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## **Contents**

1	Basi	ic Matrix Library (bml)	1
	1.1	Usage Examples	1
	1.2	Modifying the library itself	1
	1.3	Planned Features	1
2	Futu	ure Plans	3
	2.1	Matrix Types	3
	2.2	Precisions	3
	2.3	Functions	3
3	C Us	sage	5
4	Forti	ran Usage	7
5	Deve	eloper Documentation	9
	5.1	Developer Suggested Workflow	9
	5.2	Coding Style	9
6	Mod	lule Index	11
	6.1	Modules	11
7	Nam	nespace Index	13
	7.1	Namespace List	13
8	Clas	es Index	15
	8.1	Class List	15
9	File	Index	17
	9.1	File List	17
10	Mod	lule Documentation	19
	10.1	Allocation and Deallocation Functions (C interface)	19
		10.1.1 Detailed Description	19
		10.1.2 Function Documentation	19
		10.1.2.1 bml_allocate_memory	19

iv CONTENTS

			10.1.2.2	bml_deallocate	19
			10.1.2.3	bml_free_memory	20
			10.1.2.4	bml_identity_matrix	20
			10.1.2.5	bml_random_matrix	20
			10.1.2.6	bml_zero_matrix	21
	10.2	Add Fu	ınctions (C	Cinterface)	22
		10.2.1	Detailed	Description	22
		10.2.2	Function	Documentation	22
			10.2.2.1	bml_add	22
			10.2.2.2	bml_add_identity	22
	10.3	Conver	rting betwe	een Matrix Formats (C interface)	24
		10.3.1	Detailed	Description	24
		10.3.2	Function	Documentation	24
			10.3.2.1	bml_convert_from_dense	24
			10.3.2.2	bml_convert_to_dense	24
	10.4	Allocat	ion and De	eallocation Functions (Fortran interface)	26
		10.4.1	Detailed	Description	26
		10.4.2	Function	Documentation	26
			10.4.2.1	bml_deallocate	26
			10.4.2.2	bml_identity_matrix	26
			10.4.2.3	bml_random_matrix	26
			10.4.2.4	bml_zero_matrix	27
	10.5	Add Fu	ınctions (F	ortran interface)	29
		10.5.1	Detailed	Description	29
	10.6	Conver	rting betwe	een Matrix Formats (Fortran interface)	30
		10.6.1	Detailed	Description	30
		10.6.2	Function	Documentation	30
			10.6.2.1	bml_convert_from_dense_double	30
			10.6.2.2	bml_convert_from_dense_double_complex	30
			10.6.2.3	bml_convert_from_dense_single_complex	31
			10.6.2.4	bml_convert_to_dense_double	31
			10.6.2.5	bml_convert_to_dense_double_complex	31
			10.6.2.6	bml_convert_to_dense_single	31
			10.6.2.7	bml_convert_to_dense_single_complex	31
11	Nam	espace	Documer	ntation	33
•		_		rence	33
				Description	33
	11.2			Module Reference	33
				Description	33

CONTENTS

11.3 bml_copy_m Module Reference	33
11.3.1 Detailed Description	34
11.3.2 Function/Subroutine Documentation	34
11.3.2.1 bml_copy	34
11.4 bml_diagonalize_m Module Reference	34
11.4.1 Detailed Description	34
11.4.2 Function/Subroutine Documentation	34
11.4.2.1 bml_diagonalize	34
11.5 bml_error_m Module Reference	34
11.5.1 Detailed Description	35
11.5.2 Function/Subroutine Documentation	35
11.5.2.1 bml_debug	35
11.5.2.2 bml_error	35
11.5.2.3 bml_warning	35
11.6 bml_interface_m Module Reference	36
11.6.1 Detailed Description	36
11.6.2 Function/Subroutine Documentation	36
11.6.2.1 get_enum_id	36
11.7 bml_introspection_m Module Reference	36
11.7.1 Detailed Description	37
11.7.2 Function/Subroutine Documentation	37
11.7.2.1 bml_get_bandwidth	37
11.7.2.2 bml_get_size	37
11.8 bml_multiply_m Module Reference	37
11.8.1 Detailed Description	37
11.8.2 Function/Subroutine Documentation	38
11.8.2.1 bml_multiply	38
11.9 bml_scale_m Module Reference	38
11.9.1 Detailed Description	38
11.9.2 Function/Subroutine Documentation	38
11.9.2.1 scale_two	38
11.10bml_trace_m Module Reference	38
11.10.1 Detailed Description	39
11.10.2 Function/Subroutine Documentation	39
11.10.2.1 bml_trace	39
11.11bml_transpose_m Module Reference	39
11.11.1 Detailed Description	39
11.11.2 Function/Subroutine Documentation	39
11.11.2.1 bml_transpose	39
11.12bml_types_m Module Reference	39

