DD2D - Matryoshka approach 0

Generated by Doxygen 1.8.3.1

Mon Jun 3 2013 14:47:51

Contents

1	Mair	n Page			1
2	Hier	archica	l Index		3
	2.1	Class	Hierarchy		3
3	Data	Struct	ure Index		5
	3.1	Data S	Structures		5
4	File	Index			7
	4.1	File Lis	st		7
5	Data	Struct	ure Docun	nentation	9
	5.1	Defect	Class Refe	erence	9
		5.1.1	Detailed	Description	10
		5.1.2	Construc	tor & Destructor Documentation	11
			5.1.2.1	Defect	11
			5.1.2.2	Defect	11
			5.1.2.3	Defect	11
		5.1.3	Member	Function Documentation	11
			5.1.3.1	getPosition	11
			5.1.3.2	getPosition	12
			5.1.3.3	getPosition	12
			5.1.3.4	getX	12
			5.1.3.5	getY	12
			5.1.3.6	getZ	13
			5.1.3.7	setPosition	13
			5.1.3.8	setPosition	13
			5.1.3.9	setPosition	14
			5.1.3.10	setX	14
			5.1.3.11	setY	14
			5.1.3.12	setZ	14
			5.1.3.13	stressField	15
		514	Field Doo	numentation.	15

ii CONTENTS

		5.1.4.1 pos						
5.2	Disloca	tion Class Reference						
	5.2.1	Detailed Description						
	5.2.2	Constructor & Destructor Documentation						
		5.2.2.1 Dislocation						
		5.2.2.2 Dislocation						
	5.2.3	Member Function Documentation						
		5.2.3.1 calculateRotationMatrix						
		5.2.3.2 forcePeachKoehler						
		5.2.3.3 getBurgers						
		5.2.3.4 getLineVector						
		5.2.3.5 getPosition						
		5.2.3.6 getPosition						
		5.2.3.7 getPosition						
		5.2.3.8 getX						
		5.2.3.9 getY						
		5.2.3.10 getZ						
		5.2.3.11 idealTimeIncrement						
		5.2.3.12 isMobile						
		5.2.3.13 setBurgers						
		5.2.3.14 setLineVector						
		5.2.3.15 setMobile						
		5.2.3.16 setPinned						
		5.2.3.17 setPosition						
		5.2.3.18 setPosition						
		5.2.3.19 setPosition						
		5.2.3.20 setX						
		5.2.3.21 setY						
		5.2.3.22 setZ						
		5.2.3.23 stressField						
		5.2.3.24 stressFieldLocal						
	5.2.4	Field Documentation						
		5.2.4.1 bmag						
		5.2.4.2 bvec						
		5.2.4.3 lvec						
		5.2.4.4 mobile						
		5.2.4.5 pos						
		5.2.4.6 rotationMatrix						
5.3	Disloca	ationSource Class Reference						
	5.3.1	Detailed Description						

CONTENTS

5.3.2	Construc	tor & Destructor Documentation	30
	5.3.2.1	DislocationSource	30
	5.3.2.2	DislocationSource	31
5.3.3	Member I	Function Documentation	31
	5.3.3.1	dipoleNucleationLength	31
	5.3.3.2	getBurgers	32
	5.3.3.3	getBurgersMag	32
	5.3.3.4	getIterationCount	32
	5.3.3.5	getLineVector	32
	5.3.3.6	getNumIterations	33
	5.3.3.7	getPosition	33
	5.3.3.8	getPosition	33
	5.3.3.9	getPosition	34
	5.3.3.10	getTauCritical	34
	5.3.3.11	getX	34
	5.3.3.12	getY	34
	5.3.3.13	getZ	35
	5.3.3.14	ifEmitDipole	35
	5.3.3.15	incrementIterationCount	35
	5.3.3.16	resetIterationCounter	35
	5.3.3.17	setBurgers	35
	5.3.3.18	setBurgersMagnitude	36
	5.3.3.19	setLineVector	36
	5.3.3.20	setNumIterations	36
	5.3.3.21	setPosition	36
	5.3.3.22	setPosition	37
	5.3.3.23	setPosition	37
	5.3.3.24	setTauCritical	37
	5.3.3.25	setX	38
	5.3.3.26	setY	38
	5.3.3.27	setZ	38
	5.3.3.28	stressField	38
5.3.4	Field Doo	cumentation	39
	5.3.4.1	bmag	39
	5.3.4.2	bvec	39
	5.3.4.3	countIterations	39
	5.3.4.4	lvec	39
	5.3.4.5	mobile	39
	5.3.4.6	nlterations	40
	5.3.4.7	pos	40

