32) function, public mtx rank (a, tol, work, olwork, err)

Computes the rank of a matrix.

• real(dp) function, public det (a, iwork, err)

Computes the determinant of a square matrix.

• subroutine, public swap (x, y, err)

Swaps the contents of two arrays.

• subroutine, public recip\_mult\_array (a, x)

Multiplies a vector by the reciprocal of a real scalar.

• subroutine, public tri mtx mult (upper, alpha, a, beta, b, err)

Computes the triangular matrix operation: B = alpha \* A\*\*T \* A + beta \* B, or B = alpha \* A \* A\*\*T + beta \* B, where A is a triangular matrix.

#### 4.4.1 Detailed Description

## linalg\_core

## Purpose

Provides common "core" linear algebra routines.

## 4.4.2 Function/Subroutine Documentation

4.4.2.1 real(dp) function, public linalg\_core::det ( real(dp), dimension(:,:), intent(inout) a, integer(i32), dimension(:), intent(out), optional, pointer iwork, class(errors), intent(inout), optional, target err )

Computes the determinant of a square matrix.

## **Parameters**

in,out	а	On input, the N-by-N matrix on which to operate. On output the contents are overwritten by the LU factorization of the original matrix.
out	iwork	An optional input, that if provided, prevents any local memory allocation. If not provided, the memory required is allocated within. If provided, the length of the array must be at least N-elements.
out	err	An optional errors-based object that if provided can be used to retrieve information relating to any errors encountered during execution. If not provided, a default implementation of the errors class is used internally to provide error handling. Possible errors and warning messages that may be encountered are as follows.
		<ul> <li>LA_ARRAY_SIZE_ERROR: Occurs if any of the input arrays are not sized appropriately.</li> </ul>
		<ul> <li>LA_OUT_OF_MEMORY_ERROR: Occurs if local memory must be allocated, and there is insufficient memory available.</li> </ul>

## Returns

The determinant of a.

Definition at line 1086 of file linalg\_core.f90.

4.4.2.2 subroutine linalg\_core::diag\_mtx\_mult\_mtx ( logical, intent(in) *lside*, logical, intent(in) *trans*, real(dp) *alpha*, real(dp), dimension(:), intent(in) *a*, real(dp), dimension(:,:), intent(in) *b*, real(dp) *beta*, real(dp), dimension(:,:), intent(inout) *c*, class(errors), intent(inout), optional, target *err* ) [private]

Computes the matrix operation: C = alpha \* A \* op(B) + beta \* C, or C = alpha \* op(B) \* A + beta \* C.

in	Iside	Set to true to apply matrix A from the left; else, set to false to apply matrix A from the left.
in	trans	Set to true if $op(B) == B**T$ ; else, set to false if $op(B) == B$ .
in	alpha	A scalar multiplier.
in	а	A K-element array containing the diagonal elements of A where $K = MIN(M,P)$ if lside is true; else, if lside is false, $K = MIN(N,P)$ .
in	b	The LDB-by-TDB matrix B where (LDB = leading dimension of B, and TDB = trailing dimension of B):  • lside == true & trans == true: LDB = N, TDB = P  • lside == true & trans == false: LDB = P, TDB = N  • lside == false & trans == true: LDB = P, TDB = M  • lside == false & trans == false: LDB = M, TDB = P
in	beta	A scalar multiplier.
in,out	С	On input, the M-by-N matrix C. On output, the resulting M-by-N matrix.
out	err	An optional errors-based object that if provided can be used to retrieve information relating to any errors encountered during execution. If not provided, a default implementation of the errors class is used internally to provide error handling. Possible errors and warning messages that may be encountered are as follows.
		LA_ARRAY_SIZE_ERROR: Occurs if any of the input array sizes are incorrect.

Definition at line 327 of file linalg\_core.f90.

4.4.2.3 subroutine linalg\_core::diag\_mtx\_mult\_mtx2 ( logical, intent(in) *lside*, real(dp), intent(in) *alpha*, real(dp), dimension(:), intent(in) *a*, real(dp), dimension(:,:), intent(inout) *b*, class(errors), intent(inout), optional, target *err* ) [private]

Computes the matrix operation: B = alpha \* A \* op(B), or B = alpha \* op(B) \* A.

#### **Parameters**

in	Iside	Set to true to apply matrix A from the left; else, set to false to apply matrix A from the left.
in	alpha	A scalar multiplier.
in	а	A K-element array containing the diagonal elements of A where $K = MIN(M,P)$ if lside is true; else, if lside is false, $K = MIN(N,P)$ .
in	b	On input, the M-by-N matrix B. On output, the resulting M-by-N matrix.
out	err	An optional errors-based object that if provided can be used to retrieve information relating to any errors encountered during execution. If not provided, a default implementation of the errors class is used internally to provide error handling. Possible errors and warning messages that may be encountered are as follows.
		LA_ARRAY_SIZE_ERROR: Occurs if any of the input array sizes are incorrect.

Definition at line 494 of file linalg\_core.f90.

4.4.2.4 subroutine linalg\_core::diag\_mtx\_mult\_mtx3 ( logical, intent(in) *lside*, logical, intent(in) *trans*, real(dp) *alpha*, complex(dp), dimension(:,:), intent(in) *b*, real(dp) *beta*, complex(dp), dimension(:,:), intent(inout) *c*, class(errors), intent(inout), optional, target *err* ) [private]

Computes the matrix operation: C = alpha \* A \* op(B) + beta \* C, or C = alpha \* op(B) \* A + beta \* C, where A and C are complex-valued.

Iside	Set to true to apply matrix A from the left; else, set to false to apply matrix A from the left.
trans	Set to true if $op(B) == B**T$ ; else, set to false if $op(B) == B$ .
alpha	A scalar multiplier.
а	A K-element array containing the diagonal elements of A where $K = MIN(M,P)$ if lside is true; else, if lside is false, $K = MIN(N,P)$ .
b	The LDB-by-TDB matrix B where (LDB = leading dimension of B, and TDB = trailing dimension of B):  • lside == true & trans == true: LDB = N, TDB = P
	1Side == (ide & clais == (ide. LDD = N, IDD = I
	• lside == true & trans == false: LDB = P, TDB = N
	• lside == false & trans == true: LDB = P, TDB = M
	• lside == false & trans == false: LDB = M, TDB = P
beta	A scalar multiplier.
С	On input, the M-by-N matrix C. On output, the resulting M-by-N matrix.
err	An optional errors-based object that if provided can be used to retrieve information relating to any errors encountered during execution. If not provided, a default implementation of the errors class is used internally to provide error handling. Possible errors and warning messages that may be encountered are as follows.  • LA_ARRAY_SIZE_ERROR: Occurs if any of the input array sizes are incorrect.
	beta

Definition at line 577 of file linalg\_core.f90.

4.4.2.5 subroutine linalg\_core::diag\_mtx\_mult\_mtx4 ( logical, intent(in) *lside*, logical, intent(in) *trans*, real(dp) *alpha*, complex(dp), dimension(:,:), intent(in) *b*, real(dp) *beta*, complex(dp), dimension(:,:), intent(inout) *c*, class(errors), intent(inout), optional, target *err* ) [private]

Computes the matrix operation: C = alpha \* A \* op(B) + beta \* C, or C = alpha \* op(B) \* A + beta \* C, where A, B, and C are complex-valued.

## **Parameters**

in	Iside	Set to true to apply matrix A from the left; else, set to false to apply matrix A from the left.
in	trans	Set to true if $op(B) == B**T$ ; else, set to false if $op(B) == B$ .
in	alpha	A scalar multiplier.
in	а	A K-element array containing the diagonal elements of A where $K = MIN(M,P)$ if lside is true; else, if lside is false, $K = MIN(N,P)$ .
in	b	The LDB-by-TDB matrix B where:
		• lside == true & trans == true: LDA = N, TDB = P
		• lside == true & trans == false: LDA = P, TDB = N
		• lside == false & trans == true: LDA = P, TDB = M
		• lside == false & trans == false: LDA = M, TDB = P
in	beta	A scalar multiplier.
in,out	С	On input, the M-by-N matrix C. On output, the resulting M-by-N matrix.
out	err	An optional errors-based object that if provided can be used to retrieve information relating to any errors encountered during execution. If not provided, a default implementation of the errors class is used internally to provide error handling. Possible errors and warning messages that may be encountered are as follows.  • LA_ARRAY_SIZE_ERROR: Occurs if any of the input array sizes are incorrect.

Definition at line 753 of file linalg\_core.f90.

4.4.2.6 subroutine linalg\_core::mtx\_mult\_mtx ( logical, intent(in) transa, logical, intent(in) transb, real(dp), intent(in) alpha, real(dp), dimension(:,:), intent(in) a, real(dp), dimension(:,:), intent(in) b, real(dp), intent(in) beta, real(dp), dimension(:,:), intent(inout) c, class(errors), intent(inout), optional, target err ) [private]

Performs the matrix operation: C = alpha \* op(A) \* op(B) + beta \* C.

in	transa	Set to true if $op(A) = A**T$ ; else, set to false for $op(A) = A$ .
in	transb	Set to true if $op(B) = B**T$ ; else, set to false for $op(B) = B$ .
in	alpha	A scalar multiplier.
in	а	If transa is set to true, an K-by-M matrix; else, if transa is set to false, an M-by-K matrix.
in	b	If transb is set to true, an N-by-K matrix; else, if transb is set to false, a K-by-N matrix.
in	beta	A scalar multiplier.
in,out	С	On input, the M-by-N matrix C. On output, the M-by-N result.

## **Parameters**

out	err	An optional errors-based object that if provided can be used to retrieve information relating to any errors encountered during execution. If not provided, a default
		implementation of the errors class is used internally to provide error handling. Possible errors and warning messages that may be encountered are as follows.
		LA_ARRAY_SIZE_ERROR: Occurs if any of the input array sizes are incorrect.

#### Notes

This routine utilizes the BLAS routine DGEMM.

Definition at line 83 of file linalg\_core.f90.

4.4.2.7 subroutine linalg\_core::mtx\_mult\_vec ( logical, intent(in) trans, real(dp), intent(in) alpha, real(dp), dimension(:,:), intent(in) a, real(dp), dimension(:), intent(in) b, real(dp), intent(in) beta, real(dp), dimension(:), intent(inout) c, class(errors), intent(inout), optional, target err ) [private]

Performs the matrix-vector operation: c = alpha \* op(A) \* b + beta \* c.

#### **Parameters**

in	trans	Set to true if $op(A) = A**T$ ; else, set to false for $op(A) = A$ .
in	alpha	A scalar multiplier.
in	а	The M-by-N matrix A.
in	b	If trans is set to true, an M-element array; else, if trans is set to false, an N-element
		array.
in	beta	A scalar multiplier.
in, out	С	On input, if trans is set to true, an N-element array; else, if trans is set to false, an
		M-element array. On output, the results of the operation.
out	err	An optional errors-based object that if provided can be used to retrieve information relating to any errors encountered during execution. If not provided, a default implementation of the errors class is used internally to provide error handling. Possible errors and warning messages that may be encountered are as follows.  • LA_ARRAY_SIZE_ERROR: Occurs if any of the input array sizes are incorrect.

## Notes

This routine utilizes the BLAS routine DGEMV.

Definition at line 177 of file linalg\_core.f90.

4.4.2.8 integer(i32) function, public linalg\_core::mtx\_rank ( real(dp), dimension(:,:), intent(inout) a, real(dp), intent(in), optional tol, real(dp), dimension(:), intent(out), optional, pointer work, integer(i32), intent(out), optional olwork, class(errors), intent(inout), optional, target err)

Computes the rank of a matrix.

## **Parameters**

in,out	а	On input, the M-by-N matrix of interest. On output, the contents of the matrix are overwritten.
in	tol	An optional input, that if supplied, overrides the default tolerance on singular values such that singular values less than this tolerance are treated as zero. The default tolerance is: MAX(M, N) * EPS * MAX(S). If the supplied value is less than the smallest value that causes an overflow if inverted, the tolerance reverts back to its default value, and the operation continues; however, a warning message is issued.
out	work	An optional input, that if provided, prevents any local memory allocation. If not provided, the memory required is allocated within. If provided, the length of the array must be at least olwork.
out	olwork	An optional output used to determine workspace size. If supplied, the routine determines the optimal size for $\mathtt{work}$ , and returns without performing any actual calculations.
out	err	An optional errors-based object that if provided can be used to retrieve information relating to any errors encountered during execution. If not provided, a default implementation of the errors class is used internally to provide error handling. Possible errors and warning messages that may be encountered are as follows.
		<ul> <li>LA_ARRAY_SIZE_ERROR: Occurs if any of the input arrays are not sized appropriately.</li> </ul>
		<ul> <li>LA_OUT_OF_MEMORY_ERROR: Occurs if local memory must be allocated, and there is insufficient memory available.</li> </ul>
		<ul> <li>LA_CONVERGENCE_ERROR: Occurs as a warning if the QR iteration process could not converge to a zero value.</li> </ul>

## See Also

• Wolfram MathWorld

Definition at line 966 of file linalg\_core.f90.

4.4.2.9 subroutine, public linalg\_core::rank1\_update ( real(dp), intent(in) *alpha*, real(dp), dimension(:), intent(in) *x*, real(dp), dimension(:), intent(in) *y*, real(dp), dimension(:,:), intent(inout) *a*, class(errors), intent(inout), optional, target *err* )

Performs the rank-1 update to matrix A such that: A = alpha \* X \* Y \* \* T + A, where A is an M-by-N matrix, alpha is a scalar, X is an M-element array, and N is an N-element array.

in	alpha	The scalar multiplier.
in	х	An M-element array.
in	У	An N-element array.
in,out	а	On input, the M-by-N matrix to update. On output, the updated M-by-N matrix.
out	err	An optional errors-based object that if provided can be used to retrieve information relating to any errors encountered during execution. If not provided, a default implementation of the errors class is used internally to provide error handling. Possible errors and warning messages that may be encountered are as follows.  • LA_ARRAY_SIZE_ERROR: Occurs if the size of a does not match with x and y.

#### Notes

This routine is based upon the BLAS routine DGER.

Definition at line 255 of file linalg\_core.f90.

4.4.2.10 subroutine, public linalg\_core::recip\_mult\_array ( real(dp), intent(in) a, real(dp), dimension(:), intent(inout) x )

Multiplies a vector by the reciprocal of a real scalar.

## **Parameters**

in	а	The scalar which is used to divide each component of $X$ . The value must be $>= 0$ , or the	
		subroutine will divide by zero.	
in, out	Х	The vector.	

#### **Notes**

This routine is based upon the LAPACK routine DRSCL.

Definition at line 1237 of file linalg core.f90.

4.4.2.11 subroutine, public linalg\_core::swap ( real(dp), dimension(:), intent(inout) x, real(dp), dimension(:), intent(inout) y, class(errors), intent(inout), optional, target err )

Swaps the contents of two arrays.

## **Parameters**

in,out	Х	One of the N-element arrays.
in,out	У	The other N-element array.
out	err	An optional errors-based object that if provided can be used to retrieve information relating to any errors encountered during execution. If not provided, a default implementation of the errors class is used internally to provide error handling. Possible errors and warning messages that may be encountered are as follows.  • LA_ARRAY_SIZE_ERROR: Occurs if x and y are not the same size.

Definition at line 1191 of file linalg\_core.f90.

4.4.2.12 pure real(dp) function, public linalg\_core::trace ( real(dp), dimension(:,:), intent(in) x )

Computes the trace of a matrix (the sum of the main diagonal elements).

in	Χ	The matrix on which to operate.
----	---	---------------------------------

#### Returns

The trace of x.

Definition at line 910 of file linalg core.f90.

4.4.2.13 subroutine, public linalg\_core::tri\_mtx\_mult ( logical, intent(in) upper, real(dp), intent(in) alpha, real(dp), dimension(:,:), intent(in) a, real(dp), intent(in) beta, real(dp), dimension(:,:), intent(inout) b, class(errors), intent(inout), optional, target err )

Computes the triangular matrix operation: B = alpha \* A\*\*T \* A + beta \* B, or B = alpha \* A \* A\*\*T + beta \* B, where A is a triangular matrix.

#### **Parameters**

in	upper	Set to true if matrix A is upper triangular, and B = alpha $*$ A**T $*$ A + beta $*$ B is to be calculated; else, set to false if A is lower triangular, and B = alpha $*$ A $*$ A**T + beta $*$ B is to be computed.
in	alpha	A scalar multiplier.
in	а	The N-by-N triangular matrix. Notice, if upper is true only the upper triangular portion of this matrix is referenced; else, if upper is false, only the lower triangular portion of this matrix is referenced.
in	beta	A scalar multiplier.
in, out	b	On input, the N-by-N matrix B. On output, the N-by-N solution matrix.
out	err	An optional errors-based object that if provided can be used to retrieve information relating to any errors encountered during execution. If not provided, a default implementation of the errors class is used internally to provide error handling. Possible errors and warning messages that may be encountered are as follows.  • LA_ARRAY_SIZE_ERROR: Occurs if any of the input arrays are not sized appropriately.

Definition at line 1314 of file linalg core.f90.

## 4.5 linalg\_eigen Module Reference

## linalg\_eigen

## **Data Types**

• interface eigen

Computes the eigenvalues, and optionally the eigenvectors, of a matrix.

#### **Functions/Subroutines**

• subroutine eigen\_symm (vecs, a, vals, work, olwork, err)

Computes the eigenvalues, and optionally the eigenvectors of a real, symmetric matrix.

• subroutine eigen\_asymm (a, vals, vecs, work, olwork, err)

Computes the eigenvalues, and optionally the right eigenvectors of a square matrix.

• subroutine eigen\_gen (a, b, alpha, beta, vecs, work, olwork, err)

Computes the eigenvalues, and optionally the right eigenvectors of a square matrix assuming the structure of the eigenvalue problem is A\*X = lambda\*B\*X.

#### 4.5.1 Detailed Description

## linalg\_eigen

## **Purpose**

Provides routines for computing the eigenvalues and eigenvectors of matrices.

- 4.5.2 Function/Subroutine Documentation
- 4.5.2.1 subroutine linalg\_eigen::eigen\_asymm ( real(dp), dimension(:,:), intent(inout) a, complex(dp), dimension(:), intent(out) vals, complex(dp), dimension(:,:), intent(out), optional vecs, real(dp), dimension(:), intent(out), optional, pointer work, integer(i32), intent(out), optional olwork, class(errors), intent(inout), optional, target err ) [private]

Computes the eigenvalues, and optionally the right eigenvectors of a square matrix.

#### **Parameters**

in,out	а	On input, the N-by-N matrix on which to operate. On output, the contents of this matrix are overwritten.
out	vals	An N-element array containing the eigenvalues of the matrix. The eigenvalues are not sorted.
out	vecs	An optional N-by-N matrix, that if supplied, signals to compute the right eigenvectors (one per column). If not provided, only the eigenvalues will be computed.
out	work	An optional input, that if provided, prevents any local memory allocation. If not provided, the memory required is allocated within. If provided, the length of the array must be at least olwork.
out	olwork	An optional output used to determine workspace size. If supplied, the routine determines the optimal size for $work$ , and returns without performing any actual calculations.
out	err	An optional errors-based object that if provided can be used to retrieve information relating to any errors encountered during execution. If not provided, a default implementation of the errors class is used internally to provide error handling. Possible errors and warning messages that may be encountered are as follows.
		<ul> <li>LA_ARRAY_SIZE_ERROR: Occurs if any of the input arrays are not sized appropriately.</li> </ul>
		<ul> <li>LA_OUT_OF_MEMORY_ERROR: Occurs if local memory must be allocated, and there is insufficient memory available.</li> </ul>
		LA_CONVERGENCE_ERROR: Occurs if the algorithm failed to converge.

## Notes

This routine utilizes the LAPACK routine DGEEV.

Definition at line 185 of file linalg\_eigen.f90.

4.5.2.2 subroutine linalg\_eigen::eigen\_gen ( real(dp), dimension(:,:), intent(inout) a, real(dp), dimension(:,:), intent(inout) b, complex(dp), dimension(:), intent(out) alpha, real(dp), dimension(:), intent(out), optional beta, complex(dp), dimension(:,:), intent(out), optional vecs, real(dp), dimension(:), intent(out), optional, pointer work, integer(i32), intent(out), optional olwork, class(errors), intent(inout), optional, target err ) [private]

Computes the eigenvalues, and optionally the right eigenvectors of a square matrix assuming the structure of the eigenvalue problem is A\*X = lambda\*B\*X.

#### **Parameters**

in,out	а	On input, the N-by-N matrix A. On output, the contents of this matrix are overwritten.
in,out	b	On input, the N-by-N matrix B. On output, the contents of this matrix are overwritten.
out	alpha	An N-element array that, if beta is not supplied, contains the eigenvalues. If beta is supplied however, the eigenvalues must be computed as ALPHA / BETA. This however, is not as trivial as it seems as it is entirely possible, and likely, that ALPHA / BETA can overflow or underflow. With that said, the values in ALPHA will always be less than and usually comparable with the NORM(A).
out	beta	An optional N-element array that if provided forces <code>alpha</code> to return the numerator, and this array contains the denominator used to determine the eigenvalues as ALPHA / BETA. If used, the values in this array will always be less than and usually comparable with the NORM(B).
out	vecs	An optional N-by-N matrix, that if supplied, signals to compute the right eigenvectors (one per column). If not provided, only the eigenvalues will be computed.
out	work	An optional input, that if provided, prevents any local memory allocation. If not provided, the memory required is allocated within. If provided, the length of the array must be at least olwork.
out	olwork	An optional output used to determine workspace size. If supplied, the routine determines the optimal size for work, and returns without performing any actual calculations.
out	err	An optional errors-based object that if provided can be used to retrieve information relating to any errors encountered during execution. If not provided, a default implementation of the errors class is used internally to provide error handling. Possible errors and warning messages that may be encountered are as follows.
		<ul> <li>LA_ARRAY_SIZE_ERROR: Occurs if any of the input arrays are not sized appropriately.</li> </ul>
		<ul> <li>LA_OUT_OF_MEMORY_ERROR: Occurs if local memory must be allocated, and there is insufficient memory available.</li> </ul>
		LA_CONVERGENCE_ERROR: Occurs if the algorithm failed to converge.

# Usage

As an example, consider the eigenvalue problem arising from a mechanical system of masses and springs such that the masses are described by a mass matrix M, and the arrangement of springs are described by a stiffness matrix K.

```
real(dp), parameter :: k2 = 10.0d6
    real(dp), parameter :: k3 = 10.0d6
    real(dp), parameter :: k4 = 5.0d6
    ! Local Variables
    integer(i32) :: i, j
real(dp) :: m(3,3), k(3,3), natfreq(3)
   complex(dp) :: vals(3), modeshapes(3,3)
    ! Define the mass matrix m = reshape([m1, 0.0d0, 0.0d0, 0.0d0, m2, 0.0d0, 0.0d0, 0.0d0, m3], [3, 3])
    ! Define the stiffness matrix
    k = reshape([k1 + k2, -k2, 0.0d0, -k2, k2 + k3, -k3, 0.0d0, -k3, k3 + k4], &
        [3, 3])
    ! Compute the eigenvalues and eigenvectors.
    call eigen(k, m, vals, vecs = modeshapes)
    ! Compute the natural frequency values, and return them with units of Hz.
    ! Notice, all eigenvalues and eigenvectors are real for this example.
    natfreq = sqrt(real(vals)) / (2.0d0 * pi)
    ! Display the natural frequency and mode shape values. Notice, the eigen ! routine does not necessarily sort the values.
    print '(A)', "Modal Information (Not Sorted):"
    do i = 1, size(natfreq)
        print '(AIOAF8.4A)', "Mode ", i, ": (", natfreq(i), " Hz)"
        print '(F10.3)', (real(modeShapes(j,i)), j = 1, size(natfreq))
    end do
end program
```

#### Notes

This routine utilizes the LAPACK routine DGGEV.

