bml

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Contents

Chapter 1

Basic Matrix Library (bml)

This library implements a common API for linear algebra and matrix functions in C and Fortran. It offers several data structures for matrix storage and algorithms. Currently the following matrix data types are implemented:

- dense
- ellpack (sparse)
- csr (sparse)

1.1 Usage Examples

Usage examples can be found here:

- Fortran Usage
- C Usage

1.2 Modifying the library itself

If you are interested in modifying the library code itself, please have a look at the Developer Documentation.

1.3 Planned Features

We are planning to eventually support different matrix types and matrix operations on a variety of hardware platforms. For details, please have a look at our future plans.

Author

Christian Negre cnegre@lanl.gov
Jamaludin Mohd-Yusof jamal@lanl.gov
Nicolas Bock nbock@lanl.gov
Susan M. Mniszewski smm@lanl.gov

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Chapter 2

Future Plans

2.1 Matrix Types

Support types:

- bml_matrix_t
- Colinear
- Noncolinear
- Blocked Bloch Matrix

2.2 Precisions

The bml supports the following precisions:

- logical (for matrix masks)
- single real
- double real
- single complex
- double complex

2.3 Functions

The library supports the following matrix operations:

- Format Conversion
  - bml_convert::bml_convert_from_dense
  - bml_convert::bml_convert_to_dense
  - bml_convert::bml_convert
- Masking
  - Masked operations (restricted to a subgraph)
- Addition

  - $\alpha A + \beta B$: bml_add::bml_add
  - $\alpha A + \beta$: bml_add::bml_add_identity
- Copy
  - $B \leftarrow A$: bml_copy::bml_copy
- Diagonalize
  - bml_diagonalize::bml_diagonalize
- Introspection
  - bml_introspection::bml_get_type
  - bml_introspection::bml_get_size
  - bml_introspection::bml_get_bandwidth
  - bml_introspection::bml_get_spectral_range
  - bml_introspection::bml_get_HOMO_LUMO
- Matrix manipulation:
  - bml_get::bml_get
  - bml_get::bml_get_rows
  - bml_set::bml_set
  - bml_set::bml_set_rows
- Multiplication
  - $\alpha A \times B + \beta C$: bml_multiply::bml_multiply
- Printing
  - bml_utilities::bml_print_matrix
- Scaling
  - $A \leftarrow \alpha A$: bml_scale::bml_scale_one
  - $B \leftarrow \alpha A$: bml_scale::bml_scale_two
- Matrix trace
  - $\mathrm{Tr}[A]$: bml_trace::bml_trace
  - $\mathrm{Tr}[AB]$: bml_trace::bml_product_trace
- Matrix norm
  - 2-norm
  - Frobenius norm
- Matrix transpose
  - bml_transpose::bml_transpose
- Matrix commutator/anticommutator
  - bml_commutator::bml_commutator
  - bml_commutator::bml_anticommutator

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Chapter 3

C Usage

In C, the following example code does the same as the above Fortran code:

```
#include <bml.h>

bml_matrix_t *A = bml_zero_matrix(dense,
      single_real, 100);
bml_deallocate(&A);
```

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Chapter 4

Fortran Usage

The use of this library is pretty straightforward. In the application code, `use` the bml main module,

```
use bml
```

A matrix is of type

```
type(bml_matrix_t) :: a
```

There are two important things to note. First, although not explicitly state in the above example, the matrix is not yet allocated. Hence, the matrix needs to be allocated through an allocation procedure with the desired type and precision, e.g. dense:double, see the page on allocation functions for a complete list. For instance,

```
call bml_zero_matrix(BML_MATRIX_DENSE, BML_PRECISION_DOUBLE, 100, a)
```

will allocate a dense, double-precision, 100×100 matrix which is initialized to zero. Additional functions allocate special matrices,

- bml_allocate::bml_random_matrix Allocate and initialize a random matrix.
- bml_allocate::bml_identity_matrix Allocate and initialize the identity matrix.

A matrix is deallocated by calling

```
call bml_deallocate(a)
```

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Chapter 5

Developer Documentation

5.1 Developer Suggested Workflow

We try to preserve a linear history in our main (master) branch. Instead of pulling (i.e. merging), we suggest you use:

```
$ git pull --rebase
```

And then

```
$ git push
```

To push your changes back to the server.

5.2 Coding Style

Please indent your C code using

```
$ indent -gnu -nut -i4 -bli0
```

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Chapter 6

Deprecated List

globalScope> Member bml_convert_from_dense (const bml_matrix_type_t matrix_type, const bml_matrix_precision_t matrix_precision, const int N, const void *A, const double threshold, const int M)

Deprecated API.

globalScope> Member bml_convert_to_dense (const bml_matrix_t *A)

Deprecated API.

Chapter 7

Module Index

7.1 Modules

Here is a list of all modules:

Chapter 8

Namespace Index

8.1 Namespace List

Here is a list of all documented namespaces with brief descriptions:

Chapter 9

Class Index

9.1 Class List

Here are the classes, structs, unions and interfaces with brief descriptions:

Chapter 10

File Index

10.1 File List

Here is a list of all documented files with brief descriptions:

Chapter 11

Module Documentation

11.1 Allocation and Deallocation Functions (C interface)

Functions

- void * bml_allocate_memory (const size_t size)
- void bml_free_memory (void *ptr)
- void bml_deallocate (bml_matrix_t **A)
- bml_matrix_t * bml_zero_matrix (const bml_matrix_type_t matrix_type, const bml_matrix_precision_t matrix_precision, const int N, const int M)
- bml_matrix_t * bml_random_matrix (const bml_matrix_type_t matrix_type, const bml_matrix_precision_t matrix_precision, const int N, const int M)
- bml_matrix_t * bml_identity_matrix (const bml_matrix_type_t matrix_type, const bml_matrix_precision_t matrix_precision, const int N, const int M)

11.1.1 Detailed Description

11.1.2 Function Documentation

11.1.2.1 void* bml_allocate_memory (const size_t *size*)

Allocate and zero a chunk of memory.

Parameters

size	The size of the memory.

Returns

A pointer to the allocated chunk.

11.1.2.2 void bml_deallocate (bml_matrix_t ** *A*)

Deallocate a matrix.

Parameters

A	The matrix.

Here is the call graph for this function:

11.1.2.3 void bml_free_memory (void * *ptr*)

Deallocate a chunk of memory.

Parameters

ptr	A pointer to the previously allocated chunk.

11.1.2.4 bml_matrix_t* bml_identity_matrix (const bml_matrix_type_t *matrix_type*, const bml_matrix_precision_t *matrix_precision*, const int *N*, const int *M*)

Allocate the identity matrix.

Note that the matrix A will be newly allocated. The function does not check whether the matrix is already allocated.

Parameters

matrix_type	The matrix type.
matrix_precision	The precision of the matrix.
N	The matrix size.
M	The number of non-zeroes per row.

Returns

The matrix.

11.1.2.5 bml_matrix_t* bml_random_matrix (const bml_matrix_type_t *matrix_type*, const bml_matrix_precision_t *matrix_precision*, const int *N*, const int *M*)

Allocate a random matrix.

Note that the matrix A will be newly allocated. The function does not check whether the matrix is already allocated.

Parameters

matrix_type	The matrix type.
matrix_precision	The precision of the matrix.
N	The matrix size.

M	The number of non-zeroes per row.

Returns

The matrix.

11.1.2.6 bml_matrix_t* bml_zero_matrix (const bml_matrix_type_t *matrix_type*, const bml_matrix_precision_t *matrix_precision*, const int *N*, const int *M*)

Allocate the zero matrix.