iv CONTENTS

		5.3.4.8	rotationMatrix	. 40
		5.3.4.9	tauCritical	. 40
5.4	Matrix3	33 Class R	Reference	. 40
	5.4.1	Detailed	Description	. 42
	5.4.2	Construc	ctor & Destructor Documentation	. 42
		5.4.2.1	Matrix33	. 42
		5.4.2.2	Matrix33	. 42
		5.4.2.3	Matrix33	. 43
		5.4.2.4	Matrix33	. 43
	5.4.3	Member	Function Documentation	. 43
		5.4.3.1	adjugate	. 43
		5.4.3.2	getValue	. 44
		5.4.3.3	operator!	. 44
		5.4.3.4	operator*	. 45
		5.4.3.5	operator*	. 45
		5.4.3.6	operator*	. 46
		5.4.3.7	operator*=	. 46
		5.4.3.8	operator*=	. 46
		5.4.3.9	operator+	. 47
		5.4.3.10	operator+=	. 47
		5.4.3.11	operator	. 47
		5.4.3.12	operator-=	. 48
		5.4.3.13	operator [^]	. 48
		5.4.3.14	operator~	. 49
		5.4.3.15	setValue	. 49
	5.4.4	Field Doo	cumentation	. 49
		5.4.4.1	x	. 49
5.5	Rotatio	onMatrix C	lass Reference	. 50
	5.5.1	Detailed	Description	. 51
	5.5.2	Construc	ctor & Destructor Documentation	. 51
		5.5.2.1	RotationMatrix	. 51
		5.5.2.2	RotationMatrix	. 52
	5.5.3	Member	Function Documentation	. 52
		5.5.3.1	adjugate	. 52
		5.5.3.2	getValue	. 52
		5.5.3.3	operator!	. 53
		5.5.3.4	operator*	. 53
		5.5.3.5	operator*	. 54
		5.5.3.6	operator*	. 54
		5.5.3.7	operator*=	. 55

CONTENTS

		5.5.3.8	operator*=	55
		5.5.3.9	operator+	55
		5.5.3.10	operator+=	56
		5.5.3.11	operator	56
		5.5.3.12	operator-=	56
		5.5.3.13	$operator^\wedge \ldots \ldots \ldots \ldots$	57
		5.5.3.14	operator~	57
		5.5.3.15	setValue	57
	5.5.4	Field Doo	cumentation	58
		5.5.4.1	\mathbf{x}	58
5.6	SlipPla	ine Class F	Reference	58
	5.6.1	Detailed	Description	60
	5.6.2	Construc	tor & Destructor Documentation	60
		5.6.2.1	SlipPlane	60
		5.6.2.2	SlipPlane	61
	5.6.3	Member	Function Documentation	61
		5.6.3.1	calculateDislocationForces	61
		5.6.3.2	calculateDislocationStresses	62
		5.6.3.3	calculateRotationMatrix	62
		5.6.3.4	calculateTimeIncrement	63
		5.6.3.5	calculateVelocities	64
		5.6.3.6	distanceFromExtremity	65
		5.6.3.7	getAxis	65
		5.6.3.8	getDislocation	66
		5.6.3.9	getDislocationList	66
		5.6.3.10	getDislocationSource	67
		5.6.3.11	getDislocationSourceList	67
		5.6.3.12	getExtremities	68
		5.6.3.13	getExtremity	68
		5.6.3.14	getNormal	68
		5.6.3.15	getNumDislocations	68
		5.6.3.16	getNumDislocationSources	69
		5.6.3.17	getPosition	69
		5.6.3.18	getRotationMatrix	69
		5.6.3.19	moveDislocations	70
		5.6.3.20	setDislocationList	70
		5.6.3.21	setDislocationSourceList	70
		5.6.3.22	setExtremities	70
		5.6.3.23	setNormal	71
		5.6.3.24	setPosition	71