vi CONTENTS

		11.12.1	Detailed D	Description	 	 	40
	11.13			odule Reference			40
				Description			40
		11.13.2	2 Function/S	Subroutine Documentation	 	 	40
			11.13.2.1	bml_print_bml_vector	 	 	40
	11.14	1bml_uti	lities_matri	x_type_m Module Reference	 	 	41
		11.14.1	Detailed E	Description	 	 	41
12			nentation				43
	12.1			I_matrix_t Type Reference			43
				Description			43
	12.2			I_vector_t Type Reference			43
		12.2.1	Detailed L	Description	 • •	 • •	43
13	File I	Docume	entation				45
	13.1	/home/	nbock/Worl	x/bml/src-new/C-interface/bml.h File Reference	 	 	45
		13.1.1	Detailed D	Description	 	 	45
	13.2	/home/	nbock/Worl	x/bml/src-new/C-interface/bml_add.h File Reference	 	 	46
	13.3	/home/	nbock/Worl	k/bml/src-new/C-interface/bml_allocate.h File Reference	 	 	46
	13.4	/home/	nbock/Worl	x/bml/src-new/C-interface/bml_convert.h File Reference	 	 	47
	13.5	/home/	nbock/Worl	k/bml/src-new/C-interface/bml_copy.h File Reference	 	 	48
		13.5.1	Function I	Documentation	 	 	49
			13.5.1.1	bml_copy	 	 	49
			13.5.1.2	bml_copy_new	 	 	49
	13.6	/home/	nbock/Worl	k/bml/src-new/C-interface/bml_introspection.h File Reference	 	 	50
		13.6.1	Function I	Documentation	 	 	50
			13.6.1.1	bml_get_size	 	 	50
			13.6.1.2	bml_get_type	 	 	51
	13.7	/home/	nbock/Worl	x/bml/src-new/C-interface/bml_logger.h File Reference	 	 	52
		13.7.1	Macro De	finition Documentation	 	 	54
			13.7.1.1	LOG_DEBUG	 	 	54
			13.7.1.2	LOG_ERROR	 	 	54
			13.7.1.3	LOG_INFO	 	 	54
			13.7.1.4	LOG_WARN	 	 	54
		13.7.2	Enumerat	ion Type Documentation	 	 	54
			13.7.2.1	bml_log_level_t	 	 	54
		13.7.3		Documentation			54
				bml_log			54
				bml_log_location			55
	13.8			s/bml/src-new/C-interface/bml_multiply.h File Reference			55
		13.8.1	Function [	Documentation	 	 	55

CONTENTS vii

	13.8.1.1 bml_multiply	55
	13.8.1.2 bml_multiply_x2	56
13	3.9 /home/nbock/Work/bml/src-new/C-interface/bml_scale.h File Reference	56
	13.9.1 Function Documentation	57
	13.9.1.1 bml_scale	57
	13.9.1.2 bml_scale_new	58
13	3.10/home/nbock/Work/bml/src-new/C-interface/bml_trace.h File Reference	59
	13.10.1 Function Documentation	59
	13.10.1.1 bml_trace	59
13	3.11/home/nbock/Work/bml/src-new/C-interface/bml_types.h File Reference	60
	13.11.1 Typedef Documentation	60
	13.11.1.1 bml_matrix_t	60
	13.11.1.2 bml_vector_t	60
	13.11.2 Enumeration Type Documentation	60
	13.11.2.1 bml_matrix_precision_t	60
	13.11.2.2 bml_matrix_type_t	60
13	3.12/home/nbock/Work/bml/src-new/C-interface/bml_types_private.h File Reference	61
13	3.13/home/nbock/Work/bml/src-new/C-interface/bml_utilities.h File Reference	61
	13.13.1 Function Documentation	62
	13.13.1.1 bml_print_bml_matrix	62
	13.13.1.2 bml_print_bml_vector	62
	13.13.1.3 bml_print_dense_matrix	62
Index	<b>t</b>	63