Note that the matrix A will be newly allocated. The function does not check whether the matrix is already allocated.

Parameters

matrix_type	The matrix type.
matrix_precision	The precision of the matrix.
N	The matrix size.
M	The number of non-zeroes per row.

Returns

The matrix.

11.2 Add Functions (C interface)

Functions

- void bml_add (bml_matrix_t *A, const bml_matrix_t *B, const double alpha, const double beta, const double threshold)
- void bml_add_identity (bml_matrix_t *A, const double beta, const double threshold)

11.2.1 Detailed Description

11.2.2 Function Documentation

11.2.2.1 void bml_add (bml_matrix_t * *A*, const bml_matrix_t * *B*, const double *alpha*, const double *beta*, const double *threshold*)

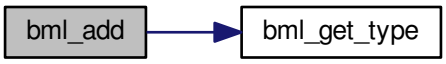
Matrix addition.

$A \leftarrow \alpha A + \beta B$

Parameters

A	Matrix A
B	Matrix B
alpha	Scalar factor multiplied by A
beta	Scalar factor multiplied by B
threshold	Threshold for matrix addition

Here is the call graph for this function:



11.2.2.2 void bml_add_identity (bml_matrix_t * *A*, const double *beta*, const double *threshold*)

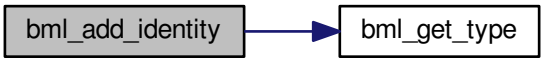
Matrix addition.

$A \leftarrow A + \beta \mathrm{Id}$

Parameters

A	Matrix A
beta	Scalar factor multiplied by A
threshold	Threshold for matrix addition

Here is the call graph for this function:



11.3 Converting between Matrix Formats (C interface)

Functions

- void * bml_export_to_dense (const bml_matrix_t *A)
- bml_matrix_t * bml_import_from_dense (const bml_matrix_type_t matrix_type, const bml_matrix_precision_t matrix_precision, const int N, const void *A, const double threshold, const int M)

11.3.1 Detailed Description

11.3.2 Function Documentation

11.3.2.1 void* bml_export_to_dense (const bml_matrix_t * A)

Export a bml matrix.

The returned pointer has to be typecase into the proper real type. If the bml matrix is a single precision matrix, then the following should be used:

```
float *A_dense = bml_convert_to_dense(A_bml);
```

The matrix size can be queried with

```
int N = bml_get_size(A_bml);
```

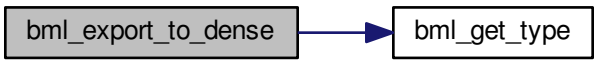
Parameters

A	The bml matrix

Returns

The dense matrix

Here is the call graph for this function:



Here is the caller graph for this function:

11.3.2.2 bml_matrix_t* bml_import_from_dense (const bml_matrix_type_t *matrix_type*, const bml_matrix_precision_t *matrix_precision*, const int *N*, const void * *A*, const double *threshold*, const int *M*)

Import a dense matrix.

Parameters

matrix_type	The matrix type
matrix_precision	The real precision
N	The number of rows/columns
A	The dense matrix
threshold	The matrix element magnited threshold
M	The number of non-zeroes per row

Returns

The bml matrix

Here is the caller graph for this function:

11.4 Allocation and Deallocation Functions (Fortran interface)

Functions

- subroutine, public bml_allocate_m::bml_deallocate (a)

  Deallocate a matrix.
- subroutine, public bml_allocate_m::bml_zero_matrix (matrix_type, matrix_precision, n, m, a)

  Create the zero matrix.
- subroutine, public bml_allocate_m::bml_random_matrix (matrix_type, matrix_precision, n, m, a)

  Create a random matrix.
- subroutine, public bml_allocate_m::bml_identity_matrix (matrix_type, matrix_precision, n, m, a)

  Create the identity matrix.

11.4.1 Detailed Description

11.4.2 Function Documentation

11.4.2.1 subroutine, public bml_allocate_m::bml_deallocate (type(bml_matrix_t) *a*)

Deallocate a matrix.

Parameters

a	The matrix.

11.4.2.2 subroutine, public bml_allocate_m::bml_identity_matrix (character(len=∗), intent(in) *matrix_type,* character(len=∗), intent(in) *matrix_precision,* integer, intent(in) *n,* integer, intent(in) *m,* type(bml_matrix_t), intent(inout) *a*)

Create the identity matrix.

Parameters

matrix_type	The matrix type.
matrix_precision	The precision of the matrix.
n	The matrix size.
a	The matrix.
m	The extra arg.

11.4.2.3 subroutine, public bml_allocate_m::bml_random_matrix (character(len=∗), intent(in) *matrix_type,* character(len=∗), intent(in) *matrix_precision,* integer, intent(in) *n,* integer, intent(in) *m,* type(bml_matrix_t), intent(inout) *a*)

Create a random matrix.

Parameters

matrix_type	The matrix type.
matrix_precision	The precision of the matrix.
n	The matrix size.
a	The matrix.
m	The extra arg.

11.4.2.4 subroutine, public bml_allocate_m::bml_zero_matrix (character(len=*), intent(in) *matrix_type,* character(len=*), intent(in) *matrix_precision,* integer, intent(in) *n,* integer, intent(in) *m,* type(**bml_matrix_t**), intent(inout) *a*)

Create the zero matrix.

Parameters

matrix_type	The matrix type.
matrix_precision	The precision of the matrix.
n	The matrix size.
a	The matrix.
m	The extra arg.

11.5 Add Functions (Fortran interface)

11.5.1 Detailed Description

11.6 Converting between Matrix Formats (Fortran interface)

Functions

- subroutine bml_convert_m::bml_convert_from_dense_double (matrix_type, a_dense, a, threshold, m)

  Convert a dense matrix into a bml matrix.
- subroutine bml_convert_m::bml_convert_from_dense_single_complex (matrix_type, a_dense, a, threshold, m)

  Convert a dense matrix into a bml matrix.
- subroutine bml_convert_m::bml_convert_from_dense_double_complex (matrix_type, a_dense, a, threshold, m)

  Convert a dense matrix into a bml matrix.
- subroutine bml_convert_m::bml_convert_to_dense_single (a, a_dense)

  Convert a matrix into a dense matrix.
- subroutine bml_convert_m::bml_convert_to_dense_double (a, a_dense)

  Convert a matrix into a dense matrix.
- subroutine bml_convert_m::bml_convert_to_dense_single_complex (a, a_dense)

  Convert a matrix into a dense matrix.
- subroutine bml_convert_m::bml_convert_to_dense_double_complex (a, a_dense)

  Convert a matrix into a dense matrix.

11.6.1 Detailed Description

11.6.2 Function Documentation

11.6.2.1 subroutine bml_convert_m::bml_convert_from_dense_double (character(len=∗), intent(in) *matrix_type,* double precision, dimension(:, :), intent(in), target *a_dense,* type(**bml_matrix_t**), intent(inout) *a,* double precision, intent(in), optional *threshold,* integer, intent(in), optional *m*)

Convert a dense matrix into a bml matrix.

Parameters

matrix_type	The matrix type
a_dense	The dense matrix
a	The bml matrix
threshold	The matrix element magnited threshold
m	the extra arg

11.6.2.2 subroutine bml_convert_m::bml_convert_from_dense_double_complex (character(len=∗), intent(in) *matrix_type,* complex(kind(0.0d0)), dimension(:, :), intent(in), target *a_dense,* type(**bml_matrix_t**), intent(inout) *a,* double precision, intent(in), optional *threshold,* integer, intent(in), optional *m*)

Convert a dense matrix into a bml matrix.