vi CONTENTS

		5.6.3.25	sortDislocations	71
	5.6.4	Field Doo	cumentation	72
		5.6.4.1	dislocationForces	72
		5.6.4.2	dislocations	72
		5.6.4.3	dislocationSources	72
		5.6.4.4	dislocationStresses	72
		5.6.4.5	dislocationVelocities	72
		5.6.4.6	$dt \ldots \ldots \ldots \ldots \ldots$	72
		5.6.4.7	extremities	73
		5.6.4.8	normalVector	73
		5.6.4.9	position	73
		5.6.4.10	rotationMatrix	73
5.7	Strain	Class Refe	erence	73
	5.7.1	Detailed	Description	75
	5.7.2	Construc	stor & Destructor Documentation	75
		5.7.2.1	Strain	75
		5.7.2.2	Strain	76
	5.7.3	Member	Function Documentation	76
		5.7.3.1	adjugate	76
		5.7.3.2	getPrincipalStrains	77
		5.7.3.3	getShearStrains	77
		5.7.3.4	getValue	77
		5.7.3.5	operator!	78
		5.7.3.6	operator*	78
		5.7.3.7	operator*	79
		5.7.3.8	operator*	79
		5.7.3.9	operator*=	80
		5.7.3.10	operator*=	80
		5.7.3.11	operator+	80
		5.7.3.12	operator+=	81
		5.7.3.13	operator	81
		5.7.3.14	operator-=	81
		5.7.3.15	operator [^]	82
		5.7.3.16	operator \sim	82
		5.7.3.17	populateMatrix	82
		5.7.3.18	rotate	83
		5.7.3.19	setValue	83
	5.7.4	Field Doo	cumentation	83
		5.7.4.1	principalStrains	83
		5.7.4.2	shearStrains	83

CONTENTS vii

		5.7.4.3 x						
5.8	Stress	Class Reference						
	5.8.1	Detailed Description						
	5.8.2	Constructor & Destructor Documentation						
		5.8.2.1 Stress						
		5.8.2.2 Stress						
	5.8.3	Member Function Documentation						
		5.8.3.1 adjugate						
		5.8.3.2 getPrincipalStresses						
		5.8.3.3 getShearStresses						
		5.8.3.4 getValue						
		5.8.3.5 operator!						
		5.8.3.6 operator*						
		5.8.3.7 operator*						
		5.8.3.8 operator*						
		5.8.3.9 operator*=						
		5.8.3.10 operator*=						
		5.8.3.11 operator+						
		5.8.3.12 operator+=						
		5.8.3.13 operator						
		5.8.3.14 operator-=						
		5.8.3.15 operator [^]						
		5.8.3.16 operator~ 92						
		5.8.3.17 populateMatrix						
		5.8.3.18 rotate						
		5.8.3.19 setValue						
	5.8.4	Field Documentation						
		5.8.4.1 principalStresses						
		5.8.4.2 shearStresses						
		5.8.4.3 x						
5.9	Vector	3d Class Reference						
	5.9.1	Detailed Description						
	5.9.2	Constructor & Destructor Documentation						
		5.9.2.1 Vector3d						
		5.9.2.2 Vector3d						
		5.9.2.3 Vector3d						
	5.9.3	Member Function Documentation						
		5.9.3.1 getValue						
		5.9.3.2 getVector						
		5.9.3.3 magnitude						

viii CONTENTS

			5.9.3.4	normalize	 	 97
			5.9.3.5	operator*	 	 98
			5.9.3.6	operator*	 	 98
			5.9.3.7	operator*=	 	 99
			5.9.3.8	operator+	 	 99
			5.9.3.9	operator+=	 	 99
			5.9.3.10	operator	 	 99
			5.9.3.11	operator-=	 	 100
			5.9.3.12	operator $^{\wedge}$	 	 100
			5.9.3.13	operator $^{\wedge}$ =	 	 100
			5.9.3.14	setValue	 	 101
			5.9.3.15	setVector	 	 101
			5.9.3.16	sum	 	 101
		5.9.4	Field Doo	mentation	 	 102
			5.9.4.1	x	 	 102
6	File	Docume	entation			103
	6.1	consta	nts.h File F	eference	 	 103
		6.1.1	Detailed	escription	 	 104
		6.1.2	Macro De	inition Documentation	 	 104
			6.1.2.1	PI	 	 104
			6.1.2.2	SQRT2	 	 104
			6.1.2.3	SQRT3	 	 104
			6.1.2.4	SQRT5	 	 104
	6.2	defect.	cpp File Re	ference	 	 105
		6.2.1	Detailed	escription	 	 105
	6.3	defect.	h File Refe	ence	 	 106
		6.3.1	Detailed	escription	 	 107
	6.4	disloca	tion.cpp Fi	Reference	 	 108
		6.4.1	Detailed	escription	 	 108
	6.5	disloca	tion.h File	Reference	 	 109
		6.5.1	Detailed	escription	 	 110
	6.6	disloca	tionDefaul	s.h File Reference	 	 110
		6.6.1	Detailed	escription	 	 112
		6.6.2	Macro De	inition Documentation	 	 112
			6.6.2.1	DEFAULT_BURGERS_0	 	 112
			6.6.2.2	DEFAULT_BURGERS_1	 	 112
			6.6.2.3	DEFAULT_BURGERS_2	 	 112
			6.6.2.4	DEFAULT_BURGERS_MAGNITUDE	 	 112
			6.6.2.5	DEFAULT_LINEVECTOR_0	 	 112