Definition at line 465 of file linalg eigen.f90.

4.5.2.3 subroutine linalg\_eigen::eigen\_symm ( logical, intent(in) *vecs*, real(dp), dimension(:,:), intent(inout) *a*, real(dp), dimension(:), intent(out), optional, pointer *work*, integer(i32), intent(out), optional *olwork*, class(errors), intent(inout), optional, target *err* ) [private]

Computes the eigenvalues, and optionally the eigenvectors of a real, symmetric matrix.

in	vecs	Set to true to compute the eigenvectors as well as the eigenvalues; else, set to false to just compute the eigenvalues.
in,out	а	On input, the N-by-N symmetric matrix on which to operate. On output, and if $vecs$ is set to true, the matrix will contain the eigenvectors (one per column) corresponding to each eigenvalue in $vals$ . If $vecs$ is set to false, the lower triangular portion of the matrix is overwritten.
out	vals	An N-element array that will contain the eigenvalues sorted into ascending order.
out	work	An optional input, that if provided, prevents any local memory allocation. If not provided, the memory required is allocated within. If provided, the length of the array must be at least olwork.
out	olwork	An optional output used to determine workspace size. If supplied, the routine determines the optimal size for work, and returns without performing any actual calculations.
out	err	An optional errors-based object that if provided can be used to retrieve information relating to any errors encountered during execution. If not provided, a default implementation of the errors class is used internally to provide error handling. Possible errors and warning messages that may be encountered are as follows.  • LA_ARRAY_SIZE_ERROR: Occurs if any of the input arrays are not sized
		appropriately.
		<ul> <li>LA_OUT_OF_MEMORY_ERROR: Occurs if local memory must be allocated, and there is insufficient memory available.</li> </ul>
Generated by Doxygen		LA_CONVERGENCE_ERROR: Occurs if the algorithm failed to converge.

#### Notes

This routine utilizes the LAPACK routine DSYEV.

Definition at line 68 of file linalg\_eigen.f90.

# 4.6 linalg\_factor Module Reference

## linalg\_factor

## **Data Types**

· interface form lu

Extracts the L and U matrices from the condensed [L\U] storage format used by the lu factor.

interface form gr

Forms the full M-by-M orthogonal matrix Q from the elementary reflectors returned by the base QR factorization algorithm.

· interface mult\_qr

Multiplies a general matrix by the orthogonal matrix Q from a QR factorization.

· interface mult rz

Multiplies a general matrix by the orthogonal matrix Z from an RZ factorization.

interface qr factor

Computes the QR factorization of an M-by-N matrix.

#### **Functions/Subroutines**

subroutine, public lu\_factor (a, ipvt, err)

Computes the LU factorization of an M-by-N matrix.

• subroutine form lu all (lu, ipvt, u, p, err)

Extracts the L, U, and P matrices from the output of the lu\_factor routine.

subroutine form\_lu\_only (lu, u, err)

Extracts the L, and U matrices from the output of the lu\_factor routine.

• subroutine qr\_factor\_no\_pivot (a, tau, work, olwork, err)

Computes the QR factorization of an M-by-N matrix without pivoting.

• subroutine qr\_factor\_pivot (a, tau, jpvt, work, olwork, err)

Computes the QR factorization of an M-by-N matrix with column pivoting such that A \* P = Q \* R.

• subroutine form\_qr\_no\_pivot (r, tau, q, work, olwork, err)

Forms the full M-by-M orthogonal matrix Q from the elementary reflectors returned by the base QR factorization algorithm.

subroutine form\_qr\_pivot (r, tau, pvt, q, p, work, olwork, err)

Forms the full M-by-M orthogonal matrix Q from the elementary reflectors returned by the base QR factorization algorithm.

• subroutine mult\_qr\_mtx (Iside, trans, a, tau, c, work, olwork, err)

Multiplies a general matrix by the orthogonal matrix Q from a QR factorization such that: C = op(Q) \* C, or C = C \* op(Q).

• subroutine mult\_qr\_vec (trans, a, tau, c, work, olwork, err)

Multiplies a vector by the orthogonal matrix Q from a QR factorization such that: C = op(Q) \* C.

• subroutine, public qr\_rank1\_update (q, r, u, v, work, err)

Computes the rank 1 update to an M-by-N QR factored matrix A (M >= N) where A = Q \* R, and A1 = A + U \* V \*\* T such that A1 = Q1 \* R1.

subroutine, public cholesky\_factor (a, upper, err)

Computes the Cholesky factorization of a symmetric, positive definite matrix.

• subroutine, public cholesky\_rank1\_update (r, u, work, err)

Computes the rank 1 update to a Cholesky factored matrix (upper triangular).

subroutine, public cholesky\_rank1\_downdate (r, u, work, err)

Computes the rank 1 downdate to a Cholesky factored matrix (upper triangular).

• subroutine, public rz\_factor (a, tau, work, olwork, err)

Factors an upper trapezoidal matrix by means of orthogonal transformations such that  $A = R * Z = (R \ 0) * Z$ . Z is an orthogonal matrix of dimension N-by-N, and R is an M-by-M upper triangular matrix.

• subroutine mult\_rz\_mtx (Iside, trans, I, a, tau, c, work, olwork, err)

Multiplies a general matrix by the orthogonal matrix Z from an RZ factorization such that: C = op(Z) \* C, or C = C \* op(Z).

• subroutine mult\_rz\_vec (trans, I, a, tau, c, work, olwork, err)

Multiplies a vector by the orthogonal matrix Z from an RZ factorization such that: C = op(Z) \* C.

• subroutine, public svd (a, s, u, vt, work, olwork, err)

Computes the singular value decomposition of a matrix A. The SVD is defined as: A = U \* S \* V \* \* T, where U is an M-by-M orthogonal matrix, S is an M-by-N diagonal matrix, and V is an N-by-N orthogonal matrix.

#### 4.6.1 Detailed Description

## linalg\_factor

#### **Purpose**

Provides a set of matrix factorization routines.

- 4.6.2 Function/Subroutine Documentation
- 4.6.2.1 subroutine, public linalg\_factor::cholesky\_factor ( real(dp), dimension(:,:), intent(inout) *a,* logical, intent(in), optional *upper,* class(errors), intent(inout), optional, target *err* )

Computes the Cholesky factorization of a symmetric, positive definite matrix.

in,out	а	On input, the N-by-N matrix to factor. On output, the factored matrix is returned in either the upper or lower triangular portion of the matrix, dependent upon the value of upper.
in	upper	An optional input that, if specified, provides control over whether the factorization is computed as $A = U**T*U$ (set to true), or as $A = L*L**T$ (set to false). The default value is true such that $A = U**T*U$ .
out	err	An optional errors-based object that if provided can be used to retrieve information relating to any errors encountered during execution. If not provided, a default implementation of the errors class is used internally to provide error handling. Possible errors and warning messages that may be encountered are as follows.  • LA_ARRAY_SIZE_ERROR: Occurs if a is not square.
		<ul> <li>LA_MATRIX_FORMAT_ERROR: Occurs if a is not positive definite.</li> </ul>

# Usage

To solve a system of N equations of N unknowns using Cholesky factorization, the following code will suffice. Notice, the system of equations must be positive definite.

```
! Solve the system: A*X = B, where A is an N-by-N matrix, and B and X are
! N-by-NRHS in size.
! Variables
real(dp), dimension(n, n) :: a
real(dp), dimension(n, nrhs) :: b
logical :: upper
! Initialize A and B...
! Specify that we're using the upper portion of A (remember positive
! definite matrices are symmetric)
upper = .true.
! Compute the factorization of A.
call cholesky_factor(a, upper)
! Solve A*X = B for X - Note: X overwrites B.
call solve_cholesky(upper, a, b)
```

#### Notes

This routine utilizes the LAPACK routine DPOTRF.

Definition at line 1308 of file linalg\_factor.f90.

4.6.2.2 subroutine, public linalg\_factor::cholesky\_rank1\_downdate ( real(dp), dimension(:,:), intent(inout) r, real(dp), dimension(:), intent(inout) u, real(dp), dimension(:), intent(out), optional, target work, class(errors), intent(inout), optional, target err )

Computes the rank 1 downdate to a Cholesky factored matrix (upper triangular).

#### **Parameters**

in,out	r	On input, the N-by-N upper triangular matrix R. On output, the updated matrix R1.
in,out	и	On input, the N-element update vector U. On output, the rotation sines used to transform R to R1.
out	work	An optional argument that if supplied prevents local memory allocation. If provided, the array must have at least N elements. Additionally, this workspace array is used to contain the rotation cosines used to transform R to R1.
out	err	An optional errors-based object that if provided can be used to retrieve information relating to any errors encountered during execution. If not provided, a default implementation of the errors class is used internally to provide error handling. Possible errors and warning messages that may be encountered are as follows.
		<ul> <li>LA_ARRAY_SIZE_ERROR: Occurs if any of the input array sizes are incorrect.</li> <li>LA_OUT_OF_MEMORY_ERROR: Occurs if local memory must be allocated, and there is insufficient memory available.</li> </ul>
		<ul> <li>LA_MATRIX_FORMAT_ERROR: Occurs if the downdated matrix is not positive definite.</li> </ul>
		LA_SINGULAR_MATRIX_ERROR: Occurs if r is singular.

# Notes

This routine utilizes the QRUPDATE routine DCH1DN.

## See Also

Source

Definition at line 1494 of file linalg\_factor.f90.

4.6.2.3 subroutine, public linalg\_factor::cholesky\_rank1\_update ( real(dp), dimension(:,:), intent(inout) r, real(dp), dimension(:), intent(inout) u, real(dp), dimension(:), intent(out), optional, target work, class(errors), intent(inout), optional, target err )

Computes the rank 1 update to a Cholesky factored matrix (upper triangular).

#### **Parameters**

in, out	r	On input, the N-by-N upper triangular matrix R. On output, the updated matrix R1.
in, out	и	On input, the N-element update vector U. On output, the rotation sines used to transform R
		to R1.
out	work	An optional argument that if supplied prevents local memory allocation. If provided, the
		array must have at least N elements. Additionally, this workspace array is used to contain
		the rotation cosines used to transform R to R1.
out	err	An optional errors-based object that if provided can be used to retrieve information relating to any errors encountered during execution. If not provided, a default implementation of the errors class is used internally to provide error handling. Possible errors and warning messages that may be encountered are as follows.
		LA_ARRAY_SIZE_ERROR: Occurs if any of the input array sizes are incorrect.
		<ul> <li>LA_OUT_OF_MEMORY_ERROR: Occurs if local memory must be allocated, and there is insufficient memory available.</li> </ul>

## Notes

This routine utilizes the QRUPDATE routine DCH1UP.

# See Also

Source

Definition at line 1400 of file linalg\_factor.f90.

4.6.2.4 subroutine linalg\_factor::form\_lu\_all ( real(dp), dimension(:,:), intent(inout) *lu*, integer(i32), dimension(:), intent(in) *ipvt*, real(dp), dimension(:,:), intent(out) *u*, real(dp), dimension(:,:), intent(out) *p*, class(errors), intent(inout), optional, target err ) [private]

Extracts the L, U, and P matrices from the output of the lu\_factor routine.

in,out	lu	On input, the N-by-N matrix as output by lu_factor. On output, the N-by-N lower triangular matrix L.
in	ipvt	The N-element pivot array as output by lu_factor.
out	и	An N-by-N matrix where the U matrix will be written.
out	р	An N-by-N matrix where the row permutation matrix will be written.
out	err	An optional errors-based object that if provided can be used to retrieve information relating to any errors encountered during execution. If not provided, a default implementation of the errors class is used internally to provide error handling. Possible errors and warning
Generated by Do	oxygen	messages that may be encountered are as follows.  • LA_ARRAY_SIZE_ERROR: Occurs if any of the input array sizes are incorrect.

#### Remarks

This routine allows extraction of the actual "L", "U", and "P" matrices of the decomposition. To use these matrices to solve the system A\*X = B, the following approach is used.

- 1. First, solve the linear system: L\*Y = P\*B for Y.
- 2. Second, solve the linear system: U\*X = Y for X.

Notice, as both L and U are triangular in structure, the above equations can be solved by forward and backward substitution.

## See Also

- Wikipedia
- Wolfram MathWorld

Definition at line 211 of file linalg\_factor.f90.

4.6.2.5 subroutine linalg\_factor::form\_lu\_only ( real(dp), dimension(:,:), intent(inout) *lu*, real(dp), dimension(:,:), intent(out) *u*, class(errors), intent(inout), optional, target *err* ) [private]

Extracts the L, and U matrices from the output of the lu\_factor routine.

## **Parameters**

in,out	lu	On input, the N-by-N matrix as output by lu_factor. On output, the N-by-N lower triangular
		matrix L.
out	и	An N-by-N matrix where the U matrix will be written.
out	err	An optional errors-based object that if provided can be used to retrieve information relating to any errors encountered during execution. If not provided, a default implementation of the errors class is used internally to provide error handling. Possible errors and warning messages that may be encountered are as follows.
		LA_ARRAY_SIZE_ERROR: Occurs if any of the input array sizes are incorrect.

Definition at line 288 of file linalg factor.f90.

4.6.2.6 subroutine linalg\_factor::form\_qr\_no\_pivot ( real(dp), dimension(:,:), intent(inout) r, real(dp), dimension(:), intent(in) tau, real(dp), dimension(:,:), intent(out) q, real(dp), dimension(:), intent(out), optional, target work, integer(i32), intent(out), optional olwork, class(errors), intent(inout), optional, target err ) [private]

Forms the full M-by-M orthogonal matrix Q from the elementary reflectors returned by the base QR factorization algorithm.

in,out	r	On input, an M-by-N matrix where the elements below the diagonal contain the elementary reflectors generated from the QR factorization. On and above the diagonal, the matrix contains the matrix R. On output, the elements below the diagonal are zeroed such that the remaining matrix is simply the M-by-N matrix R.
in	tau	A MIN(M, N)-element array containing the scalar factors of each elementary reflector defined in r.

## **Parameters**

out	q	An M-by-M matrix where the full orthogonal matrix Q will be written. In the event that $M > N$ , Q may be supplied as M-by-N, and therefore only return the useful submatrix Q1 (Q = [Q1, Q2]) as the factorization can be written as $Q * R = [Q1, Q2] * [R1; 0]$ .
out	work	An optional input, that if provided, prevents any local memory allocation. If not provided, the memory required is allocated within. If provided, the length of the array must be at least olwork.
out	olwork	An optional output used to determine workspace size. If supplied, the routine determines the optimal size for work, and returns without performing any actual calculations.
out	err	An optional errors-based object that if provided can be used to retrieve information relating to any errors encountered during execution. If not provided, a default implementation of the errors class is used internally to provide error handling. Possible errors and warning messages that may be encountered are as follows.  • LA_ARRAY_SIZE_ERROR: Occurs if any of the input arrays are not sized appropriately.  • LA_OUT_OF_MEMORY_ERROR: Occurs if local memory must be allocated, and there is insufficient memory available.

## Notes

This routine utilizes the LAPACK routine DORGQR.

Definition at line 694 of file linalg\_factor.f90.

4.6.2.7 subroutine linalg\_factor::form\_qr\_pivot ( real(dp), dimension(:,:), intent(inout) r, real(dp), dimension(:), intent(in) tau, integer(i32), dimension(:), intent(in) pvt, real(dp), dimension(:,:), intent(out) q, real(dp), dimension(:,:), intent(out) p, real(dp), dimension(:), intent(out), optional, target work, integer(i32), intent(out), optional olwork, class(errors), intent(inout), optional, target err ) [private]

Forms the full M-by-M orthogonal matrix Q from the elementary reflectors returned by the base QR factorization algorithm.

in,out	r	On input, an M-by-N matrix where the elements below the diagonal contain the elementary reflectors generated from the QR factorization. On and above the diagonal, the matrix contains the matrix R. On output, the elements below the diagonal are zeroed such that the remaining matrix is simply the M-by-N matrix R.
in	tau	A MIN(M, N)-element array containing the scalar factors of each elementary reflector defined in r.
in	pvt	An N-element column pivot array as returned by the QR factorization.
out	q	An M-by-M matrix where the full orthogonal matrix Q will be written. In the event that $M > N$ , Q may be supplied as M-by-N, and therefore only return the useful submatrix Q1 (Q = [Q1, Q2]) as the factorization can be written as Q * R = [Q1, Q2] * [R1; 0].
out	р	An N-by-N matrix where the pivot matrix will be written.
out	work	An optional input, that if provided, prevents any local memory allocation. If not provided, the memory required is allocated within. If provided, the length of the array must be at least olwork.
out	olwork	An optional output used to determine workspace size. If supplied, the routine determines the optimal size for work, and returns without performing any actual calculations.

## **Parameters**

out	err	An optional errors-based object that if provided can be used to retrieve information relating to any errors encountered during execution. If not provided, a default implementation of the errors class is used internally to provide error handling. Possible errors and warning messages that may be encountered are as follows.
		<ul> <li>LA_ARRAY_SIZE_ERROR: Occurs if any of the input arrays are not sized appropriately.</li> </ul>
		<ul> <li>LA_OUT_OF_MEMORY_ERROR: Occurs if local memory must be allocated, and there is insufficient memory available.</li> </ul>

## Notes

This routine utilizes the LAPACK routine DORGQR.

Definition at line 825 of file linalg\_factor.f90.

4.6.2.8 subroutine, public linalg\_factor::lu\_factor ( real(dp), dimension(:,:), intent(inout) a, integer(i32), dimension(:), intent(out) ipvt, class(errors), intent(inout), optional, target err )

Computes the LU factorization of an M-by-N matrix.

#### **Parameters**

in,out	а	On input, the M-by-N matrix on which to operate. On output, the LU factored matrix in the form [L\U] where the unit diagonal elements of L are not stored.
out	ipvt	An MIN(M, N)-element array used to track row-pivot operations. The array stored pivot information such that row I is interchanged with row IPVT(I).
out	err	An optional errors-based object that if provided can be used to retrieve information relating to any errors encountered during execution. If not provided, a default implementation of the errors class is used internally to provide error handling. Possible errors and warning messages that may be encountered are as follows.
		<ul> <li>LA_ARRAY_SIZE_ERROR: Occurs if ipvt is not sized appropriately.</li> </ul>
		LA_SINGULAR_MATRIX_ERROR: Occurs as a warning if a is found to be singular.
	1	

# Usage

To solve a system of N equations of N unknowns using LU factorization, the following code will suffice.

```
! Solve the system: A*X = B, where A is an N-by-N matrix, and B and X are
! N-by-NRHS in size.
! Variables
real(dp), dimension(n, n) :: a
real(dp), dimension(n, nrhs) :: b
! Define the array used to track row pivots.
integer(i32), dimension(n) :: pvt
! Initialize A and B...
! Compute the LU factorization of A. On output, A contains [L\U].
call lu_factor(a, pvt)
! Solve A*X = B for X - Note: X overwrites B.
call solve_lu(a, pvt, b)
```

#### Notes

This routine utilizes the LAPACK routine DGETRF.

## See Also

- Wikipedia
- Wolfram MathWorld

Definition at line 127 of file linalg\_factor.f90.

4.6.2.9 subroutine linalg\_factor::mult\_qr\_mtx ( logical, intent(in) *lside*, logical, intent(in) *trans*, real(dp), dimension(:,:), intent(inout) *a*, real(dp), dimension(:), intent(in) *tau*, real(dp), dimension(:,:), intent(inout) *c*, real(dp), dimension(:), intent(out), optional, target *work*, integer(i32), intent(out), optional *olwork*, class(errors), intent(inout), optional, target *err* ) [private]

Multiplies a general matrix by the orthogonal matrix Q from a QR factorization such that: C = op(Q) \* C, or C = C \* op(Q).

## **Parameters**

in	Iside	Set to true to apply Q or Q**T from the left; else, set to false to apply Q or Q**T from the right.
in	trans	Set to true to apply Q**T; else, set to false.
in	а	On input, an LDA-by-K matrix containing the elementary reflectors output from the QR factorization. If lside is set to true, LDA = M, and $M >= K >= 0$ ; else, if lside is set to false, LDA = N, and $N >= K >= 0$ . Notice, the contents of this matrix are restored on exit.
in	tau	A K-element array containing the scalar factors of each elementary reflector defined in a.
in,out	С	On input, the M-by-N matrix C. On output, the product of the orthogonal matrix Q and the original matrix C.
out	work	An optional input, that if provided, prevents any local memory allocation. If not provided, the memory required is allocated within. If provided, the length of the array must be at least olwork.
out	olwork	An optional output used to determine workspace size. If supplied, the routine determines the optimal size for work, and returns without performing any actual calculations.
out	err	An optional errors-based object that if provided can be used to retrieve information relating to any errors encountered during execution. If not provided, a default implementation of the errors class is used internally to provide error handling. Possible errors and warning messages that may be encountered are as follows.
		<ul> <li>LA_ARRAY_SIZE_ERROR: Occurs if any of the input arrays are not sized appropriately.</li> </ul>
		<ul> <li>LA_OUT_OF_MEMORY_ERROR: Occurs if local memory must be allocated, and there is insufficient memory available.</li> </ul>

#### Notes

This routine utilizes the LAPACK routine DORMQR.

Definition at line 927 of file linalg\_factor.f90.

4.6.2.10 subroutine linalg\_factor::mult\_qr\_vec ( logical, intent(in) *trans*, real(dp), dimension(:,:), intent(inout) *a*, real(dp), dimension(:), intent(inout) *c*, real(dp), dimension(:), intent(out), optional, target work, integer(i32), intent(out), optional olwork, class(errors), intent(inout), optional, target err ) [private]

Multiplies a vector by the orthogonal matrix Q from a QR factorization such that: C = op(Q) \* C.

#### **Parameters**

in	trans	Set to true to apply Q**T; else, set to false.
in	а	On input, an M-by-K matrix containing the elementary reflectors output from the QR factorization. Notice, the contents of this matrix are restored on exit.
in	tau	A K-element array containing the scalar factors of each elementary reflector defined in a.
in,out	С	On input, the M-element vector C. On output, the product of the orthogonal matrix Q and the original vector C.
out	work	An optional input, that if provided, prevents any local memory allocation. If not provided, the memory required is allocated within. If provided, the length of the array must be at least olwork.
out	olwork	An optional output used to determine workspace size. If supplied, the routine determines the optimal size for work, and returns without performing any actual calculations.
out	err	An optional errors-based object that if provided can be used to retrieve information relating to any errors encountered during execution. If not provided, a default implementation of the errors class is used internally to provide error handling. Possible errors and warning messages that may be encountered are as follows.
		<ul> <li>LA_ARRAY_SIZE_ERROR: Occurs if any of the input arrays are not sized appropriately.</li> </ul>
		<ul> <li>LA_OUT_OF_MEMORY_ERROR: Occurs if local memory must be allocated, and there is insufficient memory available.</li> </ul>

## Notes

This routine is based upon the LAPACK routine DORM2R.

Definition at line 1054 of file linalg\_factor.f90.