## **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.

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```

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2	Basic Matrix Library (bml

## **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

4 Future Plans

- $\alpha A + \beta B$ : 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
  - Tr[A]: bml\_trace::bml\_trace
  - ${\rm Tr}[AB]$ : 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.

# C Usage

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

Back to the main page.

6 C Usage

## 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,  $100 \times 100$  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.

8 Fortran Usage

# **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.

## **Module Index**

### 6.1 Modules

Here	ic	а	lict	Ωf	all	modu	المو
пеге	15	а	IISL	ΟI	all	HIOUL	แยง

Allocation and Deallocation Functions (C interface)	19
Add Functions (C interface)	22
Converting between Matrix Formats (C interface)	24
Allocation and Deallocation Functions (Fortran interface)	26
Add Functions (Fortran interface)	29
Converting between Matrix Formats (Fortran interface)	30

12 **Module Index** 

# Namespace Index

### 7.1 Namespace List

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

Offi	
Main matrix library module	33
bml_allocate_m	
Matrix allocation functions	33
bml_copy_m	
Copy operations on matrices	33
bml_diagonalize_m	
Matrix diagonalization functions	34
bml_error_m	
A module for error handling in bml	34
bml_interface_m	
	36
bml_introspection_m	
Introspection procedures	36
bml_multiply_m	
Matrix multiplication	37
bml_scale_m	
	38
bml_trace_m	
Matrix trace	38
bml_transpose_m	
Transpose functions	39
bml_types_m	
The basic bml types	39
bml_utilities_m	
,	40
bml_utilities_matrix_type_m	
Utility matrix functions	41

14 Namespace Index

## **Class Index**

### 8.1 Class List

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

bmi_types_m::bmi_matrix_t	
The bml matrix type	43
bml_types_m::bml_vector_t	
The bml vector type	43
~	

16 Class Index

## File Index

### 9.1 File List

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

/home/nbock/Work/bml/src-new/C-interface/blas.h	?
/home/nbock/Work/bml/src-new/C-interface/bml.h	5
/home/nbock/Work/bml/src-new/C-interface/bml_add.h	6
/home/nbock/Work/bml/src-new/C-interface/bml_allocate.h	6
/home/nbock/Work/bml/src-new/C-interface/bml_convert.h	7
/home/nbock/Work/bml/src-new/C-interface/bml_copy.h	8
/home/nbock/Work/bml/src-new/C-interface/bml_elemental.h	?
/home/nbock/Work/bml/src-new/C-interface/bml_introspection.h	0
/home/nbock/Work/bml/src-new/C-interface/bml_logger.h	2
/home/nbock/Work/bml/src-new/C-interface/bml_multiply.h	5
/home/nbock/Work/bml/src-new/C-interface/bml_scale.h	6
/home/nbock/Work/bml/src-new/C-interface/bml_trace.h	9
/home/nbock/Work/bml/src-new/C-interface/bml_types.h	C
/home/nbock/Work/bml/src-new/C-interface/bml_types_private.h	1
/home/nbock/Work/bml/src-new/C-interface/bml_utilities.h	1
/home/nbock/Work/bml/src-new/C-interface/ <b>lapack.h</b>	?
/home/nbock/Work/bml/src-new/C-interface/typed.h	?

18 File Index

### **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** 

20 Module Documentation

Α	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.
М	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.

_		
	М	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.
М	The number of non-zeroes per row.

#### Returns

The matrix.