Parameters

matrix_type	The matrix type
a_dense	The dense matrix
a	The bml matrix

threshold	The matrix element magnited threshold
m	the extra arg

11.6.2.3 subroutine bml_convert_m::bml_convert_from_dense_single_complex (character(len=∗), intent(in) *matrix_type,* complex, dimension(:, :), intent(in), target *a_dense,* type(**bml_matrix_t**), intent(inout) *a,* double precision, intent(in), optional *threshold,* integer, intent(in), optional *m*)

Convert a dense matrix into a bml matrix.

Parameters

matrix_type	The matrix type
a_dense	The dense matrix
a	The bml matrix
threshold	The matrix element magnited threshold
m	The extra arg

11.6.2.4 subroutine bml_convert_m::bml_convert_to_dense_double (type(**bml_matrix_t**), intent(in) *a,* double precision, dimension(:, :), intent(inout), allocatable *a_dense*)

Convert a matrix into a dense matrix.

Parameters

a	The bml matrix
a_dense	The dense matrix

11.6.2.5 subroutine bml_convert_m::bml_convert_to_dense_double_complex (type(**bml_matrix_t**), intent(in) *a,* complex(kind(0d0)), dimension(:, :), intent(out), allocatable *a_dense*)

Convert a matrix into a dense matrix.

Parameters

a	The bml matrix
a_dense	The dense matrix

11.6.2.6 subroutine bml_convert_m::bml_convert_to_dense_single (type(**bml_matrix_t**), intent(in) *a,* real, dimension(:, :), intent(inout), allocatable *a_dense*)

Convert a matrix into a dense matrix.

Parameters

a	The bml matrix
a_dense	The dense matrix

11.6.2.7 subroutine bml_convert_m::bml_convert_to_dense_single_complex (type(**bml_matrix_t**), intent(in) *a,* complex, dimension(:, :), intent(out), allocatable *a_dense*)

Convert a matrix into a dense matrix.

Parameters

a	The bml matrix
a_dense	The dense matrix

Chapter 12

Namespace Documentation

12.1 bml Module Reference

Main matrix library module.

12.1.1 Detailed Description

Main matrix library module.

Use this modules in order to use the library.

12.2 bml_allocate_m Module Reference

Matrix allocation functions.

Functions/Subroutines

- subroutine, public bml_deallocate (a)

  Deallocate a matrix.
- subroutine, public bml_zero_matrix (matrix_type, matrix_precision, n, m, a)

  Create the zero matrix.
- subroutine, public bml_random_matrix (matrix_type, matrix_precision, n, m, a)

  Create a random matrix.
- subroutine, public bml_identity_matrix (matrix_type, matrix_precision, n, m, a)

  Create the identity matrix.

12.2.1 Detailed Description

Matrix allocation functions.

12.3 bml_copy_m Module Reference

Copy operations on matrices.

Functions/Subroutines

- subroutine, public bml_copy (a, b)
  Copy a matrix - result is a new matrix.

12.3.1 Detailed Description

Copy operations on matrices.

12.3.2 Function/Subroutine Documentation

12.3.2.1 subroutine, public bml_copy_m::bml_copy (type(bml_matrix_t), intent(in) *a,* type(bml_matrix_t), intent(inout) *b*)

Copy a matrix - result is a new matrix.

Parameters

A	Matrix to copy

Returns

A Copy of A

12.4 bml_diagonalize_m Module Reference

Matrix diagonalization functions.

Functions/Subroutines

- subroutine, public bml_diagonalize (a, eigenvalues, eigenvectors)
  Diagonalize a matrix.

12.4.1 Detailed Description

Matrix diagonalization functions.

12.4.2 Function/Subroutine Documentation

12.4.2.1 subroutine, public bml_diagonalize_m::bml_diagonalize (type(bml_matrix_t), intent(in) *a,* double precision, dimension(:), intent(inout), target *eigenvalues,* type(bml_matrix_t), intent(inout) *eigenvectors*)

Diagonalize a matrix.

Parameters

a	The matrix.
eigenvalues	The corresponding eigenvalues.
eigenvectors	The set of eigenvectors.

12.5 bml_error_m Module Reference

A module for error handling in bml.

Functions/Subroutines

- subroutine, public bml_error (file, line, message)

  Common error handling of bml. This function writes out an error message and exits.
- subroutine, public bml_warning (file, line, message)

  Common error handling of bml. This function writes out a non-fatal warning message.
- subroutine, public bml_debug (file, line, message)

  Common error handling of bml. This function writes out a non-fatal warning message.

12.5.1 Detailed Description

A module for error handling in bml.

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12.5.2 Function/Subroutine Documentation

12.5.2.1 subroutine, public bml_error_m::bml_debug (character(len=∗), intent(in) *file,* integer, intent(in) *line,* character(len=∗), intent(in) *message*)

Common error handling of bml. This function writes out a non-fatal warning message.

In the future one could imagine something more like exceptions, in which the error gets passed up the call stack.

Parameters

file	The filename in which the error occurred.
line	The line number in that file.
message	The error message.

12.5.2.2 subroutine, public bml_error_m::bml_error (character(len=∗), intent(in) *file,* integer, intent(in) *line,* character(len=∗), intent(in) *message*)

Common error handling of bml. This function writes out an error message and exits.

In the future one could imagine something more like exceptions, in which the error gets passed up the call stack.

Parameters

file	The filename in which the error occurred.
line	The line number in that file.
message	The error message.

12.5.2.3 subroutine, public bml_error_m::bml_warning (character(len=∗), intent(in) *file,* integer, intent(in) *line,* character(len=∗), intent(in) *message*)

Common error handling of bml. This function writes out a non-fatal warning message.

In the future one could imagine something more like exceptions, in which the error gets passed up the call stack.

Parameters

file	The filename in which the error occurred.
line	The line number in that file.
message	The error message.

12.6 bml_interface_m Module Reference

Interface module.

Functions/Subroutines

- integer function, public get_enum_id (type_string)

  Convert the matrix type and precisions strings into enum values.

Variables

- integer, parameter bml_matrix_type_uninitialized_enum_id = 0

  The enum values of the C API. Keep this synchronized with the enum in bml_types.h.
- integer, parameter **bml_matrix_type_dense_enum_id** = 1
- integer, parameter **bml_matrix_type_ellpack_enum_id** = 2
- integer, parameter **bml_matrix_precision_uninitialized_id** = 0
- integer, parameter **bml_matrix_precision_single_real_enum_id** = 1
- integer, parameter **bml_matrix_precision_double_real_enum_id** = 2
- integer, parameter **bml_matrix_precision_single_complex_enum_id** = 3
- integer, parameter **bml_matrix_precision_double_complex_enum_id** = 4

12.6.1 Detailed Description

Interface module.

12.6.2 Function/Subroutine Documentation

12.6.2.1 integer function, public bml_interface_m::get_enum_id (character(len=∗), intent(in) *type_string*)

Convert the matrix type and precisions strings into enum values.

Parameters

type_string	The string used in the Fortran API to identify the matrix type and precision.

Returns

The corresponding integer value matching the enum values in bml_matrix_types_t and bml_matrix_↩precision_t.

12.7 bml_introspection_m Module Reference

Introspection procedures.

Functions/Subroutines

- integer function, public bml_get_n (a)

  Return the matrix size.
- integer function, public bml_get_row_bandwidth (a, i)

  Get the bandwidth of non-zero elements in a given row.

12.7.1 Detailed Description

Introspection procedures.

12.7.2 Function/Subroutine Documentation

12.7.2.1 integer function, public bml_introspection_m::bml_get_n (type(bml_matrix_t), intent(in) *a*)

Return the matrix size.

