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

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

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

Back to the main page.

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);
```

Back to the main page.

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)
```

Back to the main page.

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
```

Back to the main page.

Chapter 6

Module Index

6.1 Modules

Here is a list of all modules:

Chapter 7

Namespace Index

7.1 Namespace List

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

Chapter 8

Class Index

8.1 Class List

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

Chapter 9

File Index

9.1 File List

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

Chapter 10

Module Documentation

10.1 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)

10.1.1 Detailed Description

10.1.2 Function Documentation

10.1.2.1 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.

10.1.2.2 void bml_deallocate (bml_matrix_t ** *A*)

Deallocate a matrix.

Parameters

A	The matrix.

Here is the call graph for this function:

10.1.2.3 void bml_free_memory (void * *ptr*)

Deallocate a chunk of memory.

Parameters

ptr	A pointer to the previously allocated chunk.

10.1.2.4 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.

10.1.2.5 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.

10.1.2.6 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.

10.2 Add Functions (C interface)

Functions

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

10.2.1 Detailed Description

10.2.2 Function Documentation

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

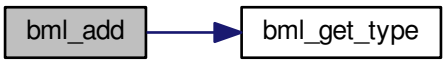
Matrix addition.

A = 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:



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

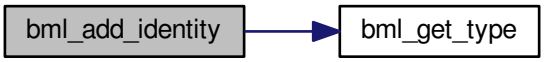
Matrix addition.

A = A + beta * I

Parameters

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

Here is the call graph for this function:



10.3 Converting between Matrix Formats (C interface)

Functions

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

10.3.1 Detailed Description

10.3.2 Function Documentation

10.3.2.1 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*)

Convert a dense matrix into a bml 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

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

Convert a bml matrix into a dense 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);
```

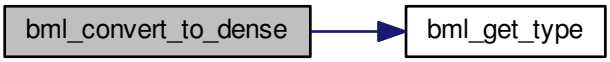
Parameters

A	The bml matrix

Returns

The dense matrix

Here is the call graph for this function:



10.4 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.

10.4.1 Detailed Description

10.4.2 Function Documentation

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

Deallocate a matrix.

Parameters

a	The matrix.

10.4.2.2 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.

10.4.2.3 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.

10.4.2.4 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.

10.5 Add Functions (Fortran interface)

10.5.1 Detailed Description

10.6 Converting between Matrix Formats (Fortran interface)

Functions

- subroutine bml_convert_m::bml_convert_from_dense_double (matrix_type, matrix_precision, 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, matrix_precision, 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, matrix_precision, 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.

10.6.1 Detailed Description

10.6.2 Function Documentation

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

Convert a dense matrix into a bml matrix.

Parameters

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

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

Convert a dense matrix into a bml matrix.

Parameters

matrix_type	The matrix type

matrix_precision	The matrix precision
a_dense	The dense matrix
a	The bml matrix
threshold	The matrix element magnited threshold
m	the extra arg

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

10.6.2.4 subroutine bml_convert_m::bml_convert_to_dense_double (type(**bml_matrix_t**), intent(in) *a,* double precision, dimension(:, :), intent(out), pointer *a_dense*)

Convert a matrix into a dense matrix.

Parameters

a	The bml matrix
a_dense	The dense matrix

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

Convert a matrix into a dense matrix.

Parameters

a	The bml matrix
a_dense	The dense matrix

10.6.2.6 subroutine bml_convert_m::bml_convert_to_dense_single (type(**bml_matrix_t**), intent(in) *a,* real, dimension(:, :), intent(out), pointer *a_dense*)

Convert a matrix into a dense matrix.

Parameters

a	The bml matrix
a_dense	The dense matrix

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

Convert a matrix into a dense matrix.

Parameters

a	The bml matrix
a_dense	The dense matrix

Chapter 11

Namespace Documentation

11.1 bml Module Reference

Main matrix library module.

11.1.1 Detailed Description

Main matrix library module.

Use this modules in order to use the library.

11.2 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.

11.2.1 Detailed Description

Matrix allocation functions.

11.3 bml_copy_m Module Reference

Copy operations on matrices.

Functions/Subroutines

- subroutine bml_copy (a, b)

  Copy (assign) a matrix to another one.

11.3.1 Detailed Description

Copy operations on matrices.

11.3.2 Function/Subroutine Documentation

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

Copy (assign) a matrix to another one.