22 Module Documentation

### 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**

Α	Matrix A
В	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**

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

Here is the call graph for this function:



24 Module Documentation

### 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
Α	The dense matrix
threshold	The matrix element magnited threshold
М	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**

Α	The bml matrix

Returns

The dense matrix

Here is the call graph for this function:



26 Module Documentation

### 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**

а	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) *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.
а	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) *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.
а	The matrix.
т	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) *m,* type(bml\_matrix\_t), intent(inout) *a* )

Create the zero matrix.

28 Module Documentation

#### **Parameters**

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

- 10.5 Add Functions (Fortran interface)
- 10.5.1 Detailed Description

30 Module Documentation

## 10.6 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.

### 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, 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
a_dense	The dense matrix
а	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*, 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
a_dense	The dense matrix
а	The bml matrix

threshold	The matrix element magnited threshold
т	the extra arg

10.6.2.3 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) threshold, integer, intent(in) m)

Convert a dense matrix into a bml matrix.

#### **Parameters**

matrix_type	The matrix type
a_dense	The dense matrix
а	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**

а	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 hml matrix
a_dens	e   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**

а	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.

32 Module Documentation

### **Parameters**

а	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**

а	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**

а	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	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\_real\_enum\_id = 0
- integer, parameter bml\_matrix\_precision\_double\_real\_enum\_id = 1
- integer, parameter bml\_matrix\_precision\_single\_complex\_enum\_id = 2
- integer, parameter bml\_matrix\_precision\_double\_complex\_enum\_id = 3

### 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\_cprecision\_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**

а	The matrix.
i	The row.

### Returns

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

 $11.7.2.2 \quad \text{integer function, public bml\_introspection\_m::bml\_get\_size ( \ \text{type(bml\_matrix\_t), intent(in)} \ a \ )$ 

Return the matrix size.

**Parameters** 

а	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  $\alpha$  and  $\beta$  default to  $\alpha=1$  and  $\beta=0$ .

### **Parameters**

а	Matrix A.
b	Matrix B.
С	Matrix $C$ .
alpha	The factor $\alpha$ .
beta	The factor $\beta$ .

## 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
а	The matrix
С	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 \operatorname{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** 

а	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\_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.

### 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	tag A string to print before the matrix.	
V	v The vector.	
<u>i_</u> I	i_/ 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