4.6.2.11 subroutine linalg\_factor::mult\_rz\_mtx ( logical, intent(in) *lside*, logical, intent(in) *trans*, integer(i32), intent(in) *l*, real(dp), dimension(:,:), intent(inout) *a*, real(dp), dimension(:), intent(in) *tau*, real(dp), dimension(:,:), intent(inout) *c*, real(dp), dimension(:), intent(out), optional, target *work*, integer(i32), intent(out), optional *olwork*, class(errors), intent(inout), optional, target *err* ) [private]

Multiplies a general matrix by the orthogonal matrix Z from an RZ factorization such that: C = op(Z) \* C, or C = C \* op(Z).

in	Iside	Set to true to apply Z or Z**T from the left; else, set to false to apply Z or Z**T from the right.
in	trans	Set to true to apply Z**T; else, set to false.
in	1	The number of columns in matrix a containing the meaningful part of the Householder vectors. If lside is true, $M >= L >= 0$ ; else, if lside is false, $N >= L >= 0$ .
in,out	а	On input the K-by-LTA matrix Z, where LTA = M if lside is true; else, LTA = N if lside is false. The I-th row must contain the Householder vector in the last k rows. Notice, the contents of this matrix are restored on exit.

## **Parameters**

in	tau	A K-element array containing the scalar factors of the elementary reflectors, where $M \ge K \ge 0$ if lside is true; else, $N \ge K \ge 0$ if lside is false.
in,out	С	On input, the M-by-N matrix C. On output, the product of the orthogonal matrix Z and the original matrix C.
out	work	An optional input, that if provided, prevents any local memory allocation. If not provided, the memory required is allocated within. If provided, the length of the array must be at least olwork.
out	olwork	An optional output used to determine workspace size. If supplied, the routine determines the optimal size for work, and returns without performing any actual calculations.
out	err	An optional errors-based object that if provided can be used to retrieve information relating to any errors encountered during execution. If not provided, a default implementation of the errors class is used internally to provide error handling. Possible errors and warning messages that may be encountered are as follows.
		<ul> <li>LA_ARRAY_SIZE_ERROR: Occurs if any of the input arrays are not sized appropriately.</li> </ul>
		<ul> <li>LA_OUT_OF_MEMORY_ERROR: Occurs if local memory must be allocated, and there is insufficient memory available.</li> </ul>

#### Notes

This routine utilizes the LAPACK routine DORMRZ.

Definition at line 1745 of file linalg\_factor.f90.

4.6.2.12 subroutine linalg\_factor::mult\_rz\_vec ( logical, intent(in) trans, integer(i32), intent(in) I, real(dp), dimension(:,:), intent(inout) a, real(dp), dimension(:), intent(in) tau, real(dp), dimension(:), intent(inout) c, real(dp), dimension(:), intent(out), optional, target work, integer(i32), intent(out), optional olwork, class(errors), intent(inout), optional, target err ) [private]

Multiplies a vector by the orthogonal matrix Z from an RZ factorization such that: C = op(Z) \* C.

in	trans	Set to true to apply Z**T; else, set to false.
in	1	The number of columns in matrix a containing the meaningful part of the Householder vectors. If lside is true, $M >= L >= 0$ ; else, if lside is false, $N >= L >= 0$ .
in,out	а	On input the K-by-LTA matrix Z, where LTA = M if lside is true; else, LTA = N if lside is false. The I-th row must contain the Householder vector in the last k rows. Notice, the contents of this matrix are restored on exit.
in	tau	A K-element array containing the scalar factors of the elementary reflectors, where $M >= K >= 0$ if lside is true; else, $N >= K >= 0$ if lside is false.
in,out	С	On input, the M-element array C. On output, the product of the orthogonal matrix Z and the original array C.
out	work	An optional input, that if provided, prevents any local memory allocation. If not provided, the memory required is allocated within. If provided, the length of the array must be at least olwork.
out	olwork	An optional output used to determine workspace size. If supplied, the routine determines the optimal size for work, and returns without performing any actual calculations.

## **Parameters**

out	err	An optional errors-based object that if provided can be used to retrieve information relating to any errors encountered during execution. If not provided, a default implementation of the errors class is used internally to provide error handling. Possible errors and warning messages that may be encountered are as follows.
		<ul> <li>LA_ARRAY_SIZE_ERROR: Occurs if any of the input arrays are not sized appropriately.</li> </ul>
		<ul> <li>LA_OUT_OF_MEMORY_ERROR: Occurs if local memory must be allocated, and there is insufficient memory available.</li> </ul>

#### Notes

This routine utilizes the LAPACK routine DORMRZ.

Definition at line 1887 of file linalg\_factor.f90.

4.6.2.13 subroutine linalg\_factor::qr\_factor\_no\_pivot ( real(dp), dimension(:,:), intent(inout) a, real(dp), dimension(:), intent(out) tau, real(dp), dimension(:), intent(out), optional, target work, integer(i32), intent(out), optional olwork, class(errors), intent(inout), optional, target err ) [private]

Computes the QR factorization of an M-by-N matrix without pivoting.

## **Parameters**

in,out	а	On input, the M-by-N matrix to factor. On output, the elements on and above the diagonal contain the MIN(M, N)-by-N upper trapezoidal matrix R (R is upper triangular if $M \ge N$ ). The elements below the diagonal, along with the array tau, represent the orthogonal matrix Q as a product of elementary reflectors.
out	tau	A MIN(M, N)-element array used to store the scalar factors of the elementary reflectors.
out	work	An optional input, that if provided, prevents any local memory allocation. If not provided, the memory required is allocated within. If provided, the length of the array must be at least olwork.
out	olwork	An optional output used to determine workspace size. If supplied, the routine determines the optimal size for work, and returns without performing any actual calculations.
out	err	An optional errors-based object that if provided can be used to retrieve information relating to any errors encountered during execution. If not provided, a default implementation of the errors class is used internally to provide error handling. Possible errors and warning messages that may be encountered are as follows.  • LA_ARRAY_SIZE_ERROR: Occurs if tau or work are not sized appropriately.  • LA_OUT_OF_MEMORY_ERROR: Occurs if local memory must be allocated, and there is insufficient memory available.

# Remarks

QR factorization without pivoting is best suited to solving an overdetermined system in least-squares terms, or to solve a normally defined system. To solve an underdetermined system, it is recommended to use either LQ factorization, or a column-pivoting based QR factorization.

#### Usage

To solve a system of M equations of N unknowns using QR factorization, the following code will suffice assuming M >= N.

```
! Solve the system: A*X = B in a least-squares sense, where A is an
! M-by-N matrix, B is an M-by-NRHS matrix, and X is an N-by-NRHS matrix.
real(dp), dimension(m, n) :: a
real(dp), dimension(m, nrhs) :: b, qtb
real(dp), dimension(n, nrhs) :: x
real(dp), dimension(n) :: tau
real(dp), dimension(m, m) :: q
! Initialize A and B...
! Compute the QR factorization. We're intentionally not forming the full
! O matrix, but instead storing it in terms of its elementary reflector
! components in the sub-diagonal portions of A, and the corresponding ! scalar factors in TAU. Additionally, we'll let the algorithm allocate ! it's own workspace array; therefore, the call to factor A is:
call qr_factor(a, tau)
! Solve A \star X = B for X. The first N rows of B are used to store X.
call solve_qr(a, tau, b)
! Also note, we could form {\tt Q} and {\tt R} explicitly. Then solution of the
  system of equations can be found. First we form Q and R.
call form_qr(a, tau, q) ! Forms Q, and R is stored in A
! Since we now have Q and R, we seek a solution to the equation:
 Q*R*X = B, but Q is an orthogonal matrix (i.e. Q**T = inv(Q)).
Then: R*X = Q**T * B, and R is upper triangular; therefore, back
! substitution will suffice for a solution procedure.
! Next, compute Q**T*B, and store in QTB. call mtx_mult(.true., .false., 1.0d0, q, b, 0.0d0, qtb)
! Copy the first N rows of Q**T*B into X for the solution process.
! Notice, only the first N rows are needed as rows N+1:M are all zero in
! matrix R.
x = qtb(1:n,nrhs)
! Compute the solution and store in \boldsymbol{X}
call solve_triangular_system(.true., .true., .false., .true., 1.0d0, &
 a(1:n,1:n), x)
```

#### Notes

This routine utilizes the LAPACK routine DGEQRF.

Definition at line 425 of file linalg\_factor.f90.

4.6.2.14 subroutine linalg\_factor::qr\_factor\_pivot ( real(dp), dimension(:,:), intent(inout) a, real(dp), dimension(:), intent(out) tau, integer(i32), dimension(:), intent(inout) jpvt, real(dp), dimension(:), intent(out), optional, target work, integer(i32), intent(out), optional olwork, class(errors), intent(inout), optional, target err ) [private]

Computes the QR factorization of an M-by-N matrix with column pivoting such that A \* P = Q \* R.

in,out	а	On input, the M-by-N matrix to factor. On output, the elements on and above the diagonal contain the MIN(M, N)-by-N upper trapezoidal matrix R (R is upper triangular if $M \ge N$ ). The elements below the diagonal, along with the array tau, represent the orthogonal matrix Q as a product of elementary reflectors.
out	tau	A MIN(M, N)-element array used to store the scalar factors of the elementary reflectors.
in,out	jpvt	On input, an N-element array that if JPVT(I) .ne. 0, the I-th column of A is permuted to the front of A $*$ P; if JPVT(I) = 0, the I-th column of A is a free column. On output, if JPVT(I) = K, then the I-th column of A $*$ P was the K-th column of A.

#### **Parameters**

out	work	An optional input, that if provided, prevents any local memory allocation. If not provided, the memory required is allocated within. If provided, the length of the array must be at least olwork.
out	olwork	An optional output used to determine workspace size. If supplied, the routine determines the optimal size for work, and returns without performing any actual calculations.
out	err	An optional errors-based object that if provided can be used to retrieve information relating to any errors encountered during execution. If not provided, a default implementation of the errors class is used internally to provide error handling. Possible errors and warning messages that may be encountered are as follows.  • LA_ARRAY_SIZE_ERROR: Occurs if any of the input arrays are not sized
		appropriately.  • LA_OUT_OF_MEMORY_ERROR: Occurs if local memory must be allocated, and
		there is insufficient memory available.

#### Usage

To solve a system of M equations of N unknowns using QR factorization, the following code will suffice for any M and N.

```
! Solve the least-squares (M >= N), or the underdetermined (M < N)
! problem A*X = B, where A is an M-by-N matrix, B is an M-by-NRHS matrix,
! and X is an N-by-NRHS matrix. In the underdetermined case, or the ! case where the rank of matrix A is less than N, the solution obtained
! contains the fewest possible non-zero entries.
real(dp), dimension(m, n) :: a
real(dp), dimension(n, nrhs) :: b
real(dp), dimension(k) :: tau ! k = min(m, n)
real(dp), dimension(m, m) :: q
real(dp), dimension(n, n) :: p
integer(i32), dimension(n) :: pvt
! Initialize A and B...
! Allow all columns to be free.
pvt = 0
! Compute the QR factorization. We're intentionally not forming the full
! Q matrix, but instead storing it in terms of its elementary reflector
! components in the sub-diagonal portions of A, and the corresponding ! scalar factors in TAU. Additionally, we'll let the algorithm allocate ! it's own workspace array; therefore, the call to factor A is:
call qr_factor(a, tau, pvt)
  Solve A \star X = B for X. If M > N, the first N rows of B are used to store
! X. If M < N, the input matrix B must be N-by-NRHS, and only the first ! M rows are used for the actual matrix B. The remaining N-M rows
! can contain whatever as they are not referenced until they are ! overwritten by the N-by-NRHS solution matrix X.
call solve_qr(a, tau, pvt, b)
! Notice, if the explicit {\tt Q} matrix from the factorization is desired,
! the form_qr routine works similarly as in the no-pivot case; ! however, the permutation matrix P is also constructed. The call would
! be as follows. Also, as with the no-pivot algorithm, the matrix R is
! stored in matrix A.
call form_qr(a, tau, pvt, q, p)
! Solution can proceed as per typical, but with a full Q matrix. Also ! note, the problem is of the form: A*P = Q*R. Solution is straight ! forward, as with the no-pivot case; however, if M < N, then R is upper
  trapezoidal, and must be appropriately partitioned to solve. The rank
! of matrix r should be considered when applying the partition.
```

#### Notes

This routine utilizes the LAPACK routine DGEQP3.

Definition at line 579 of file linalg\_factor.f90.

4.6.2.15 subroutine, public linalg\_factor::qr\_rank1\_update ( real(dp), dimension(:,:), intent(inout) q, real(dp), dimension(:,:), intent(inout) r, real(dp), dimension(:), intent(inout) u, real(dp), dimension(:), intent(inout) v, real(dp), dimension(:), intent(out), optional, target work, class(errors), intent(inout), optional, target err )

Computes the rank 1 update to an M-by-N QR factored matrix A (M >= N) where A = Q \* R, and A1 = A + U \* V\*\*T such that A1 = Q1 \* R1.

#### **Parameters**

in,out	q	On input, the original M-by-K orthogonal matrix Q. On output, the updated matrix Q1.
in, out	r	On input, the M-by-N matrix R. On output, the updated matrix R1.
in,out	и	On input, the M-element U update vector. On output, the original content of the array is overwritten.
in,out	V	On input, the N-element V update vector. On output, the original content of the array is overwritten.
out	work	An optional argument that if supplied prevents local memory allocation. If provided, the array must have at least 2*K elements.
out	err	An optional errors-based object that if provided can be used to retrieve information relating to any errors encountered during execution. If not provided, a default implementation of the errors class is used internally to provide error handling. Possible errors and warning messages that may be encountered are as follows.
		<ul> <li>LA_ARRAY_SIZE_ERROR: Occurs if any of the input arrays are not sized appropriately.</li> </ul>
		<ul> <li>LA_OUT_OF_MEMORY_ERROR: Occurs if local memory must be allocated, and there is insufficient memory available.</li> </ul>

#### Remarks

```
Notice, K must either be equal to M, or to N. In the event that K = N, only the submatrix Qa is updated. This is appropriate as the QR factorization for an overdetermined system can be written as follows: A = Q \, * \, R = [Qa, \, Qb] \, * \, [Ra] \\ [0]
```

Note: Ra is upper triangular of dimension N-by-N.

#### Notes

This routine utilizes the QRUPDATE routine DQR1UP.

## See Also

Source

Definition at line 1180 of file linalg\_factor.f90.

4.6.2.16 subroutine, public linalg\_factor::rz\_factor ( real(dp), dimension(:,:), intent(inout) a, real(dp), dimension(:), intent(out) tau, real(dp), dimension(:), intent(out), optional, target work, integer(i32), intent(out), optional olwork, class(errors), intent(inout), optional, target err )

Factors an upper trapezoidal matrix by means of orthogonal transformations such that  $A = R * Z = (R \ 0) * Z$ . Z is an orthogonal matrix of dimension N-by-N, and R is an M-by-M upper triangular matrix.

# **Parameters**

in,out	а	On input, the M-by-N upper trapezoidal matrix to factor. On output, the leading M-by-M upper triangular part of the matrix contains the upper triangular matrix R, and elements N-L+1 to N of the first M rows of A, with the array tau, represent the orthogonal matrix Z as a product of M elementary reflectors.
out	tau	An M-element array used to store the scalar factors of the elementary reflectors.
out	work	An optional input, that if provided, prevents any local memory allocation. If not provided, the memory required is allocated within. If provided, the length of the array must be at least olwork.
out	olwork	An optional output used to determine workspace size. If supplied, the routine determines the optimal size for work, and returns without performing any actual calculations.
out	err	An optional errors-based object that if provided can be used to retrieve information relating to any errors encountered during execution. If not provided, a default implementation of the errors class is used internally to provide error handling. Possible errors and warning messages that may be encountered are as follows.  • LA_ARRAY_SIZE_ERROR: Occurs if any of the input arrays are not sized
		<ul> <li>appropriately.</li> <li>LA_OUT_OF_MEMORY_ERROR: Occurs if local memory must be allocated, and there is insufficient memory available.</li> </ul>

## **Further Details**

```
The factorization is obtained by Householder's method. The kth transformation matrix, Z(k), which is used to introduce zeros into the (m-k+1)th row of A, is given in the form Z(k) = (I 0), \\ (0 T(k)) where T(k) = I - tau*u(k)*u(k)**T, u(k) = (1), \\ (0) \\ (z(k)) tau is a scalar and z(k) is an l element vector. tau and z(k) are chosen to annihilate the elements of the kth row of A2. The scalar tau is returned in the kth element of TAU and the vector u(k) in the kth row of A2, such that the elements of z(k) are in z(k) in the kth row of A2, such that the elements of z(k) are in z(k) in the kth row of A2, such that the elements of z(k) are in z(k) in the z(k) in the
```

## Notes

This routine is based upon the LAPACK routine DTZRZF.

# See Also

• LAPACK Users Manual

Definition at line 1633 of file linalg\_factor.f90.

4.6.2.17 subroutine, public linalg\_factor::svd ( real(dp), dimension(:,:), intent(inout) a, real(dp), dimension(:), intent(out) s, real(dp), dimension(:,:), intent(out), optional u, real(dp), dimension(:,:), intent(out), optional vt, real(dp), dimension(:), intent(out), optional, target work, integer(i32), intent(out), optional olwork, class(errors), intent(inout), optional, target err)

Computes the singular value decomposition of a matrix A. The SVD is defined as: A = U \* S \* V \* \* T, where U is an M-by-M orthogonal matrix, S is an M-by-N diagonal matrix, and V is an N-by-N orthogonal matrix.

# **Parameters**

in,out	а	On input, the M-by-N matrix to factor. The matrix is overwritten on output.
out	s	A MIN(M, N)-element array containing the singular values of a sorted in descending order.
out	и	An optional argument, that if supplied, is used to contain the orthogonal matrix U from the decomposition. The matrix U contains the left singular vectors, and can be either M-by-M (all left singular vectors are computed), or M-by-MIN(M,N) (only the first MIN(M, N) left singular vectors are computed).
out	vt	An optional argument, that if supplied, is used to contain the transpose of the N-by-N orthogonal matrix V. The matrix V contains the right singular vectors.
out	work	An optional input, that if provided, prevents any local memory allocation. If not provided, the memory required is allocated within. If provided, the length of the array must be at least olwork.
out	olwork	An optional output used to determine workspace size. If supplied, the routine determines the optimal size for work, and returns without performing any actual calculations.
out	err	An optional errors-based object that if provided can be used to retrieve information relating to any errors encountered during execution. If not provided, a default implementation of the errors class is used internally to provide error handling. Possible errors and warning messages that may be encountered are as follows.
		<ul> <li>LA_ARRAY_SIZE_ERROR: Occurs if any of the input arrays are not sized appropriately.</li> </ul>
		<ul> <li>LA_OUT_OF_MEMORY_ERROR: Occurs if local memory must be allocated, and there is insufficient memory available.</li> </ul>
		<ul> <li>LA_CONVERGENCE_ERROR: Occurs as a warning if the QR iteration process could not converge to a zero value.</li> </ul>

# Usage

```
! Decompose matrix the M-by-N matrix A such that A = U * S * V**T with ! M >= N.

! Variables
real(dp), dimension(m, n) :: a
real(dp), dimension(m, m) :: u
real(dp), dimension(n, n) :: vt
real(dp), dimension(n) :: s

! Initialize A...

! Compute the SVD of A. On output, S contains the MIN(M,N) singular
! values of A in descending order, U contains the left singular vectors
! (one per column), and VT contains the right singular vectors (one per row).
call svd(a, s, u, vt)

! Note: If M > N, then we can make U M-by-N, and compute the N
! left singular vectors of A, as there are at most N singular values
! of A. Also, if M < N, then there are at most M singular values of A,
! and as such, the length of the array s should be m.
```

## Notes

This routine utilizes the LAPACK routine DGESVD.

#### See Also

- · Wikipedia
- Wolfram MathWorld

Definition at line 2046 of file linalg\_factor.f90.

## 4.7 linalg\_solve Module Reference

#### linalg solve

#### **Data Types**

· interface solve\_cholesky

Solves a system of Cholesky factored equations.

• interface solve\_least\_squares

Solves the overdetermined or underdetermined system (A\*X = B) of M equations of N unknowns.

interface solve\_least\_squares\_full

Solves the overdetermined or underdetermined system (A\*X = B) of M equations of N unknowns, but uses a full orthogonal factorization of the system.

· interface solve least squares svd

Solves the overdetermined or underdetermined system (A\*X = B) of M equations of N unknowns using a singular value decomposition of matrix A.

· interface solve lu

Solves a system of LU-factored equations.

interface solve\_qr

Solves a system of M QR-factored equations of N unknowns.

• interface solve triangular system

Solves a triangular system of equations.

## **Functions/Subroutines**

• subroutine solve\_tri\_mtx (Iside, upper, trans, nounit, alpha, a, b, err)

Solves one of the matrix equations: op(A) \* X = alpha \* B, or X \* op(A) = alpha \* B, where A is a triangular matrix.

• subroutine solve\_tri\_vec (upper, trans, nounit, a, x, err)

Solves the system of equations: op(A) \* X = B, where A is a triangular matrix.

• subroutine solve\_lu\_mtx (a, ipvt, b, err)

Solves a system of LU-factored equations.

• subroutine solve\_lu\_vec (a, ipvt, b, err)

Solves a system of LU-factored equations.

subroutine solve\_qr\_no\_pivot\_mtx (a, tau, b, work, olwork, err)

Solves a system of M QR-factored equations of N unknowns where M >= N.

• subroutine solve\_qr\_no\_pivot\_vec (a, tau, b, work, olwork, err)

Solves a system of M QR-factored equations of N unknowns where M >= N.

subroutine solve\_qr\_pivot\_mtx (a, tau, jpvt, b, work, olwork, err)

Solves a system of M QR-factored equations of N unknowns where the QR factorization made use of column pivoting.

• subroutine solve qr pivot vec (a, tau, jpvt, b, work, olwork, err)

Solves a system of M QR-factored equations of N unknowns where the QR factorization made use of column pivoting.

• subroutine solve\_cholesky\_mtx (upper, a, b, err)

Solves a system of Cholesky factored equations.

subroutine solve\_cholesky\_vec (upper, a, b, err)

Solves a system of Cholesky factored equations.

• subroutine, public mtx\_inverse (a, iwork, work, olwork, err)

Computes the inverse of a square matrix.

• subroutine, public mtx\_pinverse (a, ainv, tol, work, olwork, err)

Computes the Moore-Penrose pseudo-inverse of a M-by-N matrix using the singular value decomposition of the matrix.

subroutine solve least squares mtx (a, b, work, olwork, err)

Solves the overdetermined or underdetermined system (A\*X = B) of M equations of N unknowns using a QR or LQ factorization of the matrix A. Notice, it is assumed that matrix A has full rank.

• subroutine solve\_least\_squares\_vec (a, b, work, olwork, err)

Solves the overdetermined or underdetermined system (A\*X = B) of M equations of N unknowns using a QR or LQ factorization of the matrix A. Notice, it is assumed that matrix A has full rank.

subroutine solve\_least\_squares\_mtx\_pvt (a, b, ipvt, arnk, work, olwork, err)

Solves the overdetermined or underdetermined system (A\*X = B) of M equations of N unknowns using a complete orthogonal factorization of matrix A.

• subroutine solve\_least\_squares\_vec\_pvt (a, b, ipvt, arnk, work, olwork, err)

Solves the overdetermined or underdetermined system (A\*X = B) of M equations of N unknowns using a complete orthogonal factorization of matrix A.

• subroutine solve\_least\_squares\_mtx\_svd (a, b, arnk, s, work, olwork, err)

Solves the overdetermined or underdetermined system (A\*X = B) of M equations of N unknowns using a singular value decomposition of matrix A.

• subroutine solve\_least\_squares\_vec\_svd (a, b, arnk, s, work, olwork, err)

Solves the overdetermined or underdetermined system (A\*X = B) of M equations of N unknowns using a singular value decomposition of matrix A.