This operation performs $B \leftarrow A$.

Parameters

a	Matrix to copy.
b	Matrix to copy to.

11.4 bml_diagonalize_m Module Reference

Matrix diagonalization functions.

Functions/Subroutines

- subroutine bml_diagonalize (a, eigenvectors, eigenvalues)

  Diagonalize a matrix.

11.4.1 Detailed Description

Matrix diagonalization functions.

11.4.2 Function/Subroutine Documentation

11.4.2.1 subroutine bml_diagonalize_m::bml_diagonalize (type(bml_matrix_t), intent(in) *a,* type(bml_matrix_t), intent(inout) *eigenvectors,* type(bml_vector_t), intent(inout) *eigenvalues*)

Diagonalize a matrix.

Parameters

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

11.5 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.

11.5.1 Detailed Description

A module for error handling in bml.

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11.5.2 Function/Subroutine Documentation

11.5.2.1 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.

11.5.2.2 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.

11.5.2.3 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.

11.6 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_precision_single_enum_id** = 0
- integer, parameter **bml_matrix_precision_double_enum_id** = 1

11.6.1 Detailed Description

Interface module.

11.6.2 Function/Subroutine Documentation

11.6.2.1 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.

11.7 bml_introspection_m Module Reference

Introspection procedures.

Functions/Subroutines

- integer function, public bml_get_size (a)

  Return the matrix size.

- integer function, public bml_get_bandwidth (a, i)

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

11.7.1 Detailed Description

Introspection procedures.

11.7.2 Function/Subroutine Documentation

11.7.2.1 integer function, public bml_introspection_m::bml_get_bandwidth (type(bml_matrix_t), intent(in) *a*, integer, intent(in) *i*)

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

Parameters

a	The matrix.
i	The row.

Returns

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

11.7.2.2 integer function, public bml_introspection_m::bml_get_size (type(bml_matrix_t), intent(in) *a*)

Return the matrix size.

Parameters

a	The matrix.

Returns

The matrix size.

11.8 bml_multiply_m Module Reference

Matrix multiplication.

Functions/Subroutines

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

  Multiply two matrices.

11.8.1 Detailed Description

Matrix multiplication.

11.8.2 Function/Subroutine Documentation

11.8.2.1 subroutine 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.

11.9 bml_scale_m Module Reference

Matrix scaling for matrices.

Functions/Subroutines

- subroutine scale_two (alpha, a, c)

  Scale a bml matrix.

11.9.1 Detailed Description

Matrix scaling for matrices.

11.9.2 Function/Subroutine Documentation

11.9.2.1 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

11.10 bml_trace_m Module Reference

Matrix trace.

Functions/Subroutines

- double precision function bml_trace (a)

  Calculate the trace of a matrix.

11.10.1 Detailed Description

Matrix trace.

11.10.2 Function/Subroutine Documentation

11.10.2.1 double precision function 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.

11.11 bml_transpose_m Module Reference

Transpose functions.

Functions/Subroutines

- subroutine bml_transpose (a, a_t)

  Return the transpose of a matrix.

11.11.1 Detailed Description

Transpose functions.

11.11.2 Function/Subroutine Documentation

11.11.2.1 subroutine 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.

11.12 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 = "single-precision"

  The single precision identifier.
- character(len=∗), parameter bml_precision_double = "double-precision"

  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.

11.12.1 Detailed Description

The basic bml types.

11.13 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.

11.13.1 Detailed Description

Utility matrix functions.

11.13.2 Function/Subroutine Documentation

11.13.2.1 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.

11.14 bml_utilities_matrix_type_m Module Reference

Utility matrix functions.

11.14.1 Detailed Description

Utility matrix functions.

Chapter 12

Class Documentation

12.1 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.

12.1.1 Detailed Description

The bml matrix type.

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

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

12.2 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.

12.2.1 Detailed Description

The bml vector type.