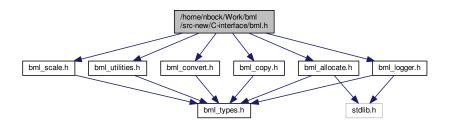
44 Class Documentation

## **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:
```



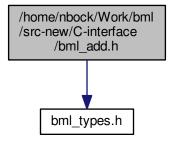
## 13.1.1 Detailed Description

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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:

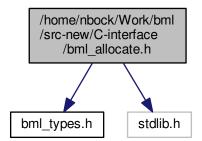


### **Functions**

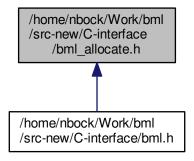
- void bml\_add (const bml\_matrix\_t \*A, const bml\_matrix\_t \*B, const double alpha, const double beta, const double threshold)
- void bml\_add\_identity (const bml\_matrix\_t \*A, const double beta, const double threshold)

## 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:

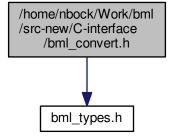


### **Functions**

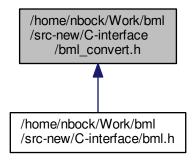
- void \* bml allocate memory (const size t s)
- void bml\_free\_memory (void \*ptr)
- void bml deallocate (bml matrix t \*\*A)
- bml\_matrix\_t \* bml\_zero\_matrix (const bml\_matrix\_type\_t matrix\_type, const bml\_matrix\_precision\_← t matrix\_precision, const int N, const int M)
- bml\_matrix\_t \* 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:

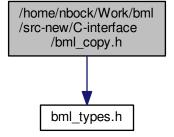


## **Functions**

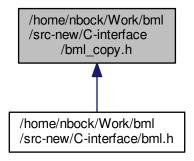
- bml\_matrix\_t \* bml\_convert\_from\_dense (const bml\_matrix\_type\_t matrix\_type, const bml\_matrix\_← precision\_t matrix\_precision, const int N, const void \*A, const double threshold, const int M)
- void \* bml\_convert\_to\_dense (const bml\_matrix\_t \*A)

## 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**

Α	Matrix to copy
В	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**

Α	Matrix to copy

### Returns

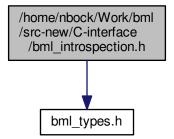
A Copy of A

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.

<b>D</b> -	 	-4	 
	m		

Α	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.

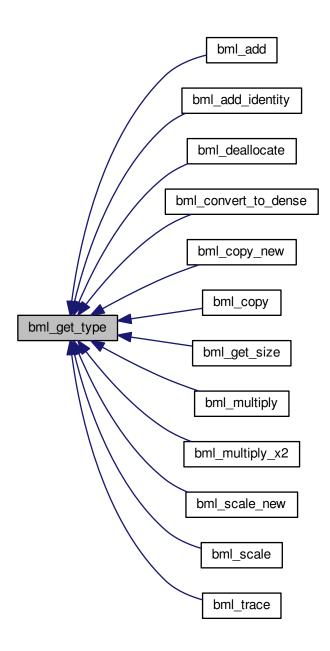
**Parameters** 

Α	The matrix.

### Returns

The matrix type.

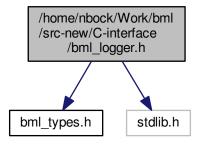
Here is the caller graph for this function:



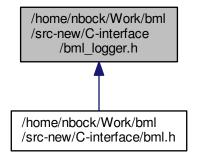
## 13.7 /home/nbock/Work/bml/src-new/C-interface/bml\_logger.h File Reference

#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 lo	og 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, ... )

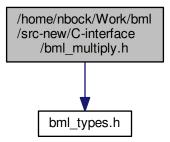
Log a message with location, i.e. filename and linenumber..

#### **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**

Α	Matrix A
В	Matrix B
С	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

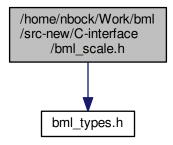
Here is the call graph for this function:



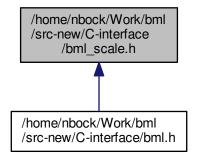
## 13.9 /home/nbock/Work/bml/src-new/C-interface/bml\_scale.h File Reference

#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

Α	Matrix to scale
В	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
Α	Matrix to scale

### Returns

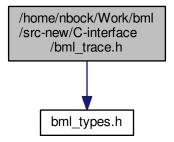
A Scaled Copy of A

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**

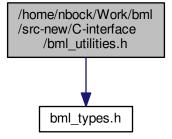
uninitialized The matrix is not initialized.

dense Dense matrix.ellpack ELLPACK matrix.csr CSR matrix.

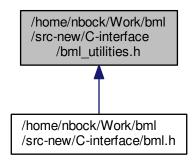
## 13.12 /home/nbock/Work/bml/src-new/C-interface/bml\_types\_private.h File Reference

## 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\_l, 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  $j_l$ , const int  $j_l$ , const int  $j_l$ , const int  $j_l$ .

Print a dense matrix.

### **Parameters**

N	The number of rows/columns.
matrix_precision	The real precision.
Α	The matrix.
<u>i_</u> I	The lower row index.
i_u	The upper row index.
<u>j_</u> I	The lower column index.
<u>j_</u> 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.
<u>i_</u> I	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  $j\_l$ , const int  $j\_l$ , const int  $j\_l$  const int j const

Print a dense matrix.

## Parameters

N	The number of rows/columns.
matrix_precision	The real precision.
Α	The matrix.
<u>i_</u> I	The lower row index.
i_u	The upper row index.
<u>j_</u> I	The lower column index.
<u>j_</u> u	The upper column index.

# Index

/home/nbock/Work/bml/src-new/C-interface/bml.h, 45	BML_LOG_WARNING
/home/nbock/Work/bml/src-new/C-interface/bml_add.h,	bml_logger.h, 54
46	bml, 33
$/home/nbock/Work/bml/src-new/C-interface/bml\_{\leftarrow}$	bml_add
allocate.h, 46	Add Functions (C interface), 22
$/home/nbock/Work/bml/src-new/C-interface/bml\_{\leftarrow}$	bml_add_identity