Parameters

a	The matrix.

Returns

The matrix size.

12.7.2.2 integer function, public bml_introspection_m::bml_get_row_bandwidth (type(bml_matrix_t), intent(in) *a*, integer, intent(in) *i*)

Get the bandwidth of non-zero elements in a given row.

Parameters

a	The matrix.
i	The row.

Returns

The bandwidth of non-zero elements (bandwidth) on that row.

12.8 bml_multiply_m Module Reference

Matrix multiplication.

Functions/Subroutines

- subroutine, public bml_multiply (a, b, c, alpha, beta)

  Multiply two matrices.

12.8.1 Detailed Description

Matrix multiplication.

12.8.2 Function/Subroutine Documentation

12.8.2.1 subroutine, public bml_multiply_m::bml_multiply (type(bml_matrix_t), intent(in) *a,* type(bml_matrix_t), intent(in) *b,* type(bml_matrix_t), intent(inout) *c,* double precision, intent(in), optional *alpha,* double precision, intent(in), optional *beta*)

Multiply two matrices.

$C \leftarrow \alpha A \times B + \beta C$

The optional scaling factors α and β default to $\alpha = 1$ and $\beta = 0$.

Parameters

a	Matrix A.
b	Matrix B.
c	Matrix C.
alpha	The factor α.
beta	The factor β.

12.9 bml_scale_m Module Reference

Matrix scaling for matrices.

Functions/Subroutines

- subroutine scale_two (alpha, a, c)

  Scale a bml matrix.

12.9.1 Detailed Description

Matrix scaling for matrices.

12.9.2 Function/Subroutine Documentation

12.9.2.1 subroutine bml_scale_m::scale_two (double precision, intent(in) *alpha,* type(bml_matrix_t), intent(in) *a,* type(bml_matrix_t), intent(inout) *c*)

Scale a bml matrix.

$C \leftarrow \alpha A$

Parameters

alpha	The factor
a	The matrix
c	The matrix

12.10 bml_trace_m Module Reference

Matrix trace.

Functions/Subroutines

- double precision function, public bml_trace (a)

  Calculate the trace of a matrix.

12.10.1 Detailed Description

Matrix trace.

12.10.2 Function/Subroutine Documentation

12.10.2.1 double precision function, public bml_trace_m::bml_trace (class(bml_matrix_t), intent(in) *a*)

Calculate the trace of a matrix.

$\leftarrow \mathrm{Tr}\left[A\right]$

Parameters

a	The matrix.

12.11 bml_transpose_m Module Reference

Transpose functions.

Functions/Subroutines

- subroutine, public bml_transpose (a, a_t)

  Return the transpose of a matrix.

12.11.1 Detailed Description

Transpose functions.

12.11.2 Function/Subroutine Documentation

12.11.2.1 subroutine, public bml_transpose_m::bml_transpose (type(bml_matrix_t), intent(in) *a*, type(bml_matrix_t), intent(inout) *a_t*)

Return the transpose of a matrix.

Parameters

a	The matrix.
a_t	The transpose.

12.12 bml_types_m Module Reference

The basic bml types.

Data Types

- type bml_matrix_t

  The bml matrix type.
- type bml_vector_t

  The bml vector type.

Variables

- character(len=∗), parameter bml_matrix_dense = "dense"

  The bml-dense matrix type identifier.
- character(len=∗), parameter bml_matrix_ellpack = "ellpack"

  The bml-ellpack matrix type identifier.
- character(len=∗), parameter bml_precision_single_real = "single_real"

  The single precision identifier.
- character(len=∗), parameter bml_precision_double_real = "double_real"

  The double-precision identifier.
- character(len=∗), parameter bml_precision_single_complex = "single_complex"

  The single precision identifier.
- character(len=∗), parameter bml_precision_double_complex = "double_complex"

  The double-precision identifier.

12.12.1 Detailed Description

The basic bml types.

12.13 bml_utilities_m Module Reference

Utility matrix functions.

Functions/Subroutines

- subroutine bml_print_bml_vector (tag, v, i_l, i_u)

  Print a bml vector.

12.13.1 Detailed Description

Utility matrix functions.

12.13.2 Function/Subroutine Documentation

12.13.2.1 subroutine bml_utilities_m::bml_print_bml_vector (character(len=∗), intent(in) *tag,* type(bml_vector_t), intent(in), target *v,* integer, intent(in) *i_l,* integer, intent(in) *i_u*)

Print a bml vector.

Parameters

tag	A string to print before the matrix.
v	The vector.
i_l	The lower row bound.
i_u	The upper row bound.

12.14 bml_utilities_matrix_type_m Module Reference

Utility matrix functions.

12.14.1 Detailed Description

Utility matrix functions.

Chapter 13

Class Documentation

13.1 bml_types_m::bml_matrix_t Type Reference

The bml matrix type.

Public Attributes

- type(c_ptr) ptr = C_NULL_PTR
  The C pointer to the matrix.

13.1.1 Detailed Description

The bml matrix type.

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

- /home/nbock/Work/bml/src/Fortran-interface/bml_types_m.F90

13.2 bml_types_m::bml_vector_t Type Reference

The bml vector type.

Public Attributes

- type(c_ptr) ptr = C_NULL_PTR
  The C pointer to the vector.

13.2.1 Detailed Description

The bml vector type.

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

- /home/nbock/Work/bml/src/Fortran-interface/bml_types_m.F90

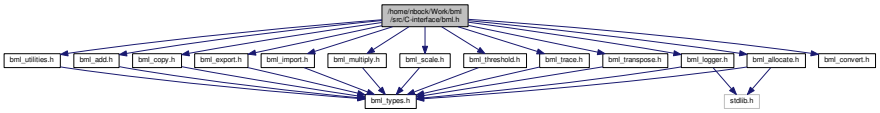
Chapter 14

File Documentation

14.1 /home/nbock/Work/bml/src/C-interface/bml.h File Reference

```
#include "bml_add.h"
#include "bml_allocate.h"
#include "bml_convert.h"
#include "bml_copy.h"
#include "bml_export.h"
#include "bml_import.h"
#include "bml_logger.h"
#include "bml_multiply.h"
#include "bml_scale.h"
#include "bml_threshold.h"
#include "bml_trace.h"
#include "bml_transpose.h"
#include "bml_utilities.h"
```

Include dependency graph for bml.h:



14.1.1 Detailed Description

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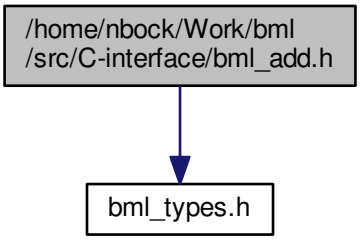
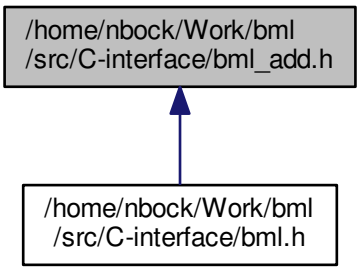
14.2 /home/nbock/Work/bml/src/C-interface/bml_add.h File Reference

```
#include "bml_types.h"
```

Include dependency graph for bml_add.h:



This graph shows which files directly or indirectly include this file:



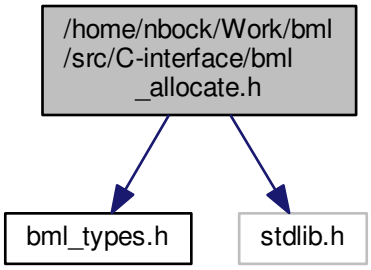
Functions

- void bml_add (bml_matrix_t *A, const bml_matrix_t *B, const double alpha, const double beta, const double threshold)
- void bml_add_identity (bml_matrix_t *A, const double beta, const double threshold)