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

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

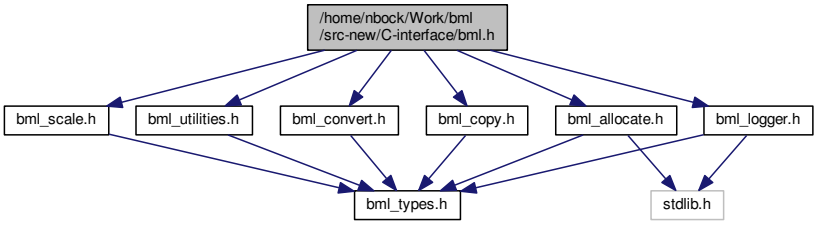
Chapter 13

File Documentation

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

```
#include "bml_allocate.h"
#include "bml_convert.h"
#include "bml_copy.h"
#include "bml_logger.h"
#include "bml_scale.h"
#include "bml_utilities.h"
```

Include dependency graph for bml.h:



13.1.1 Detailed Description

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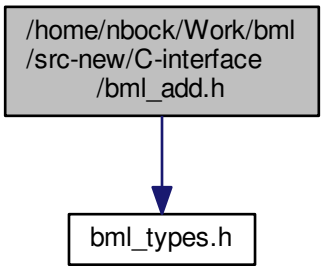
13.2 /home/nbock/Work/bml/src-new/C-interface/bml_add.h File Reference

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

Include dependency graph for bml_add.h:



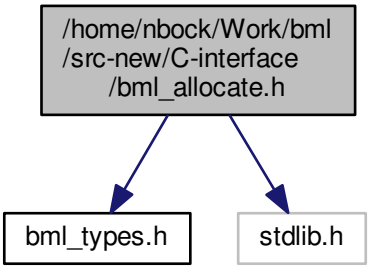
Functions

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

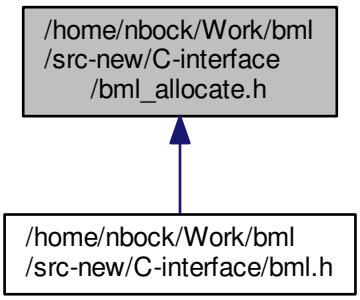
13.3 /home/nbock/Work/bml/src-new/C-interface/bml_allocate.h File Reference

```
#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:



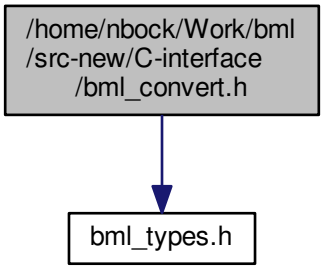
Functions

- 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)

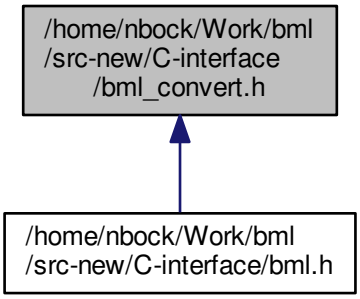
13.4 /home/nbock/Work/bml/src-new/C-interface/bml_convert.h File Reference

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

Include dependency graph for bml_convert.h:



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



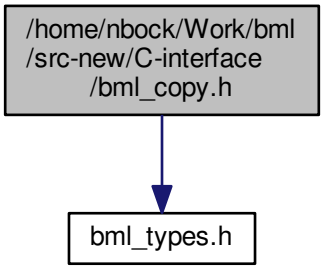
Functions

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

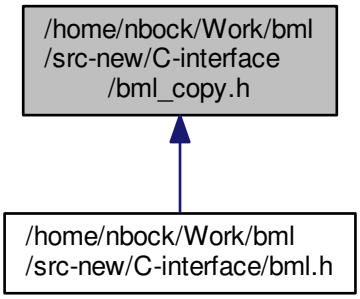
13.5 /home/nbock/Work/bml/src-new/C-interface/bml_copy.h File Reference

```
#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, const bml_matrix_t *B)

13.5.1 Function Documentation

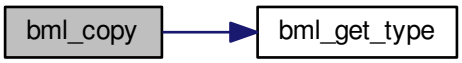
13.5.1.1 void bml_copy (const bml_matrix_t * *A*, const bml_matrix_t * *B*)

Copy a matrix.

Parameters

A	Matrix to copy
B	Copy of Matrix A

Here is the call graph for this function:



13.5.1.2 bml_matrix_t* bml_copy_new (const bml_matrix_t * *A*)

Copy a matrix - result is a new matrix.

Parameters

A	Matrix to copy

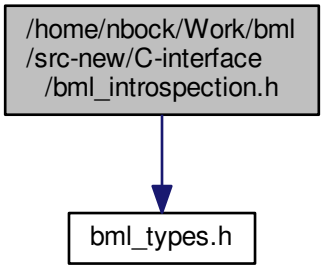
Returns

A Copy of A

Here is the call graph for this function:

13.6 /home/nbock/Work/bml/src-new/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)
- int bml_get_size (const bml_matrix_t *A)

13.6.1 Function Documentation

13.6.1.1 int bml_get_size (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:

13.6.1.2 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.