CONTENTS

		6.6.2.6	DEFAULT_I	LINEVECTO	PR_1			 	 	 . 112
		6.6.2.7	DEFAULT_I	LINEVECTO	P_2			 	 	 . 113
		6.6.2.8	DEFAULT_I	POSITION_0	0			 	 	 . 113
		6.6.2.9	DEFAULT_I	POSITION_	1			 	 	 . 113
		6.6.2.10	DEFAULT_I	POSITION_2	2			 	 	 . 113
6.7	disloca	tionSource	cpp File Ref	ference				 	 	 . 113
	6.7.1	Detailed I	Description					 	 	 . 114
6.8	disloca	tionSource	e.h File Refer	ence				 	 	 . 115
	6.8.1	Detailed I	Description					 	 	 . 116
6.9	disloca	tionSource	Defaults.h Fi	ile Reference	e			 	 	 . 116
	6.9.1	Detailed I	Description					 	 	 . 117
	6.9.2	Macro De	finition Docu	mentation .				 	 	 . 118
		6.9.2.1	DEFAULT_I	NITERATIO	NS			 	 	 . 118
		6.9.2.2	DEFAULT_	TAU_CRITIC	CAL			 	 	 . 118
6.10	mainpa	age.dox File	e Reference					 	 	 . 118
6.11	matrix3	33.cpp File	Reference					 	 	 . 118
	6.11.1	Detailed I	Description					 	 	 . 118
6.12	matrix3	33.h File R	eference					 	 	 . 119
	6.12.1	Detailed I	Description					 	 	 . 120
6.13	rotation	Matrix.cpp	File Referer	nce				 	 	 . 121
	6.13.1	Detailed I	Description					 	 	 . 121
6.14	rotation	nMatrix.h F	ile Reference	e				 	 	 . 121
	6.14.1	Detailed I	Description					 	 	 . 122
6.15	slipPla	ne.cpp File	Reference					 	 	 . 123
	6.15.1	Detailed I	Description					 	 	 . 123
6.16	slipPlai	ne.h File R	eference .					 	 	 . 124
	6.16.1	Detailed I	Description					 	 	 . 125
6.17	slipPla	neDefaults	h File Refere	ence				 	 	 . 125
	6.17.1	Detailed I	Description					 	 	 . 127
	6.17.2	Macro De	finition Docu	mentation .				 	 	 . 127
		6.17.2.1	DEFAULT_S	SLIPPLANE.	_EXTRE	MITY1_0)	 	 	 . 127
		6.17.2.2	DEFAULT_S	SLIPPLANE.	_EXTRE	MITY1_	1	 	 	 . 127
		6.17.2.3	DEFAULT_S	SLIPPLANE.	_EXTRE	MITY1_2	2	 	 	 . 127
		6.17.2.4	DEFAULT_S	SLIPPLANE.	_EXTRE	MITY2_0)	 	 	 . 127
		6.17.2.5	DEFAULT_S	SLIPPLANE.	_EXTRE	MITY2_	1	 	 	 . 128
		6.17.2.6	DEFAULT_S	SLIPPLANE.	_EXTRE	MITY2_2	2	 	 	 . 128
		6.17.2.7	DEFAULT_S	SLIPPLANE.	_NORMA	LVECT	OR_0	 	 	 . 128
		6.17.2.8	DEFAULT_S	SLIPPLANE.	_NORMA	LVECT	OR_1 .	 	 	 . 128
			DEFAULT_S				_			
		6.17.2.10	DEFAULT_S	SLIPPLANE	_POSITION	. 0_NC		 	 	 . 128