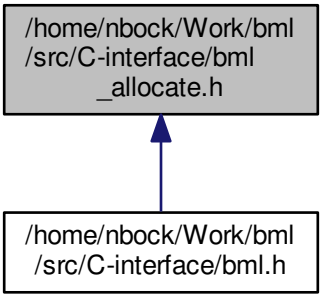
14.3 /home/nbock/Work/bml/src/C-interface/bml_allocate.h File Reference

```
#include "bml_types.h"
#include <stdlib.h>
```

Include dependency graph for bml_allocate.h:



This graph shows which files directly or indirectly include this file:

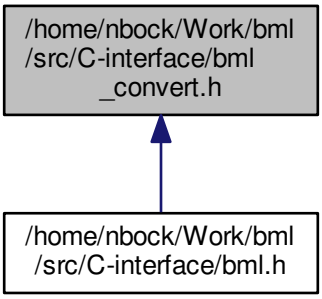


Functions

- void * bml_allocate_memory (const size_t s)
- void bml_free_memory (void *ptr)
- void bml_deallocate (bml_matrix_t **A)
- bml_matrix_t * bml_zero_matrix (const bml_matrix_type_t matrix_type, const bml_matrix_precision_t matrix_precision, const int N, const int M)
- bml_matrix_t * bml_random_matrix (const bml_matrix_type_t matrix_type, const bml_matrix_precision_t matrix_precision, const int N, const int M)
- bml_matrix_t * bml_identity_matrix (const bml_matrix_type_t matrix_type, const bml_matrix_precision_t matrix_precision, const int N, const int M)

14.4 /home/nbock/Work/bml/src/C-interface/bml_convert.h File Reference

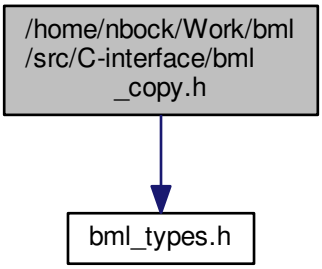
This graph shows which files directly or indirectly include this file:



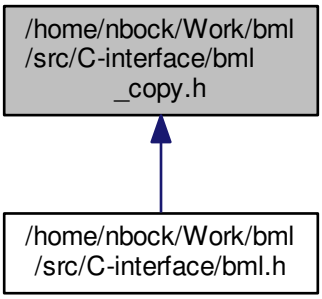
14.5 /home/nbock/Work/bml/src/C-interface/bml_copy.h File Reference

```
#include "bml_types.h"
```

Include dependency graph for bml_copy.h:



This graph shows which files directly or indirectly include this file:



Functions

- bml_matrix_t * bml_copy_new (const bml_matrix_t *A)
- void bml_copy (const bml_matrix_t *A, bml_matrix_t *B)

14.5.1 Function Documentation

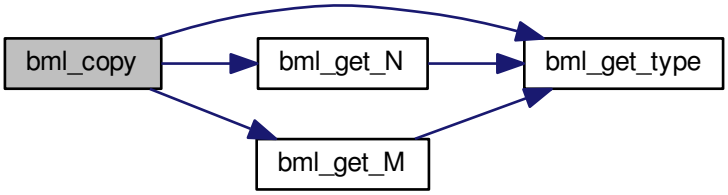
14.5.1.1 void bml_copy (const bml_matrix_t * *A*, bml_matrix_t * *B*)

Copy a matrix.

Parameters

A	Matrix to copy
B	Copy of Matrix A

Here is the call graph for this function:



14.5.1.2 bml_matrix_t* bml_copy_new (const bml_matrix_t * *A*)

Copy a matrix - result is a new matrix.

Parameters

A	Matrix to copy

Returns

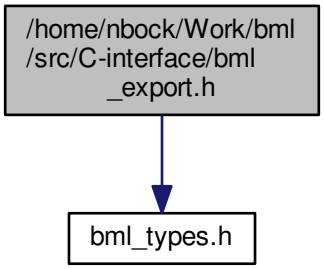
A Copy of A

Here is the call graph for this function:

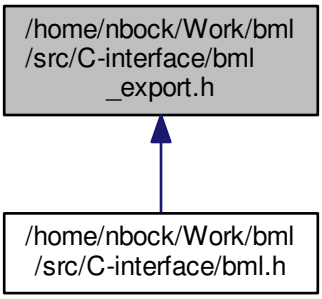
14.6 /home/nbock/Work/bml/src/C-interface/bml_export.h File Reference

```
#include "bml_types.h"
```

Include dependency graph for bml_export.h:



This graph shows which files directly or indirectly include this file:



Functions

- void * bml_convert_to_dense (const bml_matrix_t *A)
- void * bml_export_to_dense (const bml_matrix_t *A)

14.6.1 Function Documentation

14.6.1.1 void* bml_convert_to_dense (const bml_matrix_t * *A*)

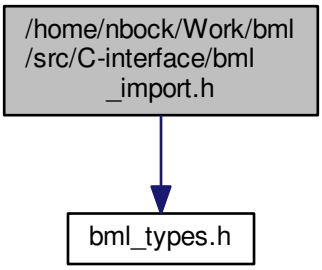
Deprecated Deprecated API.

Here is the call graph for this function:

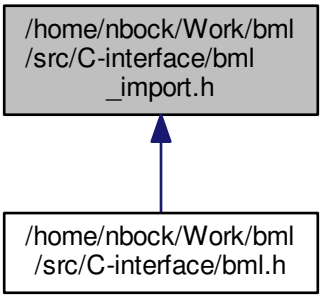
14.7 /home/nbock/Work/bml/src/C-interface/bml_import.h File Reference

```
#include "bml_types.h"
```

Include dependency graph for bml_import.h:



This graph shows which files directly or indirectly include this file:



Functions

- bml_matrix_t * bml_import_from_dense (const bml_matrix_type_t matrix_type, const bml_matrix_precision_t matrix_precision, const int N, const void *A, const double threshold, const int M)
- bml_matrix_t * bml_convert_from_dense (const bml_matrix_type_t matrix_type, const bml_matrix_precision_t matrix_precision, const int N, const void *A, const double threshold, const int M)

14.7.1 Function Documentation

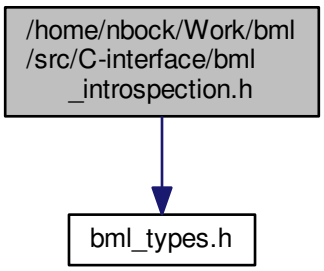
14.7.1.1 bml_matrix_t* bml_convert_from_dense (const bml_matrix_type_t *matrix_type*, const bml_matrix_precision_t *matrix_precision*, const int *N*, const void * *A*, const double *threshold*, const int *M*)

Deprecated Deprecated API.

Here is the call graph for this function:

14.8 /home/nbock/Work/bml/src/C-interface/bml_introspection.h File Reference

`#include "bml_types.h"`
Include dependency graph for bml_introspection.h:



Functions

- bml_matrix_type_t bml_get_type (const bml_matrix_t ∗A)
- bml_matrix_precision_t bml_get_precision (const bml_matrix_t ∗A)
- int bml_get_N (const bml_matrix_t ∗A)
- int bml_get_M (const bml_matrix_t ∗A)
- int bml_get_row_bandwidth (const bml_matrix_t ∗A, const int i)
- int bml_get_bandwidth (const bml_matrix_t ∗A)

14.8.1 Function Documentation

14.8.1.1 int bml_get_bandwidth (const bml_matrix_t ∗ *A*)

Return the bandwidth of a matrix.