convert.h, 47	Add Functions (C interface), 22
$/home/nbock/Work/bml/src-new/C-interface/bml\_{\leftarrow}$	bml_allocate_m, 33
copy.h, 48	bml allocate memory
$/home/nbock/Work/bml/src-new/C-interface/bml\_{\leftarrow}$	Allocation and Deallocation Functions (C interface)
introspection.h, 50	19
$/home/nbock/Work/bml/src-new/C-interface/bml\_{\leftarrow}$	bml_convert_from_dense
logger.h, 52	Converting between Matrix Formats (C interface)
$/home/nbock/Work/bml/src-new/C-interface/bml\_{\hookleftarrow}$	24
multiply.h, 55	bml_convert_from_dense_double
$/home/nbock/Work/bml/src-new/C-interface/bml\_{\leftarrow}$	Converting between Matrix Formats (Fortran inter
scale.h, 56	face), 30
$/home/nbock/Work/bml/src-new/C-interface/bml\_{\leftarrow}$	bml_convert_from_dense_double_complex
trace.h, 59	Converting between Matrix Formats (Fortran inter
$/home/nbock/Work/bml/src-new/C-interface/bml\_{\hookleftarrow}$	face), 30
types.h, 60	bml_convert_from_dense_single_complex
$/home/nbock/Work/bml/src-new/C-interface/bml\_{\hookleftarrow}$	Converting between Matrix Formats (Fortran inter
types_private.h, 61	face), 31
/home/nbock/Work/bml/src-new/C-interface/bml_←	bml_convert_to_dense
utilities.h, 61	Converting between Matrix Formats (C interface)
	24
Add Functions (C interface), 22	bml_convert_to_dense_double
bml_add, 22	Converting between Matrix Formats (Fortran inter-
bml_add_identity, 22	face), 31
Add Functions (Fortran interface), 29	bml_convert_to_dense_double_complex
Allocation and Deallocation Functions (C interface), 19	Converting between Matrix Formats (Fortran inter
bml_allocate_memory, 19	face), 31
bml_deallocate, 19	bml_convert_to_dense_single
bml_free_memory, 20	Converting between Matrix Formats (Fortran inter
bml_identity_matrix, 20	face), 31
bml_random_matrix, 20	bml_convert_to_dense_single_complex
bml_zero_matrix, 21	Converting between Matrix Formats (Fortran inter
Allocation and Deallocation Functions (Fortran inter-	face), 31
face), 26	bml_copy
bml_deallocate, 26	bml_copy.h, 49
bml_identity_matrix, 26	bml copy m, 34
bml_random_matrix, 26	bml_copy.h
bml_zero_matrix, 26	bml_copy, 49
BML_LOG_DEBUG	bml_copy_new, 49
bml_logger.h, 54	bml_copy_m, 33
BML_LOG_ERROR	bml_copy, 34
bml_logger.h, 54	bml_copy_new
BML_LOG_INFO	bml_copy.h, 49
bml_logger.h, 54	bml deallocate
ioggoini, • i	

64 INDEX

Allocation and Deallocation Functions (C interface),	bml_types.h, 60
19	bml_matrix_t
Allocation and Deallocation Functions (Fortran in-	bml_types.h, 60
terface), 26	bml_matrix_type_t
bml_debug	bml_types.h, 60
bml_error_m, 35	bml_multiply
bml_diagonalize	bml_multiply.h, 55
bml_diagonalize_m, 34	bml_multiply_m, 38
bml_diagonalize_m, 34	bml_multiply.h
bml_diagonalize, 34	bml_multiply, 55
bml_error	bml_multiply_x2, 56
bml_error_m, 35	bml_multiply_m, 37
bml_error_m, 34	bml_multiply, 38
bml_debug, 35	bml_multiply_x2
bml_error, 35	bml_multiply.h, 56
bml_warning, 35	bml_print_bml_matrix
bml free memory	bml_utilities.h, 62
Allocation and Deallocation Functions (C interface),	bml_print_bml_vector
20	bml_utilities.h, 62
bml get bandwidth	bml_utilities_m, 40
bml_introspection_m, 37	bml print dense matrix
bml_get_size	bml utilities.h, 62
bml_introspection.h, 50	bml_random_matrix
bml_introspection_m, 37	Allocation and Deallocation Functions (C interface),
bml_get_type	20
bml_introspection.h, 51	Allocation and Deallocation Functions (Fortran in-
bml_identity_matrix	terface), 26
Allocation and Deallocation Functions (C interface),	bml_scale
20	
	bml_scale.h, 57
Allocation and Deallocation Functions (Fortran in-	bml_scale.h
terface), 26	bml_scale, 57
bml_interface_m, 36	bml_scale_new, 58
get_enum_id, 36	bml_scale_m, 38
bml_introspection.h	scale_two, 38
bml_get_size, 50	bml_scale_new
bml_get_type, 51	bml_scale.h, 58
bml_introspection_m, 36	bml_trace
bml_get_bandwidth, 37	bml_trace.h, 59
bml_get_size, 37	bml_trace_m, 39
bml_log	bml_trace.h
bml_logger.h, 54	bml_trace, 59
bml_log_level_t	bml_trace_m, 38
bml_logger.h, 54	bml_trace, 39
bml_log_location	bml_transpose
bml_logger.h, 55	bml_transpose_m, 39
bml_logger.h	bml_transpose_m, 39
BML_LOG_DEBUG, 54	bml_transpose, 39
BML_LOG_ERROR, 54	bml_types.h
BML_LOG_INFO, 54	bml_matrix_precision_t, 60
BML_LOG_WARNING, 54	bml_matrix_t, 60
bml_log, 54	bml_matrix_type_t, 60
bml_log_level_t, 54	bml_vector_t, 60
bml_log_location, 55	csr, 61
LOG DEBUG, 54	dense, 60
LOG ERROR, 54	double_complex, 60
LOG_INFO, 54	double_real, 60
LOG WARN, 54	ellpack, 61
bml_matrix_precision_t	single_complex, 60
	22b.o

INDEX 65