## 4.7.1 Detailed Description

#### linalg solve

## **Purpose**

Provides a set of routines for solving systems of linear equations.

#### 4.7.2 Function/Subroutine Documentation

4.7.2.1 subroutine, public linalg\_solve::mtx\_inverse ( real(dp), dimension(:,:), intent(inout) *a,* integer(i32), dimension(:), intent(out), optional, target *iwork,* real(dp), dimension(:), intent(out), optional, target *work,* integer(i32), intent(out), optional *olwork,* class(errors), intent(inout), optional, target *err* )

Computes the inverse of a square matrix.

in,out	а	On input, the N-by-N matrix to invert. On output, the inverted matrix.
out	iwork	An optional N-element integer workspace array.
out	work	An optional input, that if provided, prevents any local memory allocation. If not provided, the memory required is allocated within. If provided, the length of the array must be at least olwork.
out	olwork	An optional output used to determine workspace size. If supplied, the routine determines the optimal size for work, and returns without performing any actual calculations.

# **Parameters**

out	err	An optional errors-based object that if provided can be used to retrieve information relating to any errors encountered during execution. If not provided, a default implementation of the errors class is used internally to provide error handling. Possible errors and warning messages that may be encountered are as follows.
		<ul> <li>LA_ARRAY_SIZE_ERROR: Occurs if a is not square. Will also occur if incorrectly sized workspace arrays are provided.</li> </ul>
		<ul> <li>LA_OUT_OF_MEMORY_ERROR: Occurs if local memory must be allocated, and there is insufficient memory available.</li> </ul>
		LA_SINGULAR_MATRIX_ERROR: Occurs if the input matrix is singular.

# Usage

```
! The following example illustrates how to solve a system of linear
! equations by matrix inversion. Notice, this is not a preferred
! solution technique (use LU factorization instead), but is merely a
! means of illustrating how to compute the inverse of a square matrix.
! Variables
real(dp), dimension(n, n) :: a
real(dp), dimension(n, nrhs) :: b, x
! Initialize A and B...
! Compute the inverse of A. The inverse will overwrite the original
! matrix.
call mtx_inverse(a)
! Solve A*X = B as X = inv(A) * B.
x = matmul(a, b)
```

# Notes

This routine utilizes the LAPACK routines DGETRF to perform an LU factorization of the matrix, and DGETRI to invert the LU factored matrix.

#### See Also

- Wikipedia
- Wolfram MathWorld

Definition at line 1240 of file linalg\_solve.f90.

4.7.2.2 subroutine, public linalg\_solve::mtx\_pinverse ( real(dp), dimension(:,:), intent(inout) *a,* real(dp), dimension(:,:), intent(out) *ainv,* real(dp), intent(in), optional *tol,* real(dp), dimension(:), intent(out), optional, target *work,* integer(i32), intent(out), optional *olwork,* class(errors), intent(inout), optional, target *err* )

Computes the Moore-Penrose pseudo-inverse of a M-by-N matrix using the singular value decomposition of the matrix.

in,out	а	On input, the M-by-N matrix to invert. The matrix is overwritten on output.
out	ainv	The N-by-M matrix where the pseudo-inverse of a will be written.
in	tol	An optional input, that if supplied, overrides the default tolerance on singular values such that singular values less than this tolerance are forced to have a reciprocal of zero, as opposed to $1/S(I)$ . The default tolerance is: MAX(M, N) $*$ EPS $*$ MAX(S). If the supplied value is less than a value that causes an overflow, the tolerance reverts back to its default
		value, and the operation continues; however, a warning message is issued.

#### **Parameters**

out	work	An optional input, that if provided, prevents any local memory allocation. If not provided, the memory required is allocated within. If provided, the length of the array must be at least olwork.
out	olwork	An optional output used to determine workspace size. If supplied, the routine determines the optimal size for work, and returns without performing any actual calculations.
out	err	An optional errors-based object that if provided can be used to retrieve information relating to any errors encountered during execution. If not provided, a default implementation of the errors class is used internally to provide error handling. Possible errors and warning messages that may be encountered are as follows.  • LA_ARRAY_SIZE_ERROR: Occurs if any of the input arrays are not sized appropriately.  • LA_OUT_OF_MEMORY_ERROR: Occurs if local memory must be allocated, and there is insufficient memory available.  • LA_CONVERGENCE_ERROR: Occurs as a warning if the QR iteration process could not converge to a zero value.

## Usage

```
! Use the pseudo-inverse to obtain a least-squares solution to the
! overdetermined problem A+X = B, where A is an M-by-N matrix (M >= N),
! B is an M-by-NRHS matrix, and X is an N-by-NRHS matrix.
! Variables
real(dp), dimension(m, n) :: a
real(dp), dimension(m, m) :: ainv
real(dp), dimension(m, nrhs) :: b
real(dp), dimension(n, nrhs) :: x
! Initialize A, and B...
! Compute the pseudo-inverse of A. Let the subroutine allocate its
! own workspace array.
call mtx_pinverse(a, ainv)
! Compute X = AINV * B to obtain the solution.
x = matmul(ainv, b)
```

## See Also

- Wikipedia
- Wolfram MathWorld
- MathWorks

Definition at line 1400 of file linalg\_solve.f90.

4.7.2.3 subroutine linalg\_solve::solve\_cholesky\_mtx ( logical, intent(in) *upper*, real(dp), dimension(:,:), intent(in) *a*, real(dp), dimension(:,:), intent(inout) *b*, class(errors), intent(inout), optional, target *err* ) [private]

Solves a system of Cholesky factored equations.

in	upper	Set to true if the original matrix A was factored such that $A = U**T*U$ ; else, set to false if
		the factorization of A was $A = L**T*L$ .
in	а	The N-by-N Cholesky factored matrix.
in,out	b	On input, the N-by-NRHS right-hand-side matrix B. On output, the solution matrix X.

#### **Parameters**

out	err	An optional errors-based object that if provided can be used to retrieve information relating to any errors encountered during execution. If not provided, a default implementation of the errors class is used internally to provide error handling. Possible errors and warning messages that may be encountered are as follows.
		LA_ARRAY_SIZE_ERROR: Occurs if any of the input array sizes are incorrect.

#### Notes

This routine utilizes the LAPACK routine DPOTRS.

Definition at line 1073 of file linalg\_solve.f90.

4.7.2.4 subroutine linalg\_solve::solve\_cholesky\_vec ( logical, intent(in) *upper*, real(dp), dimension(:,:), intent(in) *a*, real(dp), dimension(:), intent(inout) *b*, class(errors), intent(inout), optional, target *err* ) [private]

Solves a system of Cholesky factored equations.

#### **Parameters**

in	upper	Set to true if the original matrix A was factored such that $A = U**T*U$ ; else, set to false if the factorization of A was $A = L**T*L$ .
in	а	The N-by-N Cholesky factored matrix.
in,out	b	On input, the N-element right-hand-side vector B. On output, the solution vector X.
out	err	An optional errors-based object that if provided can be used to retrieve information relating to any errors encountered during execution. If not provided, a default implementation of the errors class is used internally to provide error handling. Possible errors and warning messages that may be encountered are as follows.
		<ul> <li>LA_ARRAY_SIZE_ERROR: Occurs if any of the input array sizes are incorrect.</li> </ul>

## Notes

This routine utilizes the LAPACK routine DPOTRS.

Definition at line 1139 of file linalg\_solve.f90.

4.7.2.5 subroutine linalg\_solve::solve\_least\_squares\_mtx ( real(dp), dimension(:,:), intent(inout) a, real(dp), dimension(:,:), intent(inout) b, real(dp), dimension(:), intent(out), optional, target work, integer(i32), intent(out), optional olwork, class(errors), intent(inout), optional, target err ) [private]

Solves the overdetermined or underdetermined system (A\*X = B) of M equations of N unknowns using a QR or LQ factorization of the matrix A. Notice, it is assumed that matrix A has full rank.

in,out	а	On input, the M-by-N matrix A. On output, if M >= N, the QR factorization of A in the form
		as output by $qr_factor$ ; else, if $M < N$ , the LQ factorization of A.

## **Parameters**

in,out	b	If $M >= N$ , the M-by-NRHS matrix B. On output, the first N rows contain the N-by-NRHS solution matrix X. If $M < N$ , an N-by-NRHS matrix with the first M rows containing the matrix B. On output, the N-by-NRHS solution matrix X.
out	work	An optional input, that if provided, prevents any local memory allocation. If not provided, the memory required is allocated within. If provided, the length of the array must be at least olwork.
out	olwork	An optional output used to determine workspace size. If supplied, the routine determines the optimal size for work, and returns without performing any actual calculations.
out	err	An optional errors-based object that if provided can be used to retrieve information relating to any errors encountered during execution. If not provided, a default implementation of the errors class is used internally to provide error handling. Possible errors and warning messages that may be encountered are as follows.
		<ul> <li>LA_ARRAY_SIZE_ERROR: Occurs if any of the input arrays are not sized appropriately.</li> </ul>
		<ul> <li>LA_OUT_OF_MEMORY_ERROR: Occurs if local memory must be allocated, and there is insufficient memory available.</li> </ul>
		LA_INVALID_OPERATION_ERROR: Occurs if a is not of full rank.

# Notes

This routine utilizes the LAPACK routine DGELS.

Definition at line 1568 of file linalg\_solve.f90.

4.7.2.6 subroutine linalg\_solve::solve\_least\_squares\_mtx\_pvt ( real(dp), dimension(:,:), intent(inout) a, real(dp), dimension(:,:), intent(inout) b, integer(i32), dimension(:), intent(inout), optional, target ipvt, integer(i32), intent(out), optional arnk, real(dp), dimension(:), intent(out), optional, target work, integer(i32), intent(out), optional olwork, class(errors), intent(inout), optional, target err ) [private]

Solves the overdetermined or underdetermined system (A\*X = B) of M equations of N unknowns using a complete orthogonal factorization of matrix A.

in,out	а	On input, the M-by-N matrix A. On output, the matrix is overwritten by the details of its complete orthogonal factorization.
in,out	b	If $M >= N$ , the M-by-NRHS matrix B. On output, the first N rows contain the N-by-NRHS solution matrix X. If $M < N$ , an N-by-NRHS matrix with the first M rows containing the matrix B. On output, the N-by-NRHS solution matrix X.
out	ipvt	An optional input that on input, an N-element array that if $IPVT(I)$ .ne. 0, the I-th column of A is permuted to the front of A $*$ P; if $IPVT(I) = 0$ , the I-th column of A is a free column. On output, if $IPVT(I) = K$ , then the I-th column of A $*$ P was the K-th column of A. If not supplied, memory is allocated internally, and $IPVT$ is set to all zeros such that all columns are treated as free.
out	arnk	An optional output, that if provided, will return the rank of a.
out	work	An optional input, that if provided, prevents any local memory allocation. If not provided, the memory required is allocated within. If provided, the length of the array must be at least olwork.
out	olwork	An optional output used to determine workspace size. If supplied, the routine determines the optimal size for work, and returns without performing any actual calculations.

## **Parameters**

out	err	An optional errors-based object that if provided can be used to retrieve information relating to any errors encountered during execution. If not provided, a default implementation of the errors class is used internally to provide error handling. Possible errors and warning messages that may be encountered are as follows.
		<ul> <li>LA_ARRAY_SIZE_ERROR: Occurs if any of the input arrays are not sized appropriately.</li> </ul>
		<ul> <li>LA_OUT_OF_MEMORY_ERROR: Occurs if local memory must be allocated, and there is insufficient memory available.</li> </ul>

## Notes

This routine utilizes the LAPACK routine DGELSY.

Definition at line 1786 of file linalg\_solve.f90.

4.7.2.7 subroutine linalg\_solve::solve\_least\_squares\_mtx\_svd ( real(dp), dimension(:,:), intent(inout) a, real(dp), dimension(:,:), intent(inout) b, integer(i32), intent(out), optional arnk, real(dp), dimension(:), intent(out) s, real(dp), dimension(:), intent(out), optional, target work, integer(i32), intent(out), optional olwork, class(errors), intent(inout), optional, target err ) [private]

Solves the overdetermined or underdetermined system (A\*X = B) of M equations of N unknowns using a singular value decomposition of matrix A.

in,out	а	On input, the M-by-N matrix A. On output, the matrix is overwritten by the details of its complete orthogonal factorization.
in,out	b	If M $>=$ N, the M-by-NRHS matrix B. On output, the first N rows contain the N-by-NRHS solution matrix X. If M $<$ N, an N-by-NRHS matrix with the first M rows containing the matrix B. On output, the N-by-NRHS solution matrix X.
out	arnk	An optional output, that if provided, will return the rank of a.
out	s	A MIN(M, N)-element array that on output contains the singular values of $a$ in descending order. Notice, the condition number of $a$ can be determined by S(1) / S(MIN(M, N)).
out	work	An optional input, that if provided, prevents any local memory allocation. If not provided, the memory required is allocated within. If provided, the length of the array must be at least olwork.
out	olwork	An optional output used to determine workspace size. If supplied, the routine determines the optimal size for work, and returns without performing any actual calculations.
out	err	An optional errors-based object that if provided can be used to retrieve information relating to any errors encountered during execution. If not provided, a default implementation of the errors class is used internally to provide error handling. Possible errors and warning messages that may be encountered are as follows.  • LA_ARRAY_SIZE_ERROR: Occurs if any of the input arrays are not sized
		<ul> <li>appropriately.</li> <li>LA_OUT_OF_MEMORY_ERROR: Occurs if local memory must be allocated, and there is insufficient memory available.</li> </ul>
		<ul> <li>LA_CONVERGENCE_ERROR: Occurs as a warning if the QR iteration process could not converge to a zero value.</li> </ul>

#### Notes

This routine utilizes the LAPACK routine DGELSS.

Definition at line 2076 of file linalg solve.f90.

4.7.2.8 subroutine linalg\_solve::solve\_least\_squares\_vec ( real(dp), dimension(:,:), intent(inout) a, real(dp), dimension(:), intent(inout) b, real(dp), dimension(:), intent(out), optional, target work, integer(i32), intent(out), optional olwork, class(errors), intent(inout), optional, target err ) [private]

Solves the overdetermined or underdetermined system (A\*X = B) of M equations of N unknowns using a QR or LQ factorization of the matrix A. Notice, it is assumed that matrix A has full rank.

#### **Parameters**

in,out	а	On input, the M-by-N matrix A. On output, if $M \ge N$ , the QR factorization of A in the form as output by qr_factor; else, if $M < N$ , the LQ factorization of A.
in,out	b	If $M >= N$ , the M-element array B. On output, the first N elements contain the N-element solution array X. If $M < N$ , an N-element array with the first M elements containing the array B. On output, the N-element solution array X.
out	work	An optional input, that if provided, prevents any local memory allocation. If not provided, the memory required is allocated within. If provided, the length of the array must be at least olwork.
out	olwork	An optional output used to determine workspace size. If supplied, the routine determines the optimal size for work, and returns without performing any actual calculations.
out	err	An optional errors-based object that if provided can be used to retrieve information relating to any errors encountered during execution. If not provided, a default implementation of the errors class is used internally to provide error handling. Possible errors and warning messages that may be encountered are as follows.
		<ul> <li>LA_ARRAY_SIZE_ERROR: Occurs if any of the input arrays are not sized appropriately.</li> </ul>
		<ul> <li>LA_OUT_OF_MEMORY_ERROR: Occurs if local memory must be allocated, and there is insufficient memory available.</li> </ul>
		LA_INVALID_OPERATION_ERROR: Occurs if a is not of full rank.

## Notes

This routine utilizes the LAPACK routine DGELS.

Definition at line 1674 of file linalg\_solve.f90.

4.7.2.9 subroutine linalg\_solve::solve\_least\_squares\_vec\_pvt ( real(dp), dimension(:,:), intent(inout) a, real(dp), dimension(:), intent(inout) b, integer(i32), dimension(:), intent(inout), optional, target ipvt, integer(i32), intent(out), optional arnk, real(dp), dimension(:), intent(out), optional, target work, integer(i32), intent(out), optional olwork, class(errors), intent(inout), optional, target err ) [private]

Solves the overdetermined or underdetermined system (A\*X = B) of M equations of N unknowns using a complete orthogonal factorization of matrix A.

## **Parameters**

in,out	а	On input, the M-by-N matrix A. On output, the matrix is overwritten by the details of its complete orthogonal factorization.
in,out	b	If $M >= N$ , the M-element array B. On output, the first N elements contain the N-element solution array X. If $M < N$ , an N-element array with the first M elements containing the array B. On output, the N-element solution array X.
out	ipvt	An optional input that on input, an N-element array that if $IPVT(I)$ .ne. 0, the I-th column of A is permuted to the front of A $*$ P; if $IPVT(I) = 0$ , the I-th column of A is a free column. On output, if $IPVT(I) = K$ , then the I-th column of A $*$ P was the K-th column of A. If not supplied, memory is allocated internally, and $IPVT$ is set to all zeros such that all columns are treated as free.
out	arnk	An optional output, that if provided, will return the rank of a.
out	work	An optional input, that if provided, prevents any local memory allocation. If not provided, the memory required is allocated within. If provided, the length of the array must be at least olwork.
out	olwork	An optional output used to determine workspace size. If supplied, the routine determines the optimal size for work, and returns without performing any actual calculations.
out	err	An optional errors-based object that if provided can be used to retrieve information relating to any errors encountered during execution. If not provided, a default implementation of the errors class is used internally to provide error handling. Possible errors and warning messages that may be encountered are as follows.
		<ul> <li>LA_ARRAY_SIZE_ERROR: Occurs if any of the input arrays are not sized appropriately.</li> </ul>
		<ul> <li>LA_OUT_OF_MEMORY_ERROR: Occurs if local memory must be allocated, and there is insufficient memory available.</li> </ul>

## Notes

This routine utilizes the LAPACK routine DGELSY.

Definition at line 1932 of file linalg\_solve.f90.

4.7.2.10 subroutine linalg\_solve::solve\_least\_squares\_vec\_svd ( real(dp), dimension(:,:), intent(inout) a, real(dp), dimension(:), intent(inout) b, integer(i32), intent(out), optional arnk, real(dp), dimension(:), intent(out) s, real(dp), dimension(:), intent(out), optional, target work, integer(i32), intent(out), optional olwork, class(errors), intent(inout), optional, target err ) [private]

Solves the overdetermined or underdetermined system (A\*X = B) of M equations of N unknowns using a singular value decomposition of matrix A.

in,out	а	On input, the M-by-N matrix A. On output, the matrix is overwritten by the details of its complete orthogonal factorization.
in,out	b	If $M >= N$ , the M-by-NRHS matrix B. On output, the first N rows contain the N-by-NRHS solution matrix X. If $M < N$ , an N-by-NRHS matrix with the first M rows containing the matrix B. On output, the N-by-NRHS solution matrix X.
out	arnk	An optional output, that if provided, will return the rank of a.
out	s	A MIN(M, N)-element array that on output contains the singular values of $a$ in descending order. Notice, the condition number of $a$ can be determined by S(1) / S(MIN(M, N)).

## **Parameters**

out	work	An optional input, that if provided, prevents any local memory allocation. If not provided, the memory required is allocated within. If provided, the length of the array must be at least olwork.
out	olwork	An optional output used to determine workspace size. If supplied, the routine determines the optimal size for work, and returns without performing any actual calculations.
out	err	An optional errors-based object that if provided can be used to retrieve information relating to any errors encountered during execution. If not provided, a default implementation of the errors class is used internally to provide error handling. Possible errors and warning messages that may be encountered are as follows.  • LA_ARRAY_SIZE_ERROR: Occurs if any of the input arrays are not sized appropriately.  • LA_OUT_OF_MEMORY_ERROR: Occurs if local memory must be allocated, and there is insufficient memory available.  • LA_CONVERGENCE_ERROR: Occurs as a warning if the QR iteration process could not converge to a zero value.

#### **Notes**

This routine utilizes the LAPACK routine DGELSS.

Definition at line 2204 of file linalg\_solve.f90.

4.7.2.11 subroutine linalg\_solve::solve\_lu\_mtx ( real(dp), dimension(:,:), intent(in) *a,* integer(i32), dimension(:), intent(in) *ipvt,* real(dp), dimension(:,:), intent(inout) *b,* class(errors), intent(inout), optional, target *err* ) [private]

Solves a system of LU-factored equations.

# **Parameters**

nt pivot array as output by lu_factor.
N-by-NRHS right-hand-side matrix. On output, the N-by-NRHS solution matrix.
crors-based object that if provided can be used to retrieve information relating encountered during execution. If not provided, a default implementation of the sused internally to provide error handling. Possible errors and warning at may be encountered are as follows.  RAY SIZE ERROR: Occurs if any of the input array sizes are incorrect.

# Notes

The routine is based upon the LAPACK routine DGETRS.

Definition at line 351 of file linalg\_solve.f90.

4.7.2.12 subroutine linalg\_solve::solve\_lu\_vec ( real(dp), dimension(:,:), intent(in) a, integer(i32), dimension(:), intent(in) ipvt, real(dp), dimension(:), intent(inout) b, class(errors), intent(inout), optional, target err ) [private]

Solves a system of LU-factored equations.

## **Parameters**

in	а	The N-by-N LU factored matrix as output by lu_factor.
in	ipvt	The N-element pivot array as output by lu_factor.
in,out	b	On input, the N-element right-hand-side array. On output, the N-element solution array.
out	err	An optional errors-based object that if provided can be used to retrieve information relating to any errors encountered during execution. If not provided, a default implementation of the errors class is used internally to provide error handling. Possible errors and warning messages that may be encountered are as follows.  • LA_ARRAY_SIZE_ERROR: Occurs if any of the input array sizes are incorrect.

## Notes

The routine is based upon the LAPACK routine DGETRS.

Definition at line 412 of file linalg\_solve.f90.

4.7.2.13 subroutine linalg\_solve::solve\_qr\_no\_pivot\_mtx ( real(dp), dimension(:,:), intent(inout) a, real(dp), dimension(:), intent(in) tau, real(dp), dimension(:,:), intent(inout) b, real(dp), dimension(:), intent(out), optional, target work, integer(i32), intent(out), optional olwork, class(errors), intent(inout), optional, target err ) [private]

Solves a system of M QR-factored equations of N unknowns where M >= N.

## **Parameters**

in	а	On input, the M-by-N QR factored matrix as returned by qr_factor. On output, the contents of this matrix are restored. Notice, M must be greater than or equal to N.
in	tau	A MIN(M, N)-element array containing the scalar factors of the elementary reflectors as returned by qr_factor.
in	b	On input, the M-by-NRHS right-hand-side matrix. On output, the first N columns are overwritten by the solution matrix X.
out	work	An optional input, that if provided, prevents any local memory allocation. If not provided, the memory required is allocated within. If provided, the length of the array must be at least olwork.
out	olwork	An optional output used to determine workspace size. If supplied, the routine determines the optimal size for $work$ , and returns without performing any actual calculations.
out	err	An optional errors-based object that if provided can be used to retrieve information relating to any errors encountered during execution. If not provided, a default implementation of the errors class is used internally to provide error handling. Possible errors and warning messages that may be encountered are as follows.
		<ul> <li>LA_ARRAY_SIZE_ERROR: Occurs if any of the input arrays are not sized appropriately.</li> </ul>
		<ul> <li>LA_OUT_OF_MEMORY_ERROR: Occurs if local memory must be allocated, and there is insufficient memory available.</li> </ul>

## Notes

This routine is based upon a subset of the LAPACK routine DGELS.

Definition at line 487 of file linalg\_solve.f90.