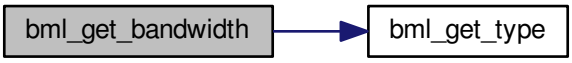
Parameters

A	The bml matrix.

Returns

The bandwidth of row i.

Here is the call graph for this function:



14.8.1.2 int bml_get_M (const bml_matrix_t * A)

Return the matrix parameter M.

Parameters

A	The matrix.

Returns

The matrix parameter M.

Here is the call graph for this function:

Here is the caller graph for this function:

14.8.1.3 int bml_get_N (const bml_matrix_t * A)

Return the matrix size.

Parameters

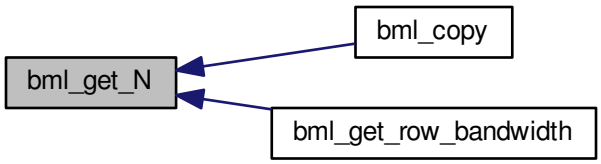
A	The matrix.

Returns

The matrix size.

Here is the call graph for this function:

Here is the caller graph for this function:



14.8.1.4 bml_matrix_precision_t bml_get_precision (const bml_matrix_t * *A*)

Return the matrix precision.

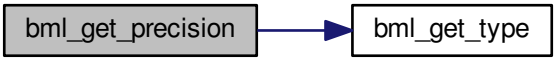
Parameters

A	The matrix.

Returns

The matrix precision.

Here is the call graph for this function:



14.8.1.5 int bml_get_row_bandwidth (const bml_matrix_t * A, const int i)

Return the bandwidth of a row in the matrix.

Parameters

A	The bml matrix.
i	The row index.

Returns

The bandwidth of row i.

Here is the call graph for this function:

14.8.1.6 bml_matrix_type_t bml_get_type (const bml_matrix_t * A)

Returns the matrix type.

If the matrix is not initialized yet, a type of "unitialized" is returned.

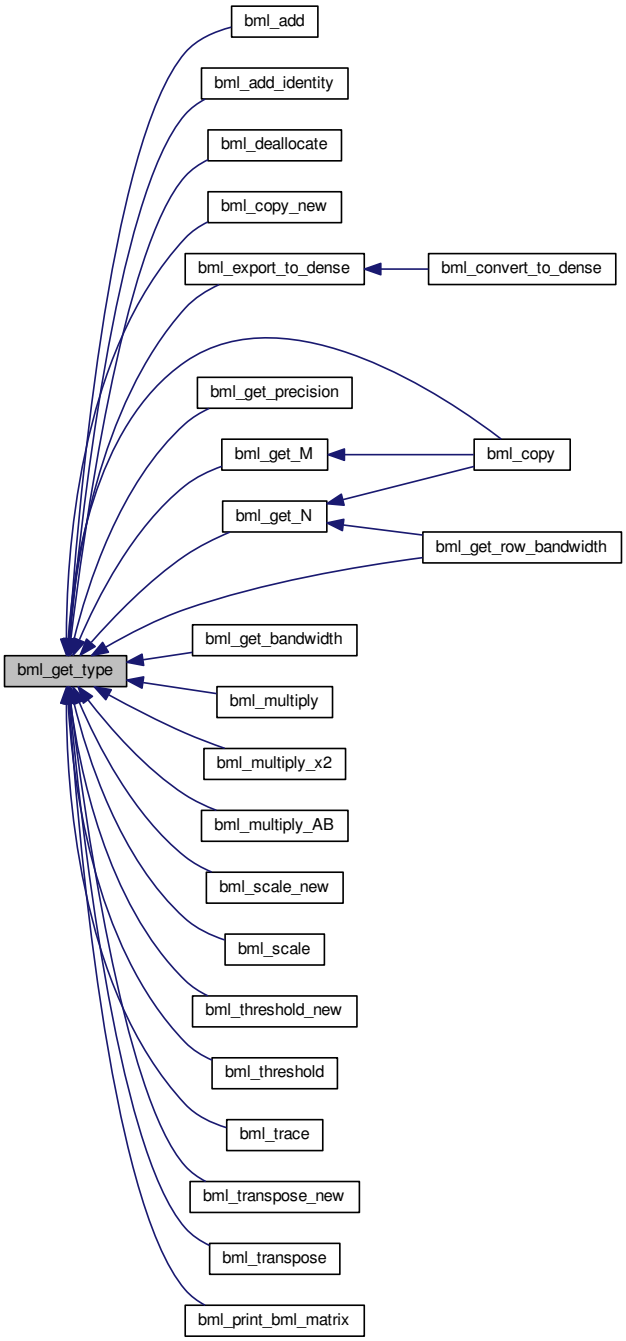
Parameters

A	The matrix.

Returns

The matrix type.

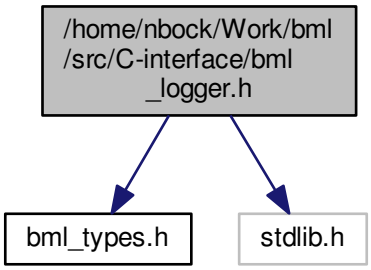
Here is the caller graph for this function:



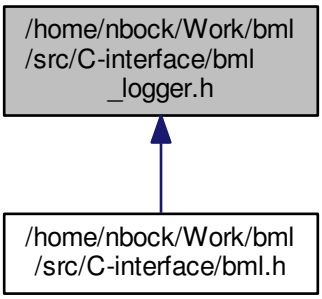
14.9 /home/nbock/Work/bml/src/C-interface/bml_logger.h File Reference

```
#include "bml_types.h"
#include <stdlib.h>
```

Include dependency graph for bml_logger.h:



This graph shows which files directly or indirectly include this file:



Macros

- #define LOG_DEBUG(format, ...) bml_log_location(BML_LOG_DEBUG, __FILE__, __LINE__, format, ##↩ __VA_ARGS__)
- #define LOG_INFO(format, ...) bml_log(BML_LOG_INFO, format, ##__VA_ARGS__)
- #define LOG_WARN(format, ...) bml_log_location(BML_LOG_WARNING, __FILE__, __LINE__, format, ##__VA_ARGS__)
- #define LOG_ERROR(format, ...) bml_log_location(BML_LOG_ERROR, __FILE__, __LINE__, format, ##↩ __VA_ARGS__)

Enumerations

- enum bml_log_level_t { BML_LOG_DEBUG, BML_LOG_INFO, BML_LOG_WARNING, BML_LOG_ERROR }

Functions

- void bml_log (const bml_log_level_t log_level, const char *format,...)
- void bml_log_location (const bml_log_level_t log_level, const char *filename, const int linenumber, const char *format,...)

14.9.1 Macro Definition Documentation

14.9.1.1 #define LOG_DEBUG(*format, ...*) bml_log_location(BML_LOG_DEBUG, __FILE__, __LINE__, format, ##__VA_ARGS__)

Convenience macro to write a BML_LOG_DEBUG level message.

14.9.1.2 #define LOG_ERROR(*format, ...*) bml_log_location(BML_LOG_ERROR, __FILE__, __LINE__, format, ##__VA_ARGS__)

Convenience macro to write a BML_LOG_ERROR level message.

14.9.1.3 #define LOG_INFO(*format, ...*) bml_log(BML_LOG_INFO, format, ##__VA_ARGS__)

Convenience macro to write a BML_LOG_INFO level message.

14.9.1.4 #define LOG_WARN(*format, ...*) bml_log_location(BML_LOG_WARNING, __FILE__, __LINE__, format, ##__VA_ARGS__)

Convenience macro to write a BML_LOG_WARNING level message.