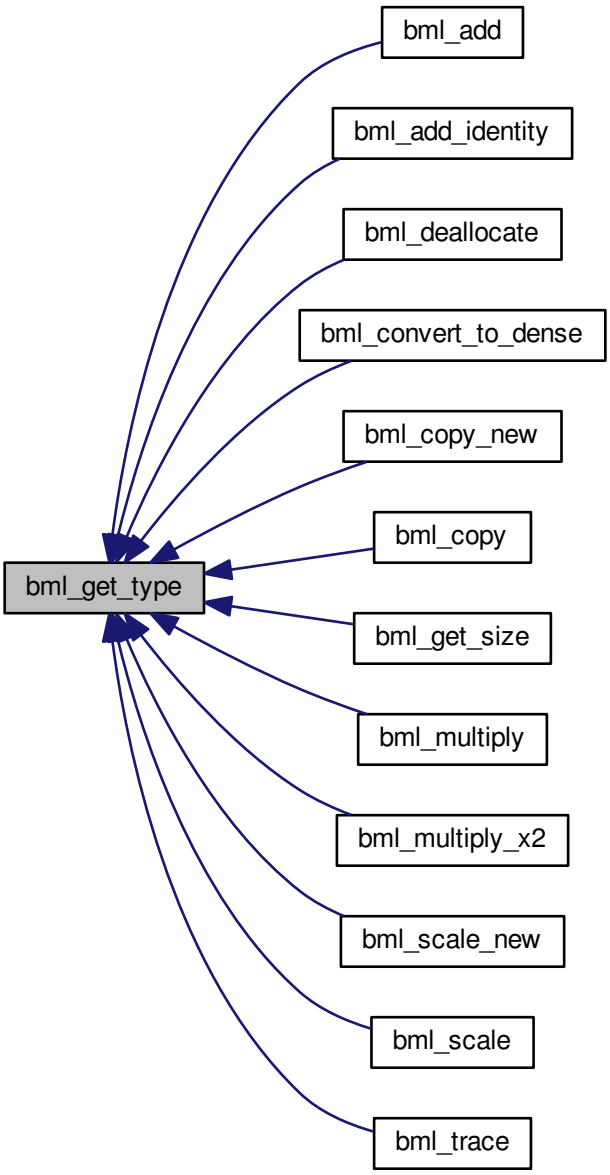
Parameters

A	The matrix.

Returns

The matrix type.

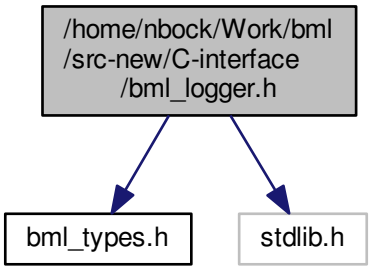
Here is the caller graph for this function:



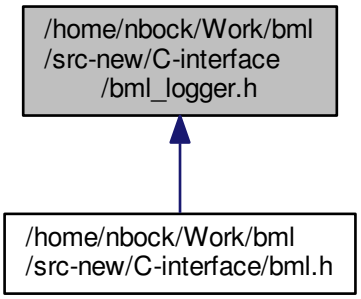
13.7 /home/nbock/Work/bml/src-new/C-interface/bml_logger.h File Reference

```
#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,...)

13.7.1 Macro Definition Documentation

13.7.1.1 #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.

13.7.1.2 #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.

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

Convenience macro to write a BML_LOG_INFO level message.

13.7.1.4 #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.

13.7.2 Enumeration Type Documentation

13.7.2.1 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.

13.7.3 Function Documentation

13.7.3.1 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()).

13.7.3.2 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..

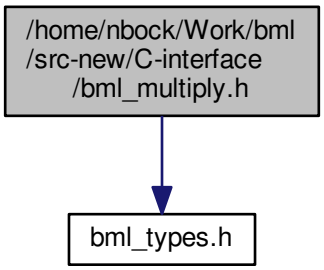
Parameters

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

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

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

Include dependency graph for bml_multiply.h:



Functions

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

13.8.1 Function Documentation

13.8.1.1 void bml_multiply (const bml_matrix_t * *A*, const bml_matrix_t * *B*, const 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:

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

Matrix multiply.

X2 = X ∗ X

Parameters

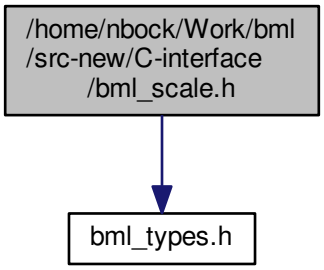
X	Matrix X
X2	MatrixX2
trX	Trace of X
trX2	Trace of X2
threshold	Threshold for multiplication

Here is the call graph for this function:

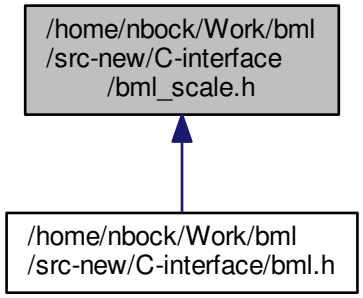
13.9 /home/nbock/Work/bml/src-new/C-interface/bml_scale.h File Reference