4.7.2.14 subroutine linalg\_solve::solve\_qr\_no\_pivot\_vec ( real(dp), dimension(:,:), intent(inout) a, real(dp), dimension(:), intent(in) tau, real(dp), dimension(:), intent(inout) b, real(dp), dimension(:), intent(out), optional, target work, integer(i32), intent(out), optional olwork, class(errors), intent(inout), optional, target err ) [private]

Solves a system of M QR-factored equations of N unknowns where  $M \ge N$ .

#### **Parameters**

in	а	On input, the M-by-N QR factored matrix as returned by qr_factor. On output, the contents of this matrix are restored. Notice, M must be greater than or equal to N.
in	tau	A MIN(M, N)-element array containing the scalar factors of the elementary reflectors as returned by qr_factor.
in	b	On input, the M-element right-hand-side vector. On output, the first N elements are overwritten by the solution vector X.
out	work	An optional input, that if provided, prevents any local memory allocation. If not provided, the memory required is allocated within. If provided, the length of the array must be at least olwork.
out	olwork	An optional output used to determine workspace size. If supplied, the routine determines the optimal size for $work$ , and returns without performing any actual calculations.
out	err	An optional errors-based object that if provided can be used to retrieve information relating to any errors encountered during execution. If not provided, a default implementation of the errors class is used internally to provide error handling. Possible errors and warning messages that may be encountered are as follows.
		<ul> <li>LA_ARRAY_SIZE_ERROR: Occurs if any of the input arrays are not sized appropriately.</li> </ul>
		<ul> <li>LA_OUT_OF_MEMORY_ERROR: Occurs if local memory must be allocated, and there is insufficient memory available.</li> </ul>

#### Notes

This routine is based upon a subset of the LAPACK routine DGELS.

Definition at line 602 of file linalg\_solve.f90.

4.7.2.15 subroutine linalg\_solve::solve\_qr\_pivot\_mtx ( real(dp), dimension(:,:), intent(inout) a, real(dp), dimension(:), intent(in) tau, integer(i32), dimension(:), intent(in) jpvt, real(dp), dimension(:,:), intent(inout) b, real(dp), dimension(:), intent(out), optional, target work, integer(i32), intent(out), optional olwork, class(errors), intent(inout), optional, target err )

[private]

Solves a system of M QR-factored equations of N unknowns where the QR factorization made use of column pivoting.

in	а	On input, the M-by-N QR factored matrix as returned by qr_factor. On output, the contents of
		this matrix are altered.
in	tau	A MIN(M, N)-element array containing the scalar factors of the elementary reflectors as
		returned by qr_factor.
in	jpvt	An N-element array, as output by qr_factor, used to track the column pivots.
in	b	On input, the MAX(M, N)-by-NRHS matrix where the first M rows contain the right-hand-side
		matrix B. On output, the first N rows are overwritten by the solution matrix X.

## **Parameters**

out	work	An optional input, that if provided, prevents any local memory allocation. If not provided, the memory required is allocated within. If provided, the length of the array must be at least olwork.
out	olwork	An optional output used to determine workspace size. If supplied, the routine determines the optimal size for work, and returns without performing any actual calculations.
out	err	An optional errors-based object that if provided can be used to retrieve information relating to any errors encountered during execution. If not provided, a default implementation of the errors class is used internally to provide error handling. Possible errors and warning messages that may be encountered are as follows.
		<ul> <li>LA_ARRAY_SIZE_ERROR: Occurs if any of the input arrays are not sized appropriately.</li> </ul>
		LA_OUT_OF_MEMORY_ERROR: Occurs if local memory must be allocated, and there is insufficient memory available.

## Notes

This routine is based upon a subset of the LAPACK routine DGELSY.

Definition at line 715 of file linalg\_solve.f90.

4.7.2.16 subroutine linalg\_solve::solve\_qr\_pivot\_vec ( real(dp), dimension(:,:), intent(inout) a, real(dp), dimension(:), intent(in) tau, integer(i32), dimension(:), intent(in) jpvt, real(dp), dimension(:), intent(inout) b, real(dp), dimension(:), intent(out), optional, target work, integer(i32), intent(out), optional olwork, class(errors), intent(inout), optional, target err )

[private]

Solves a system of M QR-factored equations of N unknowns where the QR factorization made use of column pivoting.

а	On input, the M-by-N QR factored matrix as returned by qr_factor. On output, the contents of this matrix are altered.
tau	A MIN(M, N)-element array containing the scalar factors of the elementary reflectors as returned by qr_factor.
jpvt	An N-element array, as output by qr_factor, used to track the column pivots.
b	On input, the MAX(M, N)-element array where the first M elements contain the right-hand-side vector B. On output, the first N elements are overwritten by the solution vector X.
work	An optional input, that if provided, prevents any local memory allocation. If not provided, the memory required is allocated within. If provided, the length of the array must be at least olwork.
olwork	An optional output used to determine workspace size. If supplied, the routine determines the optimal size for work, and returns without performing any actual calculations.
err	An optional errors-based object that if provided can be used to retrieve information relating to any errors encountered during execution. If not provided, a default implementation of the errors class is used internally to provide error handling. Possible errors and warning messages that may be encountered are as follows.
	<ul> <li>LA_ARRAY_SIZE_ERROR: Occurs if any of the input arrays are not sized appropriately.</li> </ul>
	<ul> <li>LA_OUT_OF_MEMORY_ERROR: Occurs if local memory must be allocated, and there is insufficient memory available.</li> </ul>
	tau  jpvt b  work  olwork

#### Notes

This routine is based upon a subset of the LAPACK routine DGELSY.

Definition at line 902 of file linalg\_solve.f90.

4.7.2.17 subroutine linalg\_solve::solve\_tri\_mtx ( logical, intent(in) *Iside,* logical, intent(in) *upper,* logical, intent(in) *trans,* logical, intent(in) *nounit,* real(dp), intent(in) *alpha,* real(dp), dimension(:,:), intent(in) *a,* real(dp), dimension(:,:), intent(inout) *b,* class(errors), intent(inout), optional, target *err* ) [private]

Solves one of the matrix equations: op(A) \* X = alpha \* B, or X \* op(A) = alpha \* B, where A is a triangular matrix.

#### **Parameters**

in	Iside	Set to true to solve $op(A) * X = alpha * B$ ; else, set to false to solve $X * op(A) = alpha * B$ .
in	upper	Set to true if A is an upper triangular matrix; else, set to false if A is a lower triangular
		matrix.
in	trans	Set to true if $op(A) = A**T$ ; else, set to false if $op(A) = A$ .
in	nounit	Set to true if A is not a unit-diagonal matrix (ones on every diagonal element); else, set to
		false if A is a unit-diagonal matrix.
in	alpha	The scalar multiplier to B.
in	а	If lside is true, the M-by-M triangular matrix on which to operate; else, if lside is
		false, the N-by-N triangular matrix on which to operate.
in,out	b	On input, the M-by-N right-hand-side. On output, the M-by-N solution.
out	err	An optional errors-based object that if provided can be used to retrieve information
		relating to any errors encountered during execution. If not provided, a default
		implementation of the errors class is used internally to provide error handling. Possible
		errors and warning messages that may be encountered are as follows.
		LA_ARRAY_SIZE_ERROR: Occurs if a is not square, or if the sizes of a and b are
		not compatible.

# **Usage**

To solve a triangular system of N equations of N unknowns A\*X = B, where A is an N-by-N upper triangular matrix, and B and X are N-by-NRHS matrices, the following code will suffice.

# Notes

This routine is based upon the BLAS routine DTRSM.

Definition at line 169 of file linalg\_solve.f90.

4.7.2.18 subroutine linalg\_solve::solve\_tri\_vec ( logical, intent(in) upper, logical, intent(in) trans, logical, intent(in) nounit, real(dp), dimension(:,:), intent(in) a, real(dp), dimension(:), intent(inout) x, class(errors), intent(inout), optional, target err ) [private]

Solves the system of equations: op(A) \* X = B, where A is a triangular matrix.

#### **Parameters**

in	upper	Set to true if A is an upper triangular matrix; else, set to false if A is a lower triangular matrix.
in	trans	Set to true if $op(A) = A**T$ ; else, set to false if $op(A) = A$ .
in	nounit	Set to true if A is not a unit-diagonal matrix (ones on every diagonal element); else, set to false if A is a unit-diagonal matrix.
in	а	The N-by-N triangular matrix.
in,out	х	On input, the N-element right-hand-side array. On output, the N-element solution array.
out	err	An optional errors-based object that if provided can be used to retrieve information relating to any errors encountered during execution. If not provided, a default implementation of the errors class is used internally to provide error handling. Possible errors and warning messages that may be encountered are as follows.  • LA_ARRAY_SIZE_ERROR: Occurs if a is not square, or if the sizes of a and b are not compatible.

#### Usage

To solve a triangular system of N equations of N unknowns A\*X = B, where A is an N-by-N upper triangular matrix, and B and X are N-element arrays, the following code will suffice.

```
! Solve the system: A*X = B, where A is an upper triangular N-by-N
! matrix, and B and X are N-elements in size.
! Variables
integer(i32) :: info
real(dp), dimension(n, n) :: a
real(dp), dimension(n) :: b
! Initialize A and B...
! Solve A*X = B for X - Note: X overwrites B.
call solve_triangular_system(.true., .false., a, b)
```

#### **Notes**

This routine is based upon the BLAS routine DTRSV.

Definition at line 275 of file linalg\_solve.f90.

# 5 Data Type Documentation

# 5.1 linalg\_core::diag\_mtx\_mult Interface Reference

Multiplies a diagonal matrix with another matrix or array.

## **Private Member Functions**

- subroutine diag\_mtx\_mult\_mtx (Iside, trans, alpha, a, b, beta, c, err)
  - Computes the matrix operation: C = alpha \* A \* op(B) + beta \* C, or C = alpha \* op(B) \* A + beta \* C.
- subroutine diag\_mtx\_mult\_mtx2 (Iside, alpha, a, b, err)
  - Computes the matrix operation: B = alpha \* A \* op(B), or B = alpha \* op(B) \* A.
- subroutine diag\_mtx\_mult\_mtx3 (Iside, trans, alpha, a, b, beta, c, err)
  - Computes the matrix operation: C = alpha \* A \* op(B) + beta \* C, or C = alpha \* op(B) \* A + beta \* C, where A and C are complex-valued.
- subroutine diag\_mtx\_mult\_mtx4 (Iside, trans, alpha, a, b, beta, c, err)
  - Computes the matrix operation: C = alpha \* A \* op(B) + beta \* C, or C = alpha \* op(B) \* A + beta \* C, where A, B, and C are complex-valued.

## 5.1.1 Detailed Description

Multiplies a diagonal matrix with another matrix or array.

Definition at line 46 of file linalg\_core.f90.

#### 5.1.2 Member Function/Subroutine Documentation

5.1.2.1 subroutine linalg\_core::diag\_mtx\_mult::diag\_mtx\_mult\_mtx ( logical, intent(in) *lside*, logical, intent(in) *trans*, real(dp) *alpha*, real(dp), dimension(:,:), intent(in) *b*, real(dp) *beta*, real(dp), dimension(:,:), intent(inout) *c*, class(errors), intent(inout), optional, target *err* ) [private]

Computes the matrix operation: C = alpha \* A \* op(B) + beta \* C, or C = alpha \* op(B) \* A + beta \* C.

#### **Parameters**

in	Iside	Set to true to apply matrix A from the left; else, set to false to apply matrix A from the left.
in	trans	Set to true if $op(B) == B**T$ ; else, set to false if $op(B) == B$ .
in	alpha	A scalar multiplier.
in	а	A K-element array containing the diagonal elements of A where $K = MIN(M,P)$ if lside is true; else, if lside is false, $K = MIN(N,P)$ .
in	b	The LDB-by-TDB matrix B where (LDB = leading dimension of B, and TDB = trailing dimension of B):
		• lside == true & trans == true: LDB = N, TDB = P
		• lside == true & trans == false: LDB = P, TDB = N
		• lside == false & trans == true: LDB = P, TDB = M
		• lside == false & trans == false: LDB = M, TDB = P
in	beta	A scalar multiplier.
in,out	С	On input, the M-by-N matrix C. On output, the resulting M-by-N matrix.
out	err	An optional errors-based object that if provided can be used to retrieve information relating to any errors encountered during execution. If not provided, a default implementation of the errors class is used internally to provide error handling. Possible errors and warning messages that may be encountered are as follows.
		LA_ARRAY_SIZE_ERROR: Occurs if any of the input array sizes are incorrect.

Definition at line 327 of file linalg\_core.f90.

5.1.2.2 subroutine linalg\_core::diag\_mtx\_mult::diag\_mtx\_mult\_mtx2 ( logical, intent(in) *lside*, real(dp), intent(in) *alpha*, real(dp), dimension(:), intent(in) *a*, real(dp), dimension(:,:), intent(inout) *b*, class(errors), intent(inout), optional, target *err* ) [private]

Computes the matrix operation: B = alpha \* A \* op(B), or B = alpha \* op(B) \* A.

in	Iside	Set to true to apply matrix A from the left; else, set to false to apply matrix A from the left.
in	alpha	A scalar multiplier.

# **Parameters**

in	а	A K-element array containing the diagonal elements of A where K = MIN(M,P) if lside is true; else, if lside is false, K = MIN(N,P).
in	b	On input, the M-by-N matrix B. On output, the resulting M-by-N matrix.
out	err	An optional errors-based object that if provided can be used to retrieve information relating to any errors encountered during execution. If not provided, a default implementation of the errors class is used internally to provide error handling. Possible errors and warning messages that may be encountered are as follows.
		LA_ARRAY_SIZE_ERROR: Occurs if any of the input array sizes are incorrect.

Definition at line 494 of file linalg\_core.f90.

5.1.2.3 subroutine linalg\_core::diag\_mtx\_mult::diag\_mtx\_mult\_mtx3 ( logical, intent(in) *lside*, logical, intent(in) *trans*, real(dp) *alpha*, complex(dp), dimension(:,:), intent(in) *a*, real(dp), dimension(:,:), intent(in) *b*, real(dp) *beta*, complex(dp), dimension(:,:), intent(inout) *c*, class(errors), intent(inout), optional, target *err* ) [private]

Computes the matrix operation: C = alpha \* A \* op(B) + beta \* C, or C = alpha \* op(B) \* A + beta \* C, where A and C are complex-valued.

#### **Parameters**

in	Iside	Set to true to apply matrix A from the left; else, set to false to apply matrix A from the left.
in	trans	Set to true if $op(B) == B**T$ ; else, set to false if $op(B) == B$ .
in	alpha	A scalar multiplier.
in	а	A K-element array containing the diagonal elements of A where $K = MIN(M,P)$ if lside is true; else, if lside is false, $K = MIN(N,P)$ .
in	b	The LDB-by-TDB matrix B where (LDB = leading dimension of B, and TDB = trailing dimension of B):
		• lside == true & trans == true: LDB = N, TDB = P
		• lside == true & trans == false: LDB = P, TDB = N
		• lside == false & trans == true: LDB = P, TDB = M
		• lside == false & trans == false: LDB = M, TDB = P
in	beta	A scalar multiplier.
in,out	С	On input, the M-by-N matrix C. On output, the resulting M-by-N matrix.
out	err	An optional errors-based object that if provided can be used to retrieve information relating to any errors encountered during execution. If not provided, a default implementation of the errors class is used internally to provide error handling. Possible errors and warning messages that may be encountered are as follows.
		LA_ARRAY_SIZE_ERROR: Occurs if any of the input array sizes are incorrect.

Definition at line 577 of file linalg\_core.f90.

5.1.2.4 subroutine linalg\_core::diag\_mtx\_mult::diag\_mtx\_mult\_mtx4 ( logical, intent(in) *lside*, logical, intent(in) *trans*, real(dp) *alpha*, complex(dp), dimension(:,:), intent(in) *a*, complex(dp), dimension(:,:), intent(in) *b*, real(dp) *beta*, complex(dp), dimension(:,:), intent(inout) *c*, class(errors), intent(inout), optional, target *err* ) [private]

Computes the matrix operation: C = alpha \* A \* op(B) + beta \* C, or C = alpha \* op(B) \* A + beta \* C, where A, B, and C are complex-valued.

#### **Parameters**

in	Iside	Set to true to apply matrix A from the left; else, set to false to apply matrix A from the left.
in	trans	Set to true if $op(B) == B**T$ ; else, set to false if $op(B) == B$ .
in	alpha	A scalar multiplier.
in	а	A K-element array containing the diagonal elements of A where $K = MIN(M,P)$ if lside is true; else, if lside is false, $K = MIN(N,P)$ .
in	b	The LDB-by-TDB matrix B where:
		• lside == true & trans == true: LDA = N, TDB = P
		• lside == true & trans == false: LDA = P, TDB = N
		• lside == false & trans == true: LDA = P, TDB = M
		• lside == false & trans == false: LDA = M, TDB = P
in	beta	A scalar multiplier.
in,out	С	On input, the M-by-N matrix C. On output, the resulting M-by-N matrix.
out	err	An optional errors-based object that if provided can be used to retrieve information relating to any errors encountered during execution. If not provided, a default implementation of the errors class is used internally to provide error handling. Possible errors and warning messages that may be encountered are as follows.  • LA_ARRAY_SIZE_ERROR: Occurs if any of the input array sizes are incorrect.

Definition at line 753 of file linalg\_core.f90.

The documentation for this interface was generated from the following file:

• /home/jason/Documents/Code/linalg/src/linalg\_core.f90

# 5.2 lapack::DLAMCH Interface Reference

**Public Member Functions** 

• real(dp) function **dlamch** (cmach)

# 5.2.1 Detailed Description

Definition at line 14 of file lapack.f90.

The documentation for this interface was generated from the following file:

• /home/jason/Documents/Code/linalg/src/lapack.f90

# 5.3 linalg\_eigen::eigen Interface Reference

Computes the eigenvalues, and optionally the eigenvectors, of a matrix.

# **Private Member Functions**

- subroutine eigen\_symm (vecs, a, vals, work, olwork, err)
  - Computes the eigenvalues, and optionally the eigenvectors of a real, symmetric matrix.
- subroutine eigen\_asymm (a, vals, vecs, work, olwork, err)
  - Computes the eigenvalues, and optionally the right eigenvectors of a square matrix.
- subroutine eigen gen (a, b, alpha, beta, vecs, work, olwork, err)

Computes the eigenvalues, and optionally the right eigenvectors of a square matrix assuming the structure of the eigenvalue problem is A\*X = lambda\*B\*X.

#### 5.3.1 Detailed Description

Computes the eigenvalues, and optionally the eigenvectors, of a matrix.

#### See Also

- Wikipedia
- Wolfram MathWorld
- LAPACK Users Manual

Definition at line 24 of file linalg\_eigen.f90.

# 5.3.2 Member Function/Subroutine Documentation

5.3.2.1 subroutine linalg\_eigen::eigen\_asymm ( real(dp), dimension(:,:), intent(inout) a, complex(dp), dimension(:), intent(out) vals, complex(dp), dimension(:,:), intent(out), optional vecs, real(dp), dimension(:), intent(out), optional, pointer work, integer(i32), intent(out), optional olwork, class(errors), intent(inout), optional, target err ) [private]

Computes the eigenvalues, and optionally the right eigenvectors of a square matrix.

in,out	а	On input, the N-by-N matrix on which to operate. On output, the contents of this matrix are overwritten.
out	vals	An N-element array containing the eigenvalues of the matrix. The eigenvalues are not sorted.
out	vecs	An optional N-by-N matrix, that if supplied, signals to compute the right eigenvectors (one per column). If not provided, only the eigenvalues will be computed.
out	work	An optional input, that if provided, prevents any local memory allocation. If not provided, the memory required is allocated within. If provided, the length of the array must be at least olwork.
out	olwork	An optional output used to determine workspace size. If supplied, the routine determines the optimal size for work, and returns without performing any actual calculations.

# **Parameters**

out	err	An optional errors-based object that if provided can be used to retrieve information relating to any errors encountered during execution. If not provided, a default implementation of the errors class is used internally to provide error handling. Possible errors and warning messages that may be encountered are as follows.
		LA_ARRAY_SIZE_ERROR: Occurs if any of the input arrays are not sized appropriately.
		LA_OUT_OF_MEMORY_ERROR: Occurs if local memory must be allocated, and there is insufficient memory available.
		LA_CONVERGENCE_ERROR: Occurs if the algorithm failed to converge.

#### Notes

This routine utilizes the LAPACK routine DGEEV.

Definition at line 185 of file linalg\_eigen.f90.

5.3.2.2 subroutine linalg\_eigen::eigen\_gen ( real(dp), dimension(:,:), intent(inout) a, real(dp), dimension(:,:), intent(inout) b, complex(dp), dimension(:), intent(out) alpha, real(dp), dimension(:), intent(out), optional beta, complex(dp), dimension(:,:), intent(out), optional vecs, real(dp), dimension(:), intent(out), optional, pointer work, integer(i32), intent(out), optional olwork, class(errors), intent(inout), optional, target err ) [private]

Computes the eigenvalues, and optionally the right eigenvectors of a square matrix assuming the structure of the eigenvalue problem is A\*X = lambda\*B\*X.

in,out	а	On input, the N-by-N matrix A. On output, the contents of this matrix are overwritten.
in,out	b	On input, the N-by-N matrix B. On output, the contents of this matrix are overwritten.
out	alpha	An N-element array that, if beta is not supplied, contains the eigenvalues. If beta is supplied however, the eigenvalues must be computed as ALPHA / BETA. This however, is not as trivial as it seems as it is entirely possible, and likely, that ALPHA / BETA can overflow or underflow. With that said, the values in ALPHA will always be less than and usually comparable with the NORM(A).
out	beta	An optional N-element array that if provided forces alpha to return the numerator, and this array contains the denominator used to determine the eigenvalues as ALPHA / BETA. If used, the values in this array will always be less than and usually comparable with the NORM(B).
out	vecs	An optional N-by-N matrix, that if supplied, signals to compute the right eigenvectors (one per column). If not provided, only the eigenvalues will be computed.
out	work	An optional input, that if provided, prevents any local memory allocation. If not provided, the memory required is allocated within. If provided, the length of the array must be at least olwork.
out	olwork	An optional output used to determine workspace size. If supplied, the routine determines the optimal size for work, and returns without performing any actual calculations.

#### **Parameters**

out	err	An optional errors-based object that if provided can be used to retrieve information relating to any errors encountered during execution. If not provided, a default implementation of the errors class is used internally to provide error handling. Possible errors and warning messages that may be encountered are as follows.
		<ul> <li>LA_ARRAY_SIZE_ERROR: Occurs if any of the input arrays are not sized appropriately.</li> </ul>
		<ul> <li>LA_OUT_OF_MEMORY_ERROR: Occurs if local memory must be allocated, and there is insufficient memory available.</li> </ul>
		LA_CONVERGENCE_ERROR: Occurs if the algorithm failed to converge.