```
single_real, 60
                                                           bml_scale_m, 38
    uninitialized, 60
                                                       single_complex
bml types m, 39
                                                           bml_types.h, 60
bml_types_m::bml_matrix_t, 43
                                                       single_real
bml_types_m::bml_vector_t, 43
                                                           bml_types.h, 60
bml utilities.h
                                                       uninitialized
    bml print bml matrix, 62
                                                           bml types.h, 60
    bml_print_bml_vector, 62
    bml print dense matrix, 62
bml utilities m, 40
    bml_print_bml_vector, 40
bml_utilities_matrix_type_m, 41
bml_vector_t
    bml_types.h, 60
bml_warning
    bml_error_m, 35
bml zero matrix
    Allocation and Deallocation Functions (C interface),
    Allocation and Deallocation Functions (Fortran in-
         terface), 26
Converting between Matrix Formats (C interface), 24
    bml_convert_from_dense, 24
    bml convert to dense, 24
Converting between Matrix Formats (Fortran interface),
    bml_convert_from_dense_double, 30
    bml_convert_from_dense_double_complex, 30
    bml_convert_from_dense_single_complex, 31
    bml_convert_to_dense_double, 31
    bml convert to dense double complex, 31
    bml convert to dense single, 31
    bml_convert_to_dense_single_complex, 31
csr
    bml types.h, 61
dense
    bml_types.h, 60
double_complex
    bml_types.h, 60
double_real
    bml types.h, 60
ellpack
    bml types.h, 61
get_enum_id
    bml_interface_m, 36
LOG DEBUG
    bml_logger.h, 54
LOG_ERROR
    bml_logger.h, 54
LOG INFO
    bml_logger.h, 54
LOG_WARN
    bml_logger.h, 54
scale_two
```