14.9.2 Enumeration Type Documentation

14.9.2.1 enum bml_log_level_t

The log-levels.

Enumerator

BML_LOG_DEBUG Debugging messages.

BML_LOG_INFO Info messages.

BML_LOG_WARNING Warning messages.

BML_LOG_ERROR Error messages.

14.9.3 Function Documentation

14.9.3.1 void bml_log (const bml_log_level_t *log_level,* const char * *format, ...*)

Log a message.

Parameters

log_level	The log level.

format	The format (as in printf()).

14.9.3.2 void bml_log_location (const bml_log_level_t *log_level*, const char * *filename*, const int *linenumber*, const char * *format*, ...)

Log a message with location, i.e. filename and linenumber..

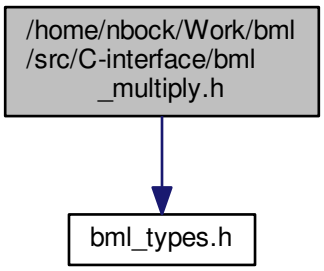
Parameters

log_level	The log level.
filename	The filename to log.
linenumber	The linenumber.
format	The format (as in printf()).

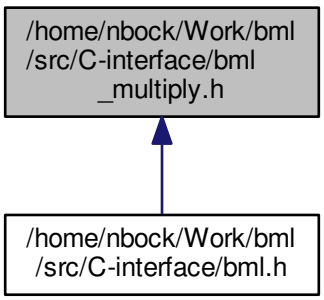
14.10 /home/nbock/Work/bml/src/C-interface/bml_multiply.h File Reference

```
#include "bml_types.h"
```

Include dependency graph for bml_multiply.h:



This graph shows which files directly or indirectly include this file:



Functions

- void bml_multiply (const bml_matrix_t *A, const bml_matrix_t *B, bml_matrix_t *C, const double alpha, const double beta, const double threshold)
- void bml_multiply_x2 (const bml_matrix_t *X, bml_matrix_t *X2, const double threshold)
- void bml_multiply_AB (const bml_matrix_t *A, const bml_matrix_t *B, bml_matrix_t *C, const double threshold)

14.10.1 Function Documentation

14.10.1.1 void bml_multiply (const bml_matrix_t * *A*, const bml_matrix_t * *B*, bml_matrix_t * *C*, const double *alpha*, const double *beta*, const double *threshold*)

Matrix multiply.

C = alpha * A * B + beat * C

Parameters

A	Matrix A
B	Matrix B
C	Matrix C
alpha	Scalar factor that multiplies A * B
beta	Scalar factor that multiplies C
threshold	Threshold for multiplication

Here is the call graph for this function:

14.10.1.2 void bml_multiply_AB (const bml_matrix_t * *A*, const bml_matrix_t * *B*, bml_matrix_t * *C*, const double *threshold*)

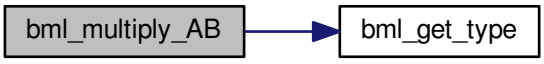
Matrix multiply.

C = A * B

Parameters

A	Matrix A
B	Matrix B
C	Matrix C
threshold	Threshold for multiplication

Here is the call graph for this function:



14.10.1.3 void bml_multiply_x2 (const bml_matrix_t * X, bml_matrix_t * X2, const double threshold)

Matrix multiply.

$X^2 \leftarrow X\,X$

Parameters

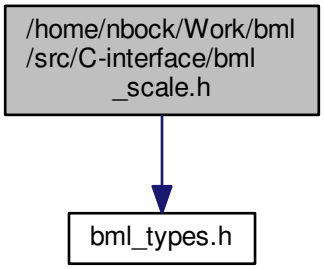
X	Matrix X
X2	MatrixX2
threshold	Threshold for multiplication

Here is the call graph for this function:

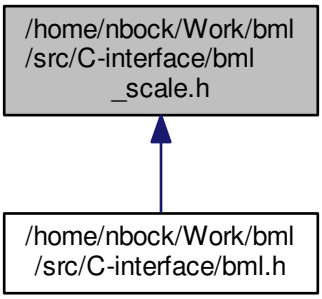
14.11 /home/nbock/Work/bml/src/C-interface/bml_scale.h File Reference

```
#include "bml_types.h"
```

Include dependency graph for bml_scale.h:



This graph shows which files directly or indirectly include this file:



Functions

- bml_matrix_t ∗ bml_scale_new (const double scale_factor, const bml_matrix_t ∗A)
- void bml_scale (const double scale_factor, const bml_matrix_t ∗A, bml_matrix_t ∗B)
- void **bml_scale_inplace** (const double scale_factor, bml_matrix_t ∗A)

14.11.1 Function Documentation

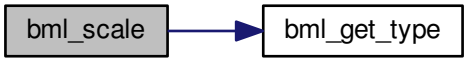
14.11.1.1 void bml_scale (const double *scale_factor,* const bml_matrix_t ∗ *A,* bml_matrix_t ∗ *B*)

Scale a matrix - resulting matrix exists.

Parameters

scale_factor	Scale factor for A
A	Matrix to scale
B	Scaled Matrix

Here is the call graph for this function:



14.11.1.2 bml_matrix_t∗ bml_scale_new (const double *scale_factor,* const bml_matrix_t ∗ *A*)

Scale a matrix - resulting matrix is new.

Parameters

scale_factor	Scale factor for A
A	Matrix to scale

Returns

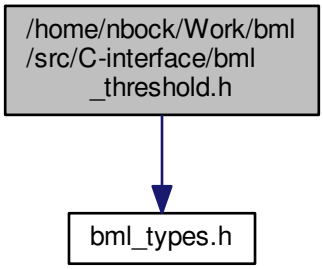
A Scaled Copy of A

Here is the call graph for this function:

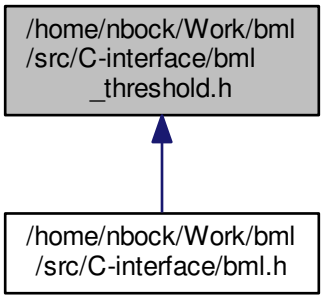
14.12 /home/nbock/Work/bml/src/C-interface/bml_threshold.h File Reference

```
#include "bml_types.h"
```

Include dependency graph for bml_threshold.h:



This graph shows which files directly or indirectly include this file:



Functions

- bml_matrix_t * bml_threshold_new (const bml_matrix_t *A, const double threshold)
- void bml_threshold (const bml_matrix_t *A, const double threshold)

14.12.1 Function Documentation

14.12.1.1 void bml_threshold (const bml_matrix_t * *A*, const double *threshold*)

Threshold matrix.

Parameters

A	Matrix to be thresholded
threshold	Threshold value

Returns

Thresholded A

Here is the call graph for this function:

14.12.1.2 bml_matrix_t* bml_threshold_new (const bml_matrix_t * *A*, const double *threshold*)

Threshold matrix.

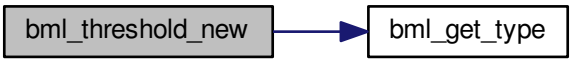
Parameters

A	Matrix to be thresholded
threshold	Threshold value

Returns

Thresholded A

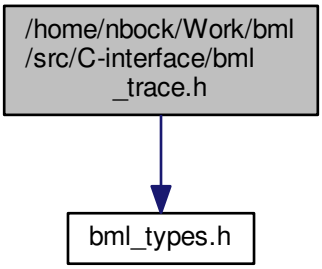
Here is the call graph for this function:



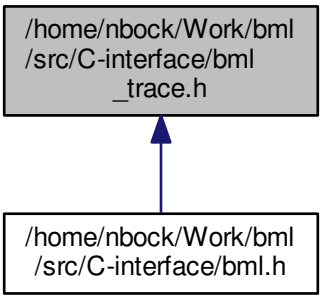
14.13 /home/nbock/Work/bml/src/C-interface/bml_trace.h File Reference

```
#include "bml_types.h"
```

Include dependency graph for bml_trace.h:



This graph shows which files directly or indirectly include this file:



Functions

- double bml_trace (const bml_matrix_t *A)

14.13.1 Function Documentation

14.13.1.1 double bml_trace (const bml_matrix_t * A)

Calculate trace of a matrix.