#### Usage

As an example, consider the eigenvalue problem arising from a mechanical system of masses and springs such that the masses are described by a mass matrix M, and the arrangement of springs are described by a stiffness matrix K.

```
! This is an example illustrating the use of the eigenvalue and eigenvector
  routines to solve a free vibration problem of 3 masses connected by springs.
  |-\/\/-| m1 |-\/\/-| m2 |-\/\/-| m3 |-\/\/-|
  As illustrated above, the system consists of 3 masses connected by springs.
  Spring k1 and spring k4 connect the end masses to ground. The equations of
  motion for this system are as follows.
 | m1 0 0 | |x1"|
                          | k1+k2 -k2

\begin{array}{c|ccccc}
0 & | & |x1| & |0| \\
-k3 & | & |x2| & = & |0|
\end{array}

! Notice: x1" = the second time derivative of x1.
program example
    use linalg_constants, only : dp, i32
    use linalg_eigen
    implicit none
    ! Define the model parameters
    real(dp), parameter :: pi = 3.14159265359d0 real(dp), parameter :: m1 = 0.5d0
    real(dp), parameter :: m2 = 2.5d0
    real(dp), parameter :: m3 = 0.75d0
    real(dp), parameter :: k1 = 5.0d6
    real(dp), parameter :: k2 = 10.0d6
    real(dp), parameter :: k3 = 10.0d6
    real(dp), parameter :: k4 = 5.0d6
    ! Local Variables
    integer(i32) :: i, j
real(dp) :: m(3,3), k(3,3), natfreq(3)
   complex(dp) :: vals(3), modeshapes(3,3)
    ! Define the mass matrix
    m = reshape([m1, 0.0d0, 0.0d0, 0.0d0, m2, 0.0d0, 0.0d0, 0.0d0, m3], [3, 3])
    ! Define the stiffness matrix
    k = reshape([k1 + k2, -k2, 0.0d0, -k2, k2 + k3, -k3, 0.0d0, -k3, k3 + k4], &
        [3, 3])
    ! Compute the eigenvalues and eigenvectors.
    call eigen(k, m, vals, vecs = modeshapes)
    ! Compute the natural frequency values, and return them with units of \ensuremath{\text{\text{Hz}}}.
    ! Notice, all eigenvalues and eigenvectors are real for this example.
    natfreq = sqrt(real(vals)) / (2.0d0 * pi)
    ! Display the natural frequency and mode shape values. Notice, the eigen
    ! routine does not necessarily sort the values.
    print '(A)', "Modal Information (Not Sorted):"
    do i = 1, size(natfreq)
    print '(AIOAF8.4A)', "Mode ", i, ": (", natfreq(i), " Hz)"
    print '(F10.3)', (real(modeShapes(j,i)), j = 1, size(natfreq))
    end do
end program
```

#### Notes

This routine utilizes the LAPACK routine DGGEV.

Definition at line 465 of file linalg\_eigen.f90.

5.3.2.3 subroutine linalg\_eigen::eigen\_symm ( logical, intent(in) *vecs*, real(dp), dimension(:,:), intent(inout) *a*, real(dp), dimension(:), intent(out) *vals*, real(dp), dimension(:), intent(out), optional, pointer *work*, integer(i32), intent(out), optional *olwork*, class(errors), intent(inout), optional, target *err* ) [private]

Computes the eigenvalues, and optionally the eigenvectors of a real, symmetric matrix.

#### **Parameters**

in	vecs	Set to true to compute the eigenvectors as well as the eigenvalues; else, set to false to just compute the eigenvalues.
in,out	а	On input, the N-by-N symmetric matrix on which to operate. On output, and if $vecs$ is set to true, the matrix will contain the eigenvectors (one per column) corresponding to each eigenvalue in $vals$ . If $vecs$ is set to false, the lower triangular portion of the matrix is overwritten.
out	vals	An N-element array that will contain the eigenvalues sorted into ascending order.
out	work	An optional input, that if provided, prevents any local memory allocation. If not provided, the memory required is allocated within. If provided, the length of the array must be at least olwork.
out	olwork	An optional output used to determine workspace size. If supplied, the routine determines the optimal size for $work$ , and returns without performing any actual calculations.
out	err	An optional errors-based object that if provided can be used to retrieve information relating to any errors encountered during execution. If not provided, a default implementation of the errors class is used internally to provide error handling. Possible errors and warning messages that may be encountered are as follows.  • LA_ARRAY_SIZE_ERROR: Occurs if any of the input arrays are not sized appropriately.
		<ul> <li>LA_OUT_OF_MEMORY_ERROR: Occurs if local memory must be allocated, and there is insufficient memory available.</li> </ul>
		LA_CONVERGENCE_ERROR: Occurs if the algorithm failed to converge.

# Notes

This routine utilizes the LAPACK routine DSYEV.

Definition at line 68 of file linalg\_eigen.f90.

The documentation for this interface was generated from the following file:

• /home/jason/Documents/Code/linalg/src/linalg\_eigen.f90

# 5.4 linalg\_factor::form\_lu Interface Reference

Extracts the L and U matrices from the condensed [L\U] storage format used by the lu\_factor.

#### **Private Member Functions**

• subroutine form\_lu\_all (lu, ipvt, u, p, err)

Extracts the L, U, and P matrices from the output of the lu factor routine.

• subroutine form\_lu\_only (lu, u, err)

Extracts the L, and U matrices from the output of the lu\_factor routine.

# 5.4.1 Detailed Description

Extracts the L and U matrices from the condensed [L\U] storage format used by the lu\_factor.

Definition at line 31 of file linalg\_factor.f90.

#### 5.4.2 Member Function/Subroutine Documentation

5.4.2.1 subroutine linalg\_factor::form\_lu::form\_lu\_all ( real(dp), dimension(:,:), intent(inout) lu, integer(i32), dimension(:), intent(in) ipvt, real(dp), dimension(:,:), intent(out) u, real(dp), dimension(:,:), intent(out) p, class(errors), intent(inout), optional, target err ) [private]

Extracts the L, U, and P matrices from the output of the lu factor routine.

#### **Parameters**

in, out	lu	On input, the N-by-N matrix as output by lu_factor. On output, the N-by-N lower triangular
, , , , , ,		matrix L.
in	ipvt	The N-element pivot array as output by lu_factor.
out	и	An N-by-N matrix where the U matrix will be written.
out	р	An N-by-N matrix where the row permutation matrix will be written.
out	err	An optional errors-based object that if provided can be used to retrieve information relating to any errors encountered during execution. If not provided, a default implementation of the errors class is used internally to provide error handling. Possible errors and warning messages that may be encountered are as follows.  • LA_ARRAY_SIZE_ERROR: Occurs if any of the input array sizes are incorrect.

#### Remarks

This routine allows extraction of the actual "L", "U", and "P" matrices of the decomposition. To use these matrices to solve the system A\*X = B, the following approach is used.

- 1. First, solve the linear system: L\*Y = P\*B for Y.
- 2. Second, solve the linear system: U\*X = Y for X.

Notice, as both L and U are triangular in structure, the above equations can be solved by forward and backward substitution.

### See Also

- Wikipedia
- Wolfram MathWorld

Definition at line 211 of file linalg\_factor.f90.

5.4.2.2 subroutine linalg\_factor::form\_lu::form\_lu\_only ( real(dp), dimension(:,:), intent(inout) lu, real(dp), dimension(:,:), intent(out) u, class(errors), intent(inout), optional, target err ) [private]

Extracts the L, and U matrices from the output of the lu\_factor routine.

#### **Parameters**

in,out	lu	On input, the N-by-N matrix as output by lu_factor. On output, the N-by-N lower triangular
		matrix L.
out	и	An N-by-N matrix where the U matrix will be written.
out	err	An optional errors-based object that if provided can be used to retrieve information relating to any errors encountered during execution. If not provided, a default implementation of the errors class is used internally to provide error handling. Possible errors and warning messages that may be encountered are as follows.
		LA_ARRAY_SIZE_ERROR: Occurs if any of the input array sizes are incorrect.

Definition at line 288 of file linalg\_factor.f90.

The documentation for this interface was generated from the following file:

/home/jason/Documents/Code/linalg/src/linalg\_factor.f90

# 5.5 linalg\_factor::form\_qr Interface Reference

Forms the full M-by-M orthogonal matrix Q from the elementary reflectors returned by the base QR factorization algorithm.

#### **Private Member Functions**

- subroutine form\_qr\_no\_pivot (r, tau, q, work, olwork, err)
  - Forms the full M-by-M orthogonal matrix Q from the elementary reflectors returned by the base QR factorization algorithm.
- subroutine form\_qr\_pivot (r, tau, pvt, q, p, work, olwork, err)
  - Forms the full M-by-M orthogonal matrix Q from the elementary reflectors returned by the base QR factorization algorithm.

# 5.5.1 Detailed Description

Forms the full M-by-M orthogonal matrix Q from the elementary reflectors returned by the base QR factorization algorithm.

# See Also

- Wikipedia
- LAPACK Users Manual

Definition at line 55 of file linalg\_factor.f90.

- 5.5.2 Member Function/Subroutine Documentation
- 5.5.2.1 subroutine linalg\_factor::form\_qr::form\_qr\_no\_pivot ( real(dp), dimension(:,:), intent(inout) r, real(dp), dimension(:), intent(in) tau, real(dp), dimension(:,:), intent(out) q, real(dp), dimension(:), intent(out), optional, target work, integer(i32), intent(out), optional olwork, class(errors), intent(inout), optional, target err ) [private]

Forms the full M-by-M orthogonal matrix Q from the elementary reflectors returned by the base QR factorization algorithm.

# **Parameters**

in,out	r	On input, an M-by-N matrix where the elements below the diagonal contain the elementary reflectors generated from the QR factorization. On and above the diagonal, the matrix contains the matrix R. On output, the elements below the diagonal are zeroed such that the remaining matrix is simply the M-by-N matrix R.
in	tau	A MIN(M, N)-element array containing the scalar factors of each elementary reflector defined in r.
out	q	An M-by-M matrix where the full orthogonal matrix Q will be written. In the event that $M > N$ , Q may be supplied as M-by-N, and therefore only return the useful submatrix Q1 (Q = [Q1, Q2]) as the factorization can be written as $Q * R = [Q1, Q2] * [R1; 0]$ .
out	work	An optional input, that if provided, prevents any local memory allocation. If not provided, the memory required is allocated within. If provided, the length of the array must be at least olwork.
out	olwork	An optional output used to determine workspace size. If supplied, the routine determines the optimal size for work, and returns without performing any actual calculations.
out	err	An optional errors-based object that if provided can be used to retrieve information relating to any errors encountered during execution. If not provided, a default implementation of the errors class is used internally to provide error handling. Possible errors and warning messages that may be encountered are as follows.  • LA_ARRAY_SIZE_ERROR: Occurs if any of the input arrays are not sized appropriately.  • LA_OUT_OF_MEMORY_ERROR: Occurs if local memory must be allocated, and there is insufficient memory available.

# Notes

This routine utilizes the LAPACK routine DORGQR.

Definition at line 694 of file linalg\_factor.f90.

5.5.2.2 subroutine linalg\_factor::form\_qr::form\_qr\_pivot ( real(dp), dimension(:,:), intent(inout) r, real(dp), dimension(:), intent(in) tau, integer(i32), dimension(:), intent(in) pvt, real(dp), dimension(:,:), intent(out) q, real(dp), dimension(:,:), intent(out) p, real(dp), dimension(:), intent(out), optional, target work, integer(i32), intent(out), optional olwork, class(errors), intent(inout), optional, target err ) [private]

Forms the full M-by-M orthogonal matrix Q from the elementary reflectors returned by the base QR factorization algorithm.

in,out	r	On input, an M-by-N matrix where the elements below the diagonal contain the elementary reflectors generated from the QR factorization. On and above the diagonal, the matrix contains the matrix R. On output, the elements below the diagonal are zeroed such that the remaining matrix is simply the M-by-N matrix R.
in	tau	A MIN(M, N)-element array containing the scalar factors of each elementary reflector defined in r.
in	pvt	An N-element column pivot array as returned by the QR factorization.
out	q	An M-by-M matrix where the full orthogonal matrix Q will be written. In the event that $M > N$ , Q may be supplied as M-by-N, and therefore only return the useful submatrix Q1 (Q = [Q1, Q2]) as the factorization can be written as Q * R = [Q1, Q2] * [R1; 0].
out	р	An N-by-N matrix where the pivot matrix will be written.

#### **Parameters**

out	work	An optional input, that if provided, prevents any local memory allocation. If not provided, the memory required is allocated within. If provided, the length of the array must be at least olwork.
out	olwork	An optional output used to determine workspace size. If supplied, the routine determines the optimal size for work, and returns without performing any actual calculations.
out	err	An optional errors-based object that if provided can be used to retrieve information relating to any errors encountered during execution. If not provided, a default implementation of the errors class is used internally to provide error handling. Possible errors and warning messages that may be encountered are as follows.  • LA_ARRAY_SIZE_ERROR: Occurs if any of the input arrays are not sized appropriately.  • LA_OUT_OF_MEMORY_ERROR: Occurs if local memory must be allocated, and there is insufficient memory available.

#### Notes

This routine utilizes the LAPACK routine DORGQR.

Definition at line 825 of file linalg\_factor.f90.

The documentation for this interface was generated from the following file:

/home/jason/Documents/Code/linalg/src/linalg factor.f90

# 5.6 linalg\_core::mtx\_mult Interface Reference

Performs the matrix operation: C = alpha \* op(A) \* op(B) + beta \* C.

### **Private Member Functions**

- subroutine mtx\_mult\_mtx (transa, transb, alpha, a, b, beta, c, err)
- subroutine mtx\_mult\_vec (trans, alpha, a, b, beta, c, err)

Performs the matrix-vector operation: c = alpha \* op(A) \* b + beta \* c.

Performs the matrix operation: C = alpha \* op(A) \* op(B) + beta \* C.

# 5.6.1 Detailed Description

Performs the matrix operation: C = alpha \* op(A) \* op(B) + beta \* C.

Definition at line 39 of file linalg core.f90.

# 5.6.2 Member Function/Subroutine Documentation

5.6.2.1 subroutine linalg\_core::mtx\_mult::mtx ( logical, intent(in) *transa,* logical, intent(in) *transb,* real(dp), intent(in) *alpha,* real(dp), dimension(:,:), intent(in) *a,* real(dp), dimension(:,:), intent(in) *b,* real(dp), intent(in) *beta,* real(dp), dimension(:,:), intent(inout) *c,* class(errors), intent(inout), optional, target *err* ) [private]

Performs the matrix operation: C = alpha \* op(A) \* op(B) + beta \* C.

# **Parameters**

in	transa	Set to true if $op(A) = A**T$ ; else, set to false for $op(A) = A$ .
in	transb	Set to true if $op(B) = B**T$ ; else, set to false for $op(B) = B$ .
in	alpha	A scalar multiplier.
in	а	If transa is set to true, an K-by-M matrix; else, if transa is set to false, an M-by-K matrix.
in	b	If transb is set to true, an N-by-K matrix; else, if transb is set to false, a K-by-N matrix.
in	beta	A scalar multiplier.
in,out	С	On input, the M-by-N matrix C. On output, the M-by-N result.
out	err	An optional errors-based object that if provided can be used to retrieve information relating to any errors encountered during execution. If not provided, a default implementation of the errors class is used internally to provide error handling. Possible errors and warning messages that may be encountered are as follows.  • LA_ARRAY_SIZE_ERROR: Occurs if any of the input array sizes are incorrect.

# Notes

This routine utilizes the BLAS routine DGEMM.

Definition at line 83 of file linalg\_core.f90.

5.6.2.2 subroutine linalg\_core::mtx\_mult::mtx\_mult\_vec ( logical, intent(in) trans, real(dp), intent(in) alpha, real(dp), dimension(:), intent(in) b, real(dp), intent(in) beta, real(dp), dimension(:), intent(inout) c, class(errors), intent(inout), optional, target err ) [private]

Performs the matrix-vector operation: c = alpha \* op(A) \* b + beta \* c.

# **Parameters**

in	trans	Set to true if $op(A) = A**T$ ; else, set to false for $op(A) = A$ .
in	alpha	A scalar multiplier.
in	а	The M-by-N matrix A.
in	b	If trans is set to true, an M-element array; else, if trans is set to false, an N-element array.
in	beta	A scalar multiplier.
in,out	С	On input, if trans is set to true, an N-element array; else, if trans is set to false, an M-element array. On output, the results of the operation.
out	err	An optional errors-based object that if provided can be used to retrieve information relating to any errors encountered during execution. If not provided, a default implementation of the errors class is used internally to provide error handling. Possible errors and warning messages that may be encountered are as follows.  • LA_ARRAY_SIZE_ERROR: Occurs if any of the input array sizes are incorrect.

# Notes

This routine utilizes the BLAS routine DGEMV.

Definition at line 177 of file linalg\_core.f90.

The documentation for this interface was generated from the following file:

/home/jason/Documents/Code/linalg/src/linalg\_core.f90

# 5.7 linalg\_factor::mult\_qr Interface Reference

Multiplies a general matrix by the orthogonal matrix Q from a QR factorization.

#### **Private Member Functions**

- subroutine mult\_qr\_mtx (Iside, trans, a, tau, c, work, olwork, err)
   Multiplies a general matrix by the orthogonal matrix Q from a QR factorization such that: C = op(Q) \* C, or C = C \* op(Q).
- subroutine mult\_qr\_vec (trans, a, tau, c, work, olwork, err)
   Multiplies a vector by the orthogonal matrix Q from a QR factorization such that: C = op(Q) \* C.

# 5.7.1 Detailed Description

Multiplies a general matrix by the orthogonal matrix Q from a QR factorization.

Definition at line 63 of file linalg\_factor.f90.

# 5.7.2 Member Function/Subroutine Documentation

5.7.2.1 subroutine linalg\_factor::mult\_qr::mult\_qr\_mtx ( logical, intent(in) *lside*, logical, intent(in) *trans*, real(dp), dimension(:,:), intent(inout) *a*, real(dp), dimension(:), intent(inout) *a*, real(dp), dimension(:), intent(inout) *c*, real(dp), dimension(:), intent(out), optional, target *work*, integer(i32), intent(out), optional *olwork*, class(errors), intent(inout), optional, target *err* ) [private]

Multiplies a general matrix by the orthogonal matrix Q from a QR factorization such that: C = op(Q) \* C, or C = C \* op(Q).

in	Iside	Set to true to apply Q or Q**T from the left; else, set to false to apply Q or Q**T from the right.
in	trans	Set to true to apply Q**T; else, set to false.
in	а	On input, an LDA-by-K matrix containing the elementary reflectors output from the QR factorization. If lside is set to true, LDA = M, and $M >= K >= 0$ ; else, if lside is set to false, LDA = N, and $N >= K >= 0$ . Notice, the contents of this matrix are restored on exit.
in	tau	A K-element array containing the scalar factors of each elementary reflector defined in a.
in,out	С	On input, the M-by-N matrix C. On output, the product of the orthogonal matrix Q and the original matrix C.
out	work	An optional input, that if provided, prevents any local memory allocation. If not provided, the memory required is allocated within. If provided, the length of the array must be at least olwork.

# **Parameters**

out	olwork	An optional output used to determine workspace size. If supplied, the routine determines the optimal size for $\mathtt{work}$ , and returns without performing any actual calculations.
out	err	An optional errors-based object that if provided can be used to retrieve information relating to any errors encountered during execution. If not provided, a default implementation of the errors class is used internally to provide error handling. Possible errors and warning messages that may be encountered are as follows.  • LA_ARRAY_SIZE_ERROR: Occurs if any of the input arrays are not sized appropriately.
		<ul> <li>LA_OUT_OF_MEMORY_ERROR: Occurs if local memory must be allocated, and there is insufficient memory available.</li> </ul>

# Notes

This routine utilizes the LAPACK routine DORMQR.

Definition at line 927 of file linalg\_factor.f90.

5.7.2.2 subroutine linalg\_factor::mult\_qr::mult\_qr\_vec ( logical, intent(in) *trans*, real(dp), dimension(:,:), intent(inout) *a*, real(dp), dimension(:), intent(in) *tau*, real(dp), dimension(:), intent(inout) *c*, real(dp), dimension(:), intent(out), optional, target *work*, integer(i32), intent(out), optional *olwork*, class(errors), intent(inout), optional, target *err* ) [private]

Multiplies a vector by the orthogonal matrix Q from a QR factorization such that: C = op(Q) \* C.

### **Parameters**

in	trans	Set to true to apply Q**T; else, set to false.
in	а	On input, an M-by-K matrix containing the elementary reflectors output from the QR factorization. Notice, the contents of this matrix are restored on exit.
in	tau	A K-element array containing the scalar factors of each elementary reflector defined in a.
in,out	С	On input, the M-element vector C. On output, the product of the orthogonal matrix Q and the original vector C.
out	work	An optional input, that if provided, prevents any local memory allocation. If not provided, the memory required is allocated within. If provided, the length of the array must be at least olwork.
out	olwork	An optional output used to determine workspace size. If supplied, the routine determines the optimal size for $work$ , and returns without performing any actual calculations.
out	err	An optional errors-based object that if provided can be used to retrieve information relating to any errors encountered during execution. If not provided, a default implementation of the errors class is used internally to provide error handling. Possible errors and warning messages that may be encountered are as follows.  • LA_ARRAY_SIZE_ERROR: Occurs if any of the input arrays are not sized appropriately.
		<ul> <li>LA_OUT_OF_MEMORY_ERROR: Occurs if local memory must be allocated, and there is insufficient memory available.</li> </ul>

# Notes

This routine is based upon the LAPACK routine DORM2R.

Definition at line 1054 of file linalg\_factor.f90.

The documentation for this interface was generated from the following file:

• /home/jason/Documents/Code/linalg/src/linalg\_factor.f90

# 5.8 linalg\_factor::mult\_rz Interface Reference

Multiplies a general matrix by the orthogonal matrix Z from an RZ factorization.

#### **Private Member Functions**

- subroutine mult\_rz\_mtx (Iside, trans, I, a, tau, c, work, olwork, err)
   Multiplies a general matrix by the orthogonal matrix Z from an RZ factorization such that: C = op(Z) \* C, or C = C \* op(Z).
- subroutine mult\_rz\_vec (trans, I, a, tau, c, work, olwork, err)
   Multiplies a vector by the orthogonal matrix Z from an RZ factorization such that: C = op(Z) \* C.

# 5.8.1 Detailed Description

Multiplies a general matrix by the orthogonal matrix Z from an RZ factorization.

Definition at line 71 of file linalg\_factor.f90.

# 5.8.2 Member Function/Subroutine Documentation

5.8.2.1 subroutine linalg\_factor::mult\_rz::mult\_rz\_mtx ( logical, intent(in) *lside*, logical, intent(in) *trans*, integer(i32), intent(in) *l*, real(dp), dimension(:,:), intent(inout) *a*, real(dp), dimension(:), intent(in) *tau*, real(dp), dimension(:,:), intent(inout) *c*, real(dp), dimension(:), intent(out), optional, target *work*, integer(i32), intent(out), optional *olwork*, class(errors), intent(inout), optional, target *err* ) [private]

Multiplies a general matrix by the orthogonal matrix Z from an RZ factorization such that: C = op(Z) \* C, or C = C \* op(Z).

in	Iside	Set to true to apply Z or Z**T from the left; else, set to false to apply Z or Z**T from the right.
in	trans	Set to true to apply Z**T; else, set to false.
in	1	The number of columns in matrix a containing the meaningful part of the Householder vectors. If $lside$ is true, $M >= L >= 0$ ; else, if $lside$ is false, $N >= L >= 0$ .
in,out	а	On input the K-by-LTA matrix Z, where LTA = M if lside is true; else, LTA = N if lside is false. The I-th row must contain the Householder vector in the last k rows. Notice, the contents of this matrix are restored on exit.
in	tau	A K-element array containing the scalar factors of the elementary reflectors, where $M \ge K \ge 0$ if lside is true; else, $N \ge K \ge 0$ if lside is false.
in,out	С	On input, the M-by-N matrix C. On output, the product of the orthogonal matrix Z and the original matrix C.