```
#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, const bml_matrix_t ∗B)

13.9.1 Function Documentation

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

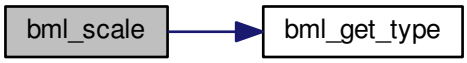
Scale a matrix - resulting matrix exists.

Parameters

scale_factor	Scale factor for A

A	Matrix to scale
B	Scaled Matrix

Here is the call graph for this function:



13.9.1.2 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

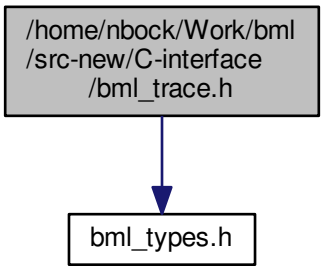
A Scaled Copy of A

Here is the call graph for this function:

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

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

Include dependency graph for bml_trace.h:



Functions

- double bml_trace (const bml_matrix_t *A)

13.10.1 Function Documentation

13.10.1.1 double bml_trace (const bml_matrix_t * A)

Calculate trace of a matrix.

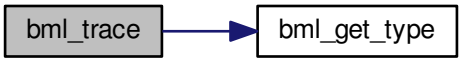
Parameters

A	Matrix tocalculate trace for

Returns

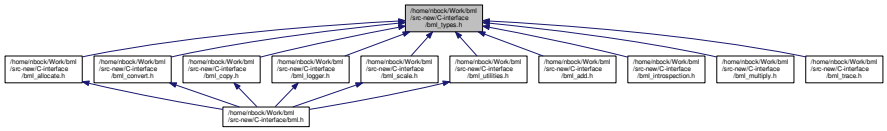
Trace of A

Here is the call graph for this function:



13.11 /home/nbock/Work/bml/src-new/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 { uninitialized, dense, ellpack, csr }
- enum bml_matrix_precision_t { single_real, double_real, single_complex, double_complex }

13.11.1 Typedef Documentation

13.11.1.1 typedef void bml_matrix_t

The matrix type.

13.11.1.2 typedef void bml_vector_t

The vector type.

13.11.2 Enumeration Type Documentation

13.11.2.1 enum bml_matrix_precision_t

The supported real precisions.

Enumerator

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).

13.11.2.2 enum bml_matrix_type_t

The supported matrix types.

Enumerator

uninitialized The matrix is not initialized.

dense Dense matrix.

ellpack ELLPACK matrix.

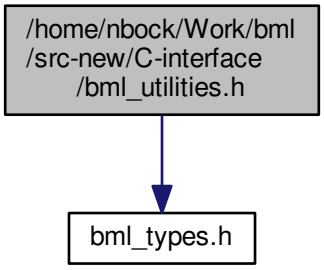
csr CSR matrix.

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

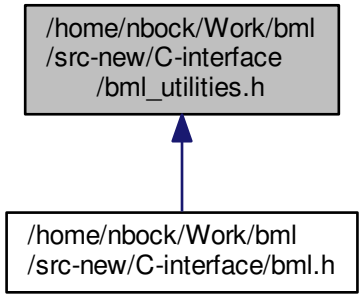
13.13 /home/nbock/Work/bml/src-new/C-interface/bml_utilities.h File Reference

```
#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_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)

13.13.1 Function Documentation

13.13.1.1 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.

13.13.1.2 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.

13.13.1.3 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.

Index