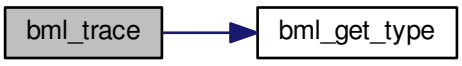
Parameters

A	Matrix tocalculate trace for

Returns

Trace of A

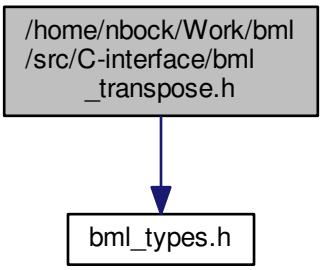
Here is the call graph for this function:



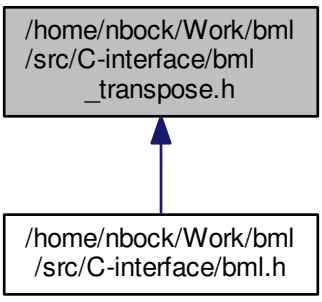
14.14 /home/nbock/Work/bml/src/C-interface/bml_transpose.h File Reference

```
#include "bml_types.h"
```

Include dependency graph for bml_transpose.h:



This graph shows which files directly or indirectly include this file:



Functions

- bml_matrix_t * bml_transpose_new (const bml_matrix_t *A)
- void bml_transpose (const bml_matrix_t *A)

14.14.1 Function Documentation

14.14.1.1 void bml_transpose (const bml_matrix_t * *A*)

Transpose matrix.

Parameters

A	Matrix to be transposed

Returns

Transposed A

Here is the call graph for this function:

14.14.1.2 bml_matrix_t* bml_transpose_new (const bml_matrix_t * *A*)

Transpose matrix.

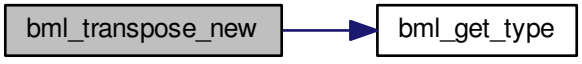
Parameters

A	Matrix to be transposed

Returns

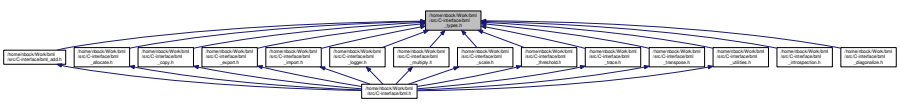
Transposed A

Here is the call graph for this function:



14.15 /home/nbock/Work/bml/src/C-interface/bml_types.h File Reference

This graph shows which files directly or indirectly include this file:



Typedefs

- typedef void bml_vector_t
- typedef void bml_matrix_t

Enumerations

- enum bml_matrix_type_t { type_uninitialized, dense, ellpack, csr }
- enum bml_matrix_precision_t { precision_uninitialized, single_real, double_real, single_complex, double_complex }

14.15.1 Typedef Documentation

14.15.1.1 typedef void bml_matrix_t

The matrix type.

14.15.1.2 typedef void bml_vector_t

The vector type.

14.15.2 Enumeration Type Documentation

14.15.2.1 enum bml_matrix_precision_t

The supported real precisions.

Enumerator

precision_uninitialized The matrix is not initialized.

single_real Matrix data is stored in single precision (float).

double_real Matrix data is stored in double precision (double).

single_complex Matrix data is stored in single-complex precision (float).

double_complex Matrix data is stored in double-complex precision (double).

14.15.2.2 enum bml_matrix_type_t

The supported matrix types.

Enumerator

type_uninitialized The matrix is not initialized.

dense Dense matrix.

ellpack ELLPACK matrix.

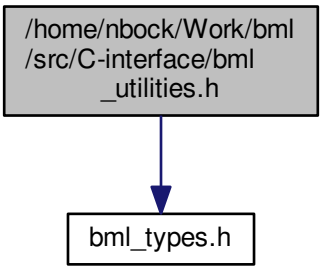
csr CSR matrix.

14.16 /home/nbock/Work/bml/src/C-interface/bml_types_private.h File Reference

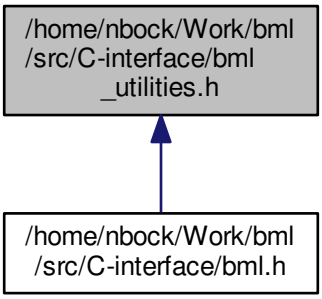
14.17 /home/nbock/Work/bml/src/C-interface/bml_utilities.h File Reference

```
#include "bml_types.h"
```

Include dependency graph for bml_utilities.h:



This graph shows which files directly or indirectly include this file:



Functions

- void bml_print_dense_matrix (const int N, bml_matrix_precision_t matrix_precision, const void ∗A, const int i_l, const int i_u, const int j_l, const int j_u)
- void bml_print_dense_vector (const int N, bml_matrix_precision_t matrix_precision, const void ∗v, const int i_l, const int i_u)
- void bml_print_bml_vector (const bml_vector_t ∗v, const int i_l, const int i_u)
- void bml_print_bml_matrix (const bml_matrix_t ∗A, const int i_l, const int i_u, const int j_l, const int j_u)

14.17.1 Function Documentation

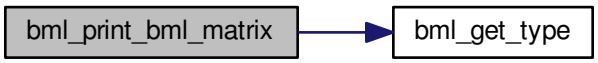
14.17.1.1 void bml_print_bml_matrix (const bml_matrix_t * A, const int i_l, const int i_u, const int j_l, const int j_u)

Print a dense matrix.

Parameters

N	The number of rows/columns.
matrix_precision	The real precision.
A	The matrix.
i_l	The lower row index.
i_u	The upper row index.
j_l	The lower column index.
j_u	The upper column index.

Here is the call graph for this function:



14.17.1.2 void bml_print_bml_vector (const bml_vector_t * v, const int i_l, const int i_u)

Print a bml vector.

Parameters

N	The number of rows/columns.
matrix_precision	The real precision.
v	The vector.
i_l	The lower row index.
i_u	The upper row index.

14.17.1.3 void bml_print_dense_matrix (const int N, bml_matrix_precision_t matrix_precision, const void * A, const int i_l, const int i_u, const int j_l, const int j_u)

Print a dense matrix.

Parameters

N	The number of rows/columns.
matrix_precision	The real precision.
A	The matrix.
i_l	The lower row index.
i_u	The upper row index.
j_l	The lower column index.
j_u	The upper column index.

14.17.1.4 void bml_print_dense_vector (const int N, bml_matrix_precision_t matrix_precision, const void * v, const int i_l, const int i_u)

Print a dense vector.

Parameters

N	The number of rows/columns.
matrix_precision	The real precision.
v	The vector.
i_l	The lower row index.
i_u	The upper row index.

14.18 /home/nbock/Work/bml/src/C-interface/macros.h File Reference

Macros

- #define ROWMAJOR(i, j, N) (i) ∗ (N) + (j)
- #define COLMAJOR(i, j, N) (i) + (N) ∗ (j)

14.18.1 Macro Definition Documentation

14.18.1.1 #define COLMAJOR(*i, j, N*) (i) + (N) ∗ (j)

Column major access.

14.18.1.2 #define ROWMAJOR(*i, j, N*) (i) ∗ (N) + (j)

Row major access.

Index