# **Parameters**

out	work	An optional input, that if provided, prevents any local memory allocation. If not provided, the memory required is allocated within. If provided, the length of the array must be at least olwork.
out	olwork	An optional output used to determine workspace size. If supplied, the routine determines the optimal size for work, and returns without performing any actual calculations.
out	err	An optional errors-based object that if provided can be used to retrieve information relating to any errors encountered during execution. If not provided, a default implementation of the errors class is used internally to provide error handling. Possible errors and warning messages that may be encountered are as follows.  • LA_ARRAY_SIZE_ERROR: Occurs if any of the input arrays are not sized appropriately.  • LA_OUT_OF_MEMORY_ERROR: Occurs if local memory must be allocated, and there is insufficient memory available.

# Notes

This routine utilizes the LAPACK routine DORMRZ.

Definition at line 1745 of file linalg\_factor.f90.

5.8.2.2 subroutine linalg\_factor::mult\_rz::mult\_rz\_vec ( logical, intent(in) trans, integer(i32), intent(in) l, real(dp), dimension(:,:), intent(inout) a, real(dp), dimension(:), intent(in) tau, real(dp), dimension(:), intent(inout) c, real(dp), dimension(:), intent(out), optional, target work, integer(i32), intent(out), optional olwork, class(errors), intent(inout), optional, target err ) [private]

Multiplies a vector by the orthogonal matrix Z from an RZ factorization such that: C = op(Z) \* C.

in	trans	Set to true to apply Z**T; else, set to false.
in	1	The number of columns in matrix a containing the meaningful part of the Householder vectors. If lside is true, $M >= L >= 0$ ; else, if lside is false, $N >= L >= 0$ .
in,out	а	On input the K-by-LTA matrix Z, where LTA = M if lside is true; else, LTA = N if lside is false. The I-th row must contain the Householder vector in the last k rows. Notice, the contents of this matrix are restored on exit.
in	tau	A K-element array containing the scalar factors of the elementary reflectors, where $M >= K >= 0$ if lside is true; else, $N >= K >= 0$ if lside is false.
in,out	С	On input, the M-element array C. On output, the product of the orthogonal matrix Z and the original array C.
out	work	An optional input, that if provided, prevents any local memory allocation. If not provided, the memory required is allocated within. If provided, the length of the array must be at least olwork.
out	olwork	An optional output used to determine workspace size. If supplied, the routine determines the optimal size for work, and returns without performing any actual calculations.
out	err	An optional errors-based object that if provided can be used to retrieve information relating to any errors encountered during execution. If not provided, a default implementation of the errors class is used internally to provide error handling. Possible errors and warning messages that may be encountered are as follows.
		<ul> <li>LA_ARRAY_SIZE_ERROR: Occurs if any of the input arrays are not sized appropriately.</li> </ul>
		LA_OUT_OF_MEMORY_ERROR: Occurs if local memory must be allocated, and there is insufficient memory available.  Generated by Doxygen  Generated by Doxygen

#### Notes

This routine utilizes the LAPACK routine DORMRZ.

Definition at line 1887 of file linalg\_factor.f90.

The documentation for this interface was generated from the following file:

/home/jason/Documents/Code/linalg/src/linalg factor.f90

# 5.9 linalg\_factor::qr\_factor Interface Reference

Computes the QR factorization of an M-by-N matrix.

#### **Private Member Functions**

- subroutine qr\_factor\_no\_pivot (a, tau, work, olwork, err)
   Computes the QR factorization of an M-by-N matrix without pivoting.
- subroutine qr\_factor\_pivot (a, tau, jpvt, work, olwork, err)
   Computes the QR factorization of an M-by-N matrix with column pivoting such that A \* P = Q \* R.

# 5.9.1 Detailed Description

Computes the QR factorization of an M-by-N matrix.

# See Also

- Wikipedia
- Wolfram MathWorld
- LAPACK Users Manual

Definition at line 43 of file linalg\_factor.f90.

# 5.9.2 Member Function/Subroutine Documentation

5.9.2.1 subroutine linalg\_factor::qr\_factor::qr\_factor\_no\_pivot ( real(dp), dimension(:,:), intent(inout) a, real(dp), dimension(:), intent(out) tau, real(dp), dimension(:), intent(out), optional, target work, integer(i32), intent(out), optional olwork, class(errors), intent(inout), optional, target err ) [private]

Computes the QR factorization of an M-by-N matrix without pivoting.

in,ou	t <b>a</b>	On input, the M-by-N matrix to factor. On output, the elements on and above the diagonal contain the MIN(M, N)-by-N upper trapezoidal matrix R (R is upper triangular if $M \ge N$ ). The elements below the diagonal, along with the array tau, represent the orthogonal matrix Q as a product of elementary reflectors.
out	tau	A MIN(M, N)-element array used to store the scalar factors of the elementary reflectors.

#### **Parameters**

out	work	An optional input, that if provided, prevents any local memory allocation. If not provided, the memory required is allocated within. If provided, the length of the array must be at least olwork.
out	olwork	An optional output used to determine workspace size. If supplied, the routine determines the optimal size for $work$ , and returns without performing any actual calculations.
out	err	An optional errors-based object that if provided can be used to retrieve information relating to any errors encountered during execution. If not provided, a default implementation of the errors class is used internally to provide error handling. Possible errors and warning messages that may be encountered are as follows.
		LA_ARRAY_SIZE_ERROR: Occurs if tau or work are not sized appropriately.
		<ul> <li>LA_OUT_OF_MEMORY_ERROR: Occurs if local memory must be allocated, and there is insufficient memory available.</li> </ul>

#### Remarks

QR factorization without pivoting is best suited to solving an overdetermined system in least-squares terms, or to solve a normally defined system. To solve an underdetermined system, it is recommended to use either LQ factorization, or a column-pivoting based QR factorization.

### Usage

To solve a system of M equations of N unknowns using QR factorization, the following code will suffice assuming M >= N.

```
! Solve the system: A \star X = B in a least-squares sense, where A is an
! M-by-N matrix, B is an M-by-NRHS matrix, and X is an N-by-NRHS matrix.
! Variables
real(dp), dimension(m, n) :: a
real(dp), dimension(m, nrhs) :: b, qtb
real(dp), dimension(n, nrhs) :: x
real(dp), dimension(n) :: tau
real(dp), dimension(m, m) :: q
! Initialize A and B...
! Compute the QR factorization. We're intentionally not forming the full
! Q matrix, but instead storing it in terms of its elementary reflector ! components in the sub-diagonal portions of A, and the corresponding ! scalar factors in TAU. Additionally, we'll let the algorithm allocate ! it's own workspace array; therefore, the call to factor A is:
call qr_factor(a, tau)
! Solve A \star X = B for X. The first N rows of B are used to store X.
call solve_qr(a, tau, b)
! Also note, we could form {\tt Q} and {\tt R} explicitly. Then solution of the
! system of equations can be found. First we form {\bf Q} and {\bf R}.
call form_qr(a, tau, q) ! Forms Q, and R is stored in A
! Since we now have Q and R, we seek a solution to the equation:
! Then: R*X = Q**T * B, and R is upper triangular; therefore, back
  substitution will suffice for a solution procedure.
! Next, compute Q**T*B, and store in QTB.
call mtx\_mult(.true., .false., 1.0d0, q, b, 0.0d0, qtb)
! Copy the first N rows of Q**T*B into X for the solution process.
! Notice, only the first N rows are needed as rows N+1:M are all zero in
! matrix R.
x = qtb(1:n,nrhs)
! Compute the solution and store in X
call solve_triangular_system(.true., .true., .false., .true., 1.0d0, &
 a(1:n,1:n), x)
```

#### Notes

This routine utilizes the LAPACK routine DGEQRF.

Definition at line 425 of file linalg\_factor.f90.

5.9.2.2 subroutine linalg\_factor::qr\_factor::qr\_factor\_pivot ( real(dp), dimension(:,:), intent(inout) a, real(dp), dimension(:), intent(out) tau, integer(i32), dimension(:), intent(inout) jpvt, real(dp), dimension(:), intent(out), optional, target work, integer(i32), intent(out), optional olwork, class(errors), intent(inout), optional, target err ) [private]

Computes the QR factorization of an M-by-N matrix with column pivoting such that A \* P = Q \* R.

#### **Parameters**

in,out	а	On input, the M-by-N matrix to factor. On output, the elements on and above the diagonal contain the MIN(M, N)-by-N upper trapezoidal matrix R (R is upper triangular if $M \ge N$ ). The elements below the diagonal, along with the array tau, represent the orthogonal matrix Q as a product of elementary reflectors.
out	tau	A MIN(M, N)-element array used to store the scalar factors of the elementary reflectors.
in,out	jpvt	On input, an N-element array that if $JPVT(I)$ .ne. 0, the I-th column of A is permuted to the front of A $*$ P; if $JPVT(I) = 0$ , the I-th column of A is a free column. On output, if $JPVT(I) = K$ , then the I-th column of A $*$ P was the K-th column of A.
out	work	An optional input, that if provided, prevents any local memory allocation. If not provided, the memory required is allocated within. If provided, the length of the array must be at least olwork.
out	olwork	An optional output used to determine workspace size. If supplied, the routine determines the optimal size for work, and returns without performing any actual calculations.
out	err	An optional errors-based object that if provided can be used to retrieve information relating to any errors encountered during execution. If not provided, a default implementation of the errors class is used internally to provide error handling. Possible errors and warning messages that may be encountered are as follows.
		<ul> <li>LA_ARRAY_SIZE_ERROR: Occurs if any of the input arrays are not sized appropriately.</li> </ul>
		<ul> <li>LA_OUT_OF_MEMORY_ERROR: Occurs if local memory must be allocated, and there is insufficient memory available.</li> </ul>

# Usage

To solve a system of M equations of N unknowns using QR factorization, the following code will suffice for any M and N.

```
! Solve the least-squares (M >= N), or the underdetermined (M < N)
! problem A*X = B, where A is an M-by-N matrix, B is an M-by-NRHS matrix,
! and X is an N-by-NRHS matrix. In the underdetermined case, or the
! case where the rank of matrix A is less than N, the solution obtained
! contains the fewest possible non-zero entries.

! Variables
real(dp), dimension(m, n) :: a
real(dp), dimension(h) :: tau ! k = min(m, n)
real(dp), dimension(m, m) :: q
real(dp), dimension(n, n) :: p
integer(i32), dimension(n) :: pvt
! Initialize A and B...
! Allow all columns to be free.
pvt = 0</pre>
```

```
! Compute the QR factorization. We're intentionally not forming the full
! Q matrix, but instead storing it in terms of its elementary reflector
! components in the sub-diagonal portions of A, and the corresponding
! scalar factors in TAU. Additionally, we'll let the algorithm allocate
! it's own workspace array; therefore, the call to factor A is:
call qr_factor(a, tau, pvt)
! Solve A \star X = B for X. If M > N, the first N rows of B are used to store
! X. If M < N, the input matrix B must be N-by-NRHS, and only the first
! M rows are used for the actual matrix B. The remaining N-M rows
!\ \mbox{\it can} contain whatever as they are not referenced until they are
! overwritten by the N-by-NRHS solution matrix X.
call solve_qr(a, tau, pvt, b)
! Notice, if the explicit Q matrix from the factorization is desired,
! the form_qr routine works similarly as in the no-pivot case; ! however, the permutation matrix P is also constructed. The call would
! be as follows. Also, as with the no-pivot algorithm, the matrix \ensuremath{\mathbf{R}} is
! stored in matrix A.
call form_qr(a, tau, pvt, q, p)
! Solution can proceed as per typical, but with a full {\tt Q} matrix. Also
! note, the problem is of the form: A*P = Q*R. Solution is straight ! forward, as with the no-pivot case; however, if M < N, then R is upper
  trapezoidal, and must be appropriately partitioned to solve. The rank
! of matrix r should be considered when applying the partition.
```

#### **Notes**

This routine utilizes the LAPACK routine DGEQP3.

Definition at line 579 of file linalg factor.f90.

The documentation for this interface was generated from the following file:

/home/jason/Documents/Code/linalg/src/linalg factor.f90

# 5.10 linalg\_solve::solve\_cholesky Interface Reference

Solves a system of Cholesky factored equations.

# **Private Member Functions**

- subroutine solve\_cholesky\_mtx (upper, a, b, err)
   Solves a system of Cholesky factored equations.
- subroutine solve\_cholesky\_vec (upper, a, b, err)
   Solves a system of Cholesky factored equations.

# 5.10.1 Detailed Description

Solves a system of Cholesky factored equations.

Definition at line 83 of file linalg solve.f90.

#### 5.10.2 Member Function/Subroutine Documentation

5.10.2.1 subroutine linalg\_solve::solve\_cholesky::solve\_cholesky\_mtx ( logical, intent(in) *upper*, real(dp), dimension(:,:), intent(in) *a*, real(dp), dimension(:,:), intent(inout) *b*, class(errors), intent(inout), optional, target *err* ) [private]

Solves a system of Cholesky factored equations.

# **Parameters**

in	upper	Set to true if the original matrix A was factored such that $A = U**T*U$ ; else, set to false if
		the factorization of A was $A = L**T*L$ .
in	а	The N-by-N Cholesky factored matrix.
in,out	b	On input, the N-by-NRHS right-hand-side matrix B. On output, the solution matrix X.
out	err	An optional errors-based object that if provided can be used to retrieve information relating to any errors encountered during execution. If not provided, a default implementation of the errors class is used internally to provide error handling. Possible errors and warning messages that may be encountered are as follows.
		LA_ARRAY_SIZE_ERROR: Occurs if any of the input array sizes are incorrect.

# Notes

This routine utilizes the LAPACK routine DPOTRS.

Definition at line 1073 of file linalg\_solve.f90.

5.10.2.2 subroutine linalg\_solve::solve\_cholesky::solve\_cholesky\_vec ( logical, intent(in) *upper*, real(dp), dimension(:,:), intent(in) *a*, real(dp), dimension(:), intent(inout) *b*, class(errors), intent(inout), optional, target *err* ) [private]

Solves a system of Cholesky factored equations.

#### **Parameters**

in	upper	Set to true if the original matrix A was factored such that $A = U**T*U$ ; else, set to false if
		the factorization of A was $A = L**T*L$ .
in	а	The N-by-N Cholesky factored matrix.
in, out	b	On input, the N-element right-hand-side vector B. On output, the solution vector X.
out	err	An optional errors-based object that if provided can be used to retrieve information relating to any errors encountered during execution. If not provided, a default implementation of the errors class is used internally to provide error handling. Possible errors and warning messages that may be encountered are as follows.  • LA_ARRAY_SIZE_ERROR: Occurs if any of the input array sizes are incorrect.

# Notes

This routine utilizes the LAPACK routine DPOTRS.

Definition at line 1139 of file linalg\_solve.f90.

The documentation for this interface was generated from the following file:

• /home/jason/Documents/Code/linalg/src/linalg\_solve.f90

# 5.11 linalg\_solve::solve\_least\_squares Interface Reference

Solves the overdetermined or underdetermined system (A\*X = B) of M equations of N unknowns.

#### **Private Member Functions**

• subroutine solve\_least\_squares\_mtx (a, b, work, olwork, err)

Solves the overdetermined or underdetermined system (A\*X = B) of M equations of N unknowns using a QR or LQ factorization of the matrix A. Notice, it is assumed that matrix A has full rank.

• subroutine solve\_least\_squares\_vec (a, b, work, olwork, err)

Solves the overdetermined or underdetermined system (A\*X = B) of M equations of N unknowns using a QR or LQ factorization of the matrix A. Notice, it is assumed that matrix A has full rank.

# 5.11.1 Detailed Description

Solves the overdetermined or underdetermined system (A\*X = B) of M equations of N unknowns.

Definition at line 91 of file linalg\_solve.f90.

### 5.11.2 Member Function/Subroutine Documentation

5.11.2.1 subroutine linalg\_solve::solve\_least\_squares::solve\_least\_squares\_mtx ( real(dp), dimension(:,:), intent(inout) *a*, real(dp), dimension(:,:), intent(inout) *b*, real(dp), dimension(:), intent(out), optional, target *work*, integer(i32), intent(out), optional *olwork*, class(errors), intent(inout), optional, target *err* ) [private]

Solves the overdetermined or underdetermined system (A\*X = B) of M equations of N unknowns using a QR or LQ factorization of the matrix A. Notice, it is assumed that matrix A has full rank.

# **Parameters**

in,out	а	On input, the M-by-N matrix A. On output, if $M \ge N$ , the QR factorization of A in the form as output by qr_factor; else, if $M < N$ , the LQ factorization of A.
in,out	b	If $M >= N$ , the M-by-NRHS matrix B. On output, the first N rows contain the N-by-NRHS solution matrix X. If $M < N$ , an N-by-NRHS matrix with the first M rows containing the matrix B. On output, the N-by-NRHS solution matrix X.
out	work	An optional input, that if provided, prevents any local memory allocation. If not provided, the memory required is allocated within. If provided, the length of the array must be at least olwork.
out	olwork	An optional output used to determine workspace size. If supplied, the routine determines the optimal size for work, and returns without performing any actual calculations.
out	err	An optional errors-based object that if provided can be used to retrieve information relating to any errors encountered during execution. If not provided, a default implementation of the errors class is used internally to provide error handling. Possible errors and warning messages that may be encountered are as follows.
		<ul> <li>LA_ARRAY_SIZE_ERROR: Occurs if any of the input arrays are not sized appropriately.</li> </ul>
		<ul> <li>LA_OUT_OF_MEMORY_ERROR: Occurs if local memory must be allocated, and there is insufficient memory available.</li> </ul>
		LA_INVALID_OPERATION_ERROR: Occurs if a is not of full rank.

# Notes

This routine utilizes the LAPACK routine DGELS.

Definition at line 1568 of file linalg\_solve.f90.

5.11.2.2 subroutine linalg\_solve::solve\_least\_squares::solve\_least\_squares\_vec ( real(dp), dimension(:,:), intent(inout) *a*, real(dp), dimension(:), intent(inout) *b*, real(dp), dimension(:), intent(out), optional, target *work*, integer(i32), intent(out), optional *olwork*, class(errors), intent(inout), optional, target *err* ) [private]

Solves the overdetermined or underdetermined system (A\*X = B) of M equations of N unknowns using a QR or LQ factorization of the matrix A. Notice, it is assumed that matrix A has full rank.

#### **Parameters**

in,out	а	On input, the M-by-N matrix A. On output, if $M \ge N$ , the QR factorization of A in the form as output by qr_factor; else, if $M < N$ , the LQ factorization of A.
in,out	b	If $M >= N$ , the M-element array B. On output, the first N elements contain the N-element solution array X. If $M < N$ , an N-element array with the first M elements containing the array B. On output, the N-element solution array X.
out	work	An optional input, that if provided, prevents any local memory allocation. If not provided, the memory required is allocated within. If provided, the length of the array must be at least olwork.
out	olwork	An optional output used to determine workspace size. If supplied, the routine determines the optimal size for work, and returns without performing any actual calculations.
out	err	An optional errors-based object that if provided can be used to retrieve information relating to any errors encountered during execution. If not provided, a default implementation of the errors class is used internally to provide error handling. Possible errors and warning messages that may be encountered are as follows.
		<ul> <li>LA_ARRAY_SIZE_ERROR: Occurs if any of the input arrays are not sized appropriately.</li> </ul>
		<ul> <li>LA_OUT_OF_MEMORY_ERROR: Occurs if local memory must be allocated, and there is insufficient memory available.</li> </ul>
		LA_INVALID_OPERATION_ERROR: Occurs if a is not of full rank.

### Notes

This routine utilizes the LAPACK routine DGELS.

Definition at line 1674 of file linalg\_solve.f90.

The documentation for this interface was generated from the following file:

- $\bullet \ \ / home/jason/Documents/Code/linalg/src/linalg\_solve.f90$
- 5.12 linalg\_solve::solve\_least\_squares\_full Interface Reference

Solves the overdetermined or underdetermined system (A\*X = B) of M equations of N unknowns, but uses a full orthogonal factorization of the system.

#### **Private Member Functions**

• subroutine solve\_least\_squares\_mtx\_pvt (a, b, ipvt, arnk, work, olwork, err)

Solves the overdetermined or underdetermined system (A\*X = B) of M equations of N unknowns using a complete orthogonal factorization of matrix A.

• subroutine solve\_least\_squares\_vec\_pvt (a, b, ipvt, arnk, work, olwork, err)

Solves the overdetermined or underdetermined system (A\*X = B) of M equations of N unknowns using a complete orthogonal factorization of matrix A.

# 5.12.1 Detailed Description

Solves the overdetermined or underdetermined system (A\*X = B) of M equations of N unknowns, but uses a full orthogonal factorization of the system.

Definition at line 100 of file linalg\_solve.f90.

#### 5.12.2 Member Function/Subroutine Documentation

5.12.2.1 subroutine linalg\_solve::solve\_least\_squares\_full::solve\_least\_squares\_mtx\_pvt ( real(dp), dimension(:,:), intent(inout) a, real(dp), dimension(:,:), intent(inout) b, integer(i32), dimension(:), intent(inout), optional, target ipvt, integer(i32), intent(out), optional arnk, real(dp), dimension(:), intent(out), optional, target work, integer(i32), intent(out), optional olwork, class(errors), intent(inout), optional, target err ) [private]

Solves the overdetermined or underdetermined system (A\*X = B) of M equations of N unknowns using a complete orthogonal factorization of matrix A.

а	On input, the M-by-N matrix A. On output, the matrix is overwritten by the details of its
	complete orthogonal factorization.
b	If $M >= N$ , the M-by-NRHS matrix B. On output, the first N rows contain the N-by-NRHS solution matrix X. If $M < N$ , an N-by-NRHS matrix with the first M rows containing the matrix B. On output, the N-by-NRHS solution matrix X.
ipvt	An optional input that on input, an N-element array that if $IPVT(I)$ .ne. 0, the I-th column of A is permuted to the front of A $*$ P; if $IPVT(I) = 0$ , the I-th column of A is a free column. On output, if $IPVT(I) = K$ , then the I-th column of A $*$ P was the K-th column of A. If not supplied, memory is allocated internally, and $IPVT$ is set to all zeros such that all columns are treated as free.
arnk	An optional output, that if provided, will return the rank of a.
work	An optional input, that if provided, prevents any local memory allocation. If not provided, the memory required is allocated within. If provided, the length of the array must be at least olwork.
olwork	An optional output used to determine workspace size. If supplied, the routine determines the optimal size for work, and returns without performing any actual calculations.
err	An optional errors-based object that if provided can be used to retrieve information relating to any errors encountered during execution. If not provided, a default implementation of the errors class is used internally to provide error handling. Possible errors and warning messages that may be encountered are as follows.
	<ul> <li>LA_ARRAY_SIZE_ERROR: Occurs if any of the input arrays are not sized appropriately.</li> </ul>
	<ul> <li>LA_OUT_OF_MEMORY_ERROR: Occurs if local memory must be allocated, and there is insufficient memory available.</li> </ul>
	b ipvt arnk work olwork

#### Notes

This routine utilizes the LAPACK routine DGELSY.

Definition at line 1786 of file linalg\_solve.f90.

5.12.2.2 subroutine linalg\_solve::solve\_least\_squares\_full::solve\_least\_squares\_vec\_pvt ( real(dp), dimension(:,:), intent(inout) a, real(dp), dimension(:), intent(inout) b, integer(i32), dimension(:), intent(inout), optional, target ipvt, integer(i32), intent(out), optional arnk, real(dp), dimension(:), intent(out), optional, target work, integer(i32), intent(out), optional olwork, class(errors), intent(inout), optional, target err ) [private]

Solves the overdetermined or underdetermined system (A\*X = B) of M equations of N unknowns using a complete orthogonal factorization of matrix A.

#### **Parameters**

in,out	а	On input, the M-by-N matrix A. On output, the matrix is overwritten by the details of its complete orthogonal factorization.
in,out	b	If $M >= N$ , the M-element array B. On output, the first N elements contain the N-element solution array X. If $M < N$ , an N-element array with the first M elements containing the array B. On output, the N-element solution array X.
out	ipvt	An optional input that on input, an N-element array that if $IPVT(I)$ .ne. 0, the I-th column of A is permuted to the front of A $*$ P; if $IPVT(I) = 0$ , the I-th column of A is a free column. On output, if $IPVT(I) = K$ , then the I-th column of A $*$ P was the K-th column of A. If not supplied, memory is allocated internally, and $IPVT$ is set to all zeros such that all columns are treated as free.
out	arnk	An optional output, that if provided, will return the rank of a.
out	work	An optional input, that if provided, prevents any local memory allocation. If not provided, the memory required is allocated within. If provided, the length of the array must be at least olwork.
out	olwork	An optional output used to determine workspace size. If supplied, the routine determines the optimal size for work, and returns without performing any actual calculations.
out	err	An optional errors-based object that if provided can be used to retrieve information relating to any errors encountered during execution. If not provided, a default implementation of the errors class is used internally to provide error handling. Possible errors and warning messages that may be encountered are as follows.
		<ul> <li>LA_ARRAY_SIZE_ERROR: Occurs if any of the input arrays are not sized appropriately.</li> </ul>
		<ul> <li>LA_OUT_OF_MEMORY_ERROR: Occurs if local memory must be allocated, and there is insufficient memory available.</li> </ul>

#### Notes

This routine utilizes the LAPACK routine DGELSY.

Definition at line 1932 of file linalg\_solve.f90.

The documentation for this interface was generated from the following file:

• /home/jason/Documents/Code/linalg/src/linalg\_solve.f90

# 5.13 linalg\_solve::solve\_least\_squares\_svd Interface Reference

Solves the overdetermined or underdetermined system (A\*X = B) of M equations of N unknowns using a singular value decomposition of matrix A.

#### **Private Member Functions**

- subroutine solve\_least\_squares\_mtx\_svd (a, b, arnk, s, work, olwork, err)

  Solves the overdetermined or underdetermined system (A\*X = B) of M equations of N unknowns using a singular value decomposition of matrix A.
- subroutine solve\_least\_squares\_vec\_svd (a, b, arnk, s, work, olwork, err)

  Solves the overdetermined or underdetermined system (A\*X = B) of M equations of N unknowns using a singular value decomposition of matrix A.

# 5.13.1 Detailed Description

Solves the overdetermined or underdetermined system (A\*X = B) of M equations of N unknowns using a singular value decomposition of matrix A.

Definition at line 109 of file linalg solve.f90.

# 5.13.2 Member Function/Subroutine Documentation

5.13.2.1 subroutine linalg\_solve::solve\_least\_squares\_svd::solve\_least\_squares\_mtx\_svd ( real(dp), dimension(:,:), intent(inout) a, real(dp), dimension(:,:), intent(inout) b, integer(i32), intent(out), optional arnk, real(dp), dimension(:), intent(out) s, real(dp), dimension(:), intent(out), optional, target work, integer(i32), intent(out), optional olwork, class(errors), intent(inout), optional, target err ) [private]

Solves the overdetermined or underdetermined system (A\*X = B) of M equations of N unknowns using a singular value decomposition of matrix A.

in,out	а	On input, the M-by-N matrix A. On output, the matrix is overwritten by the details of its complete orthogonal factorization.
in,out	b	If $M >= N$ , the M-by-NRHS matrix B. On output, the first N rows contain the N-by-NRHS solution matrix X. If $M < N$ , an N-by-NRHS matrix with the first M rows containing the matrix B. On output, the N-by-NRHS solution matrix X.
out	arnk	An optional output, that if provided, will return the rank of a.
out	s	A MIN(M, N)-element array that on output contains the singular values of $a$ in descending order. Notice, the condition number of $a$ can be determined by S(1) / S(MIN(M, N)).
out	work	An optional input, that if provided, prevents any local memory allocation. If not provided, the memory required is allocated within. If provided, the length of the array must be at least olwork.
out	olwork	An optional output used to determine workspace size. If supplied, the routine determines the optimal size for work, and returns without performing any actual calculations.

# **Parameters**

out	err	An optional errors-based object that if provided can be used to retrieve information relating to any errors encountered during execution. If not provided, a default implementation of the errors class is used internally to provide error handling. Possible errors and warning messages that may be encountered are as follows.
		<ul> <li>LA_ARRAY_SIZE_ERROR: Occurs if any of the input arrays are not sized appropriately.</li> </ul>
		<ul> <li>LA_OUT_OF_MEMORY_ERROR: Occurs if local memory must be allocated, and there is insufficient memory available.</li> </ul>
		<ul> <li>LA_CONVERGENCE_ERROR: Occurs as a warning if the QR iteration process could not converge to a zero value.</li> </ul>

# Notes

This routine utilizes the LAPACK routine DGELSS.

Definition at line 2076 of file linalg\_solve.f90.

5.13.2.2 subroutine linalg\_solve::solve\_least\_squares\_svd::solve\_least\_squares\_vec\_svd ( real(dp), dimension(:,:), intent(inout) a, real(dp), dimension(:), intent(inout) b, integer(i32), intent(out), optional arnk, real(dp), dimension(:), intent(out) s, real(dp), dimension(:), intent(out), optional, target work, integer(i32), intent(out), optional olwork, class(errors), intent(inout), optional, target err ) [private]

Solves the overdetermined or underdetermined system (A\*X = B) of M equations of N unknowns using a singular value decomposition of matrix A.

in,out	а	On input, the M-by-N matrix A. On output, the matrix is overwritten by the details of its complete orthogonal factorization.
in,out	b	If $M >= N$ , the M-by-NRHS matrix B. On output, the first N rows contain the N-by-NRHS solution matrix X. If $M < N$ , an N-by-NRHS matrix with the first M rows containing the matrix B. On output, the N-by-NRHS solution matrix X.
out	arnk	An optional output, that if provided, will return the rank of a.
out	S	A MIN(M, N)-element array that on output contains the singular values of $a$ in descending order. Notice, the condition number of $a$ can be determined by S(1) / S(MIN(M, N)).
out	work	An optional input, that if provided, prevents any local memory allocation. If not provided, the memory required is allocated within. If provided, the length of the array must be at least olwork.
out	olwork	An optional output used to determine workspace size. If supplied, the routine determines the optimal size for work, and returns without performing any actual calculations.
out	err	An optional errors-based object that if provided can be used to retrieve information relating to any errors encountered during execution. If not provided, a default implementation of the errors class is used internally to provide error handling. Possible errors and warning messages that may be encountered are as follows.  • LA_ARRAY_SIZE_ERROR: Occurs if any of the input arrays are not sized appropriately.
		<ul> <li>LA_OUT_OF_MEMORY_ERROR: Occurs if local memory must be allocated, and there is insufficient memory available.</li> </ul>
		LA_CONVERGENCE_ERROR: Occurs as a warning if the QR iteration process could not converge to a zero value.
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#### Notes

This routine utilizes the LAPACK routine DGELSS.

Definition at line 2204 of file linalg\_solve.f90.

The documentation for this interface was generated from the following file:

/home/jason/Documents/Code/linalg/src/linalg\_solve.f90

# 5.14 linalg\_solve::solve\_lu Interface Reference

Solves a system of LU-factored equations.

**Private Member Functions** 

```
    subroutine solve_lu_mtx (a, ipvt, b, err)
    Solves a system of LU-factored equations.
```

subroutine solve\_lu\_vec (a, ipvt, b, err)
 Solves a system of LU-factored equations.

# 5.14.1 Detailed Description

Solves a system of LU-factored equations.

#### Usage

To solve a system of N equations of N unknowns using LU factorization, the following code will suffice.

```
! Solve the system: A*X = B, where A is an N-by-N matrix, and B and X are
! N-by-NRHS in size.
! Variables
real(dp), dimension(n, n) :: a
real(dp), dimension(n, nrhs) :: b
! Define the array used to track row pivots.
integer(i32), dimension(n) :: pvt
! Initialize A and B...
! Compute the LU factorization of A. On output, A contains [L\U].
call lu_factor(a, pvt)
! Solve A*X = B for X - Note: X overwrites B.
call solve_lu(a, pvt, b)
```

#### See Also

- Wikipedia
- Wolfram MathWorld

Definition at line 63 of file linalg\_solve.f90.

- 5.14.2 Member Function/Subroutine Documentation
- 5.14.2.1 subroutine linalg\_solve::solve\_lu::solve\_lu\_mtx ( real(dp), dimension(:,:), intent(in) a, integer(i32), dimension(:), intent(in) ipvt, real(dp), dimension(:,:), intent(inout) b, class(errors), intent(inout), optional, target err )

  [private]

Solves a system of LU-factored equations.

# **Parameters**

in	а	The N-by-N LU factored matrix as output by lu_factor.
in	ipvt	The N-element pivot array as output by lu_factor.
in, out	b	On input, the N-by-NRHS right-hand-side matrix. On output, the N-by-NRHS solution matrix.
out	err	An optional errors-based object that if provided can be used to retrieve information relating to any errors encountered during execution. If not provided, a default implementation of the errors class is used internally to provide error handling. Possible errors and warning messages that may be encountered are as follows.  • LA_ARRAY_SIZE_ERROR: Occurs if any of the input array sizes are incorrect.

### Notes

The routine is based upon the LAPACK routine DGETRS.

Definition at line 351 of file linalg\_solve.f90.

5.14.2.2 subroutine linalg\_solve::solve\_lu::solve\_lu\_vec ( real(dp), dimension(:,:), intent(in) a, integer(i32), dimension(:), intent(in) ipvt, real(dp), dimension(:), intent(inout) b, class(errors), intent(inout), optional, target err ) [private]

Solves a system of LU-factored equations.

### **Parameters**

in	а	The N-by-N LU factored matrix as output by lu_factor.
in	ipvt	The N-element pivot array as output by lu_factor.
in,out	b	On input, the N-element right-hand-side array. On output, the N-element solution array.
out	err	An optional errors-based object that if provided can be used to retrieve information relating to any errors encountered during execution. If not provided, a default implementation of the errors class is used internally to provide error handling. Possible errors and warning messages that may be encountered are as follows.  • LA_ARRAY_SIZE_ERROR: Occurs if any of the input array sizes are incorrect.

# Notes

The routine is based upon the LAPACK routine DGETRS.

Definition at line 412 of file linalg\_solve.f90.

The documentation for this interface was generated from the following file:

• /home/jason/Documents/Code/linalg/src/linalg\_solve.f90

# 5.15 linalg\_solve::solve\_qr Interface Reference

Solves a system of M QR-factored equations of N unknowns.

#### **Private Member Functions**

• subroutine solve\_qr\_no\_pivot\_mtx (a, tau, b, work, olwork, err)

Solves a system of M QR-factored equations of N unknowns where M >= N.

• subroutine solve\_qr\_no\_pivot\_vec (a, tau, b, work, olwork, err)

Solves a system of M QR-factored equations of N unknowns where M >= N.

• subroutine solve\_qr\_pivot\_mtx (a, tau, jpvt, b, work, olwork, err)

Solves a system of M QR-factored equations of N unknowns where the QR factorization made use of column pivoting.

• subroutine solve\_qr\_pivot\_vec (a, tau, jpvt, b, work, olwork, err)

Solves a system of M QR-factored equations of N unknowns where the QR factorization made use of column pivoting.

# 5.15.1 Detailed Description

Solves a system of M QR-factored equations of N unknowns.

#### See Also

- Wikipedia
- LAPACK Users Manual

Definition at line 74 of file linalg\_solve.f90.

# 5.15.2 Member Function/Subroutine Documentation

5.15.2.1 subroutine linalg\_solve::solve\_qr::solve\_qr\_no\_pivot\_mtx ( real(dp), dimension(:,:), intent(inout) a, real(dp), dimension(:), intent(inout) b, real(dp), dimension(:), intent(out), optional, target work, integer(i32), intent(out), optional olwork, class(errors), intent(inout), optional, target err ) [private]

Solves a system of M QR-factored equations of N unknowns where  $M \ge N$ .

in	а	On input, the M-by-N QR factored matrix as returned by qr_factor. On output, the contents of this matrix are restored. Notice, M must be greater than or equal to N.
in	tau	A MIN(M, N)-element array containing the scalar factors of the elementary reflectors as returned by qr_factor.
in	b	On input, the M-by-NRHS right-hand-side matrix. On output, the first N columns are overwritten by the solution matrix X.
out	work	An optional input, that if provided, prevents any local memory allocation. If not provided, the memory required is allocated within. If provided, the length of the array must be at least olwork.
out	olwork	An optional output used to determine workspace size. If supplied, the routine determines the optimal size for work, and returns without performing any actual calculations.
out	err	An optional errors-based object that if provided can be used to retrieve information relating to any errors encountered during execution. If not provided, a default implementation of the errors class is used internally to provide error handling. Possible errors and warning messages that may be encountered are as follows.
		<ul> <li>LA_ARRAY_SIZE_ERROR: Occurs if any of the input arrays are not sized appropriately.</li> </ul>
		<ul> <li>LA_OUT_OF_MEMORY_ERROR: Occurs if local memory must be allocated, and there is insufficient memory available.</li> </ul>
		Generated by Poweren

#### Notes

This routine is based upon a subset of the LAPACK routine DGELS.

Definition at line 487 of file linalg\_solve.f90.

5.15.2.2 subroutine linalg\_solve::solve\_qr::solve\_qr\_no\_pivot\_vec ( real(dp), dimension(:,:), intent(inout) *a,* real(dp), dimension(:), intent(inout) *b,* real(dp), dimension(:), intent(out), optional, target work, integer(i32), intent(out), optional olwork, class(errors), intent(inout), optional, target err ) [private]

Solves a system of M QR-factored equations of N unknowns where  $M \ge N$ .

#### **Parameters**

in	а	On input, the M-by-N QR factored matrix as returned by qr_factor. On output, the contents of this matrix are restored. Notice, M must be greater than or equal to N.
in	tau	A MIN(M, N)-element array containing the scalar factors of the elementary reflectors as returned by qr_factor.
in	b	On input, the M-element right-hand-side vector. On output, the first N elements are overwritten by the solution vector X.
out	work	An optional input, that if provided, prevents any local memory allocation. If not provided, the memory required is allocated within. If provided, the length of the array must be at least olwork.
out	olwork	An optional output used to determine workspace size. If supplied, the routine determines the optimal size for $work$ , and returns without performing any actual calculations.
out	err	An optional errors-based object that if provided can be used to retrieve information relating to any errors encountered during execution. If not provided, a default implementation of the errors class is used internally to provide error handling. Possible errors and warning messages that may be encountered are as follows.
		<ul> <li>LA_ARRAY_SIZE_ERROR: Occurs if any of the input arrays are not sized appropriately.</li> </ul>
		<ul> <li>LA_OUT_OF_MEMORY_ERROR: Occurs if local memory must be allocated, and there is insufficient memory available.</li> </ul>

#### Notes

This routine is based upon a subset of the LAPACK routine DGELS.

Definition at line 602 of file linalg\_solve.f90.

5.15.2.3 subroutine linalg\_solve::solve\_qr::solve\_qr\_pivot\_mtx ( real(dp), dimension(:,:), intent(inout) a, real(dp), dimension(:), intent(in) tau, integer(i32), dimension(:), intent(in) jpvt, real(dp), dimension(:,:), intent(inout) b, real(dp), dimension(:), intent(out), optional, target work, integer(i32), intent(out), optional olwork, class(errors), intent(inout), optional, target err ) [private]

Solves a system of M QR-factored equations of N unknowns where the QR factorization made use of column pivoting.

in	а	On input, the M-by-N QR factored matrix as returned by qr_factor. On output, the contents of
		this matrix are altered.

# **Parameters**

An N-element array, as output by gr factor, used to track the column pivots.
An in-element array, as output by qi_lactor, used to track the column pivots.
On input, the MAX(M, N)-by-NRHS matrix where the first M rows contain the right-hand-side matrix B. On output, the first N rows are overwritten by the solution matrix X.
An optional input, that if provided, prevents any local memory allocation. If not provided, the memory required is allocated within. If provided, the length of the array must be at least olwork.
An optional output used to determine workspace size. If supplied, the routine determines the optimal size for work, and returns without performing any actual calculations.
<ul> <li>An optional errors-based object that if provided can be used to retrieve information relating to any errors encountered during execution. If not provided, a default implementation of the errors class is used internally to provide error handling. Possible errors and warning messages that may be encountered are as follows.</li> <li>LA_ARRAY_SIZE_ERROR: Occurs if any of the input arrays are not sized appropriately.</li> <li>LA_OUT_OF_MEMORY_ERROR: Occurs if local memory must be allocated, and there is insufficient memory available.</li> </ul>

# Notes

This routine is based upon a subset of the LAPACK routine DGELSY.

Definition at line 715 of file linalg\_solve.f90.

5.15.2.4 subroutine linalg\_solve::solve\_qr::solve\_qr\_pivot\_vec ( real(dp), dimension(:,:), intent(inout) a, real(dp), dimension(:), intent(in) tau, integer(i32), dimension(:), intent(in) jpvt, real(dp), dimension(:), intent(inout) b, real(dp), dimension(:), intent(out), optional, target work, integer(i32), intent(out), optional olwork, class(errors), intent(inout), optional, target err ) [private]

Solves a system of M QR-factored equations of N unknowns where the QR factorization made use of column pivoting.

in	а	On input, the M-by-N QR factored matrix as returned by qr_factor. On output, the contents of this matrix are altered.
in	tau	A MIN(M, N)-element array containing the scalar factors of the elementary reflectors as returned by qr_factor.
in	jpvt	An N-element array, as output by qr_factor, used to track the column pivots.
in	b	On input, the MAX(M, N)-element array where the first M elements contain the right-hand-side vector B. On output, the first N elements are overwritten by the solution vector X.
out	work	An optional input, that if provided, prevents any local memory allocation. If not provided, the memory required is allocated within. If provided, the length of the array must be at least olwork.
out	olwork	An optional output used to determine workspace size. If supplied, the routine determines the optimal size for $work$ , and returns without performing any actual calculations.

#### **Parameters**

out	err	An optional errors-based object that if provided can be used to retrieve information relating to any errors encountered during execution. If not provided, a default implementation of the errors class is used internally to provide error handling. Possible errors and warning messages that may be encountered are as follows.
		<ul> <li>LA_ARRAY_SIZE_ERROR: Occurs if any of the input arrays are not sized appropriately.</li> </ul>
		<ul> <li>LA_OUT_OF_MEMORY_ERROR: Occurs if local memory must be allocated, and there is insufficient memory available.</li> </ul>

#### Notes

This routine is based upon a subset of the LAPACK routine DGELSY.

Definition at line 902 of file linalg\_solve.f90.

The documentation for this interface was generated from the following file:

• /home/jason/Documents/Code/linalg/src/linalg\_solve.f90

# 5.16 linalg\_solve::solve\_triangular\_system Interface Reference

Solves a triangular system of equations.

### **Private Member Functions**

- subroutine solve\_tri\_mtx (Iside, upper, trans, nounit, alpha, a, b, err)

  Solves one of the matrix equations: op(A) \* X = alpha \* B, or X \* op(A) = alpha \* B, where A is a triangular matrix.
- subroutine solve\_tri\_vec (upper, trans, nounit, a, x, err)

Solves the system of equations: op(A) \* X = B, where A is a triangular matrix.

# 5.16.1 Detailed Description

Solves a triangular system of equations.

Definition at line 29 of file linalg\_solve.f90.

# 5.16.2 Member Function/Subroutine Documentation

5.16.2.1 subroutine linalg\_solve::solve\_triangular\_system::solve\_tri\_mtx ( logical, intent(in) *lside,* logical, intent(in) *upper,* logical, intent(in) *trans,* logical, intent(in) *nounit,* real(dp), intent(in) *alpha,* real(dp), dimension(:,:), intent(in) *a,* real(dp), dimension(:,:), intent(inout) *b,* class(errors), intent(inout), optional, target *err* ) [private]

Solves one of the matrix equations: op(A) \* X = alpha \* B, or X \* op(A) = alpha \* B, where A is a triangular matrix.

#### **Parameters**

in	Iside	Set to true to solve $op(A) * X = alpha * B$ ; else, set to false to solve $X * op(A) = alpha * B$ .
in	upper	Set to true if A is an upper triangular matrix; else, set to false if A is a lower triangular matrix.
in	trans	Set to true if $op(A) = A**T$ ; else, set to false if $op(A) = A$ .
in	nounit	Set to true if A is not a unit-diagonal matrix (ones on every diagonal element); else, set to false if A is a unit-diagonal matrix.
in	alpha	The scalar multiplier to B.
in	а	If lside is true, the M-by-M triangular matrix on which to operate; else, if lside is false, the N-by-N triangular matrix on which to operate.
in,out	b	On input, the M-by-N right-hand-side. On output, the M-by-N solution.
out	err	An optional errors-based object that if provided can be used to retrieve information relating to any errors encountered during execution. If not provided, a default implementation of the errors class is used internally to provide error handling. Possible errors and warning messages that may be encountered are as follows.  • LA_ARRAY_SIZE_ERROR: Occurs if a is not square, or if the sizes of a and b are not compatible.

# Usage

To solve a triangular system of N equations of N unknowns A\*X = B, where A is an N-by-N upper triangular matrix, and B and X are N-by-NRHS matrices, the following code will suffice.

# Notes

This routine is based upon the BLAS routine DTRSM.

Definition at line 169 of file linalg\_solve.f90.

5.16.2.2 subroutine linalg\_solve::solve\_triangular\_system::solve\_tri\_vec ( logical, intent(in) upper, logical, intent(in) trans, logical, intent(in) nounit, real(dp), dimension(:,:), intent(in) a, real(dp), dimension(:), intent(inout) x, class(errors), intent(inout), optional, target err ) [private]

Solves the system of equations: op(A) \* X = B, where A is a triangular matrix.

in	upper	Set to true if A is an upper triangular matrix; else, set to false if A is a lower triangular	
		matrix.	
in	trans	Set to true if $op(A) = A**T$ ; else, set to false if $op(A) = A$ .	
in	nounit	Set to true if A is not a unit-diagonal matrix (ones on every diagonal element); else, set to false if A is a unit-diagonal matrix.	

# **Parameters**

in	а	The N-by-N triangular matrix.
in,out	х	On input, the N-element right-hand-side array. On output, the N-element solution array.
out	err	An optional errors-based object that if provided can be used to retrieve information relating to any errors encountered during execution. If not provided, a default implementation of the errors class is used internally to provide error handling. Possible errors and warning messages that may be encountered are as follows.  • LA_ARRAY_SIZE_ERROR: Occurs if a is not square, or if the sizes of a and b are not compatible.

# Usage

To solve a triangular system of N equations of N unknowns A\*X = B, where A is an N-by-N upper triangular matrix, and B and X are N-element arrays, the following code will suffice.

```
! Solve the system: A*X = B, where A is an upper triangular N-by-N
! matrix, and B and X are N-elements in size.
! Variables
integer(i32) :: info
real(dp), dimension(n, n) :: a
real(dp), dimension(n) :: b
! Initialize A and B...
! Solve A*X = B for X - Note: X overwrites B.
call solve_triangular_system(.true., .false., a, b)
```

# Notes

This routine is based upon the BLAS routine DTRSV.

Definition at line 275 of file linalg\_solve.f90.

The documentation for this interface was generated from the following file:

• /home/jason/Documents/Code/linalg/src/linalg\_solve.f90

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