CONTENTS

	6.17.2.11 DEFAULT_SLIPPLANE_POSITION_1	128
	6.17.2.12 DEFAULT_SLIPPLANE_POSITION_2	128
6.18	strain.cpp File Reference	128
	6.18.1 Detailed Description	129
6.19	strain.h File Reference	130
	6.19.1 Detailed Description	131
6.20	stress.cpp File Reference	131
	6.20.1 Detailed Description	132
6.21	stress.h File Reference	133
	6.21.1 Detailed Description	134
6.22	vector3d.cpp File Reference	135
	6.22.1 Detailed Description	135
6.23	vector3d.h File Reference	135
	6.23.1 Detailed Description	137
Indev	-	137
Index	- Table 1	137

Chapter 1

Main Page

The files in this program provide a heirarchical data structure system for carrying out dislocation dynamics simulations in two dimensions. The base class is Defect, which represents a generic defect in a metallic crystal. All other defects, such as dislocations, dislocation sources, precipitates, etc., are represented by their own classes which inherit certain functions from the Defect class.

The goal of carrying out these simulations in two dimensions is to be able to simulate plastic deformation of up to a few percent. Current three dimensional dislocation dynamics simulations are computationally expensive. This approach hopes to sacrifice some of the precision in order to gain in speed and flexibility.

The program is under development now, with the data structures being defined. When it will be complete, it is intended to have data structures nested within each other, hence the name Matryoshka. For example, a polycrystal is a collection of grains; a grain is a collection of slip systems; a slip system is a collection of slip planes; a slip plane is a collection of dislocations, dislocation sources and other defects. This program will also take advantage of the functionality provided by the C++ STL to manage lists of various objects in the simulation. Once the base simulations execute successfully, other defects will be introduced.

To view the hierarchical structure, go to the section labeled Data Structures > Class Hierarchy. A good place to start would be the Defect class, which is the generic base class for most of the entities present in the simulation.

2 Main Page

Chapter 2

Hierarchical Index

2.1 Class Hierarchy

This inheritance list is sorted roughly, but not completely, alphabetically:

efect	9
Dislocation	15
DislocationSource	27
latrix33	40
RotationMatrix	50
Strain	73
Stress	84
lipPlane	
ector3d	94

Hierarchical Index

Chapter 3

Data Structure Index

3.1 Data Structures

Here are the data structures with brief descriptions:

Class Defect representing a generic defect in a material	9
on Control of the Con	
Dislocation class representing a dislocation in the simulation	15
onSource	
DislocationSource class representing a source of dislocations in the simulation	27
Matrix33 class representing a 3x3 square matrix	40
Matrix Matrix	
RotationMatrix class to represent a rotation matrix	50
SlipPlane class representing a slip plane in the simulation	58
Strain class to represent the strain tensor	73
Stress class to represent the stress tensor	84
Vector3d class representing a single 3-dimensional vector in the simulation	94
	Class Defect representing a generic defect in a material

6 **Data Structure Index**

Chapter 4

File Index

4.1 File List

Here is a list of all files with brief descriptions:

constants.h	
Definition of constants used in the program	103
defect.cpp	
Definition of member functions of the Defect class	105
defect.h	
Definition of the Defect class	106
dislocation.cpp	
Definition of constructors and member functions of the Dislocation class	108
dislocation.h	
	109
dislocationDefaults.h	
Definition of certain default values for members of the Dislocation class	110
dislocationSource.cpp	
	113
dislocationSource.h	
	115
dislocationSourceDefaults.h	
	116
matrix33.cpp	
•	118
matrix33.h	
	119
rotationMatrix.cpp	101
	121
rotationMatrix.h	121
Definition of the RotationMatrix class	121
	123
slipPlane.h	23
·	124
slipPlaneDefaults.h	
	125
strain.cpp	20
	128
strain.h	
	130
stress.cpp	
	131

8 File Index

stress.h	
Definition of the Stress class	 133
vector3d.cpp	
Definition of member functions and operators of the Vector3d class	 135
vector3d.h	
Definition of the Vector3d class	 135

Chapter 5

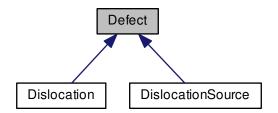
Data Structure Documentation

5.1 Defect Class Reference

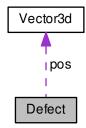
Class Defect representing a generic defect in a material.

#include <defect.h>

Inheritance diagram for Defect:



Collaboration diagram for Defect:



Public Member Functions

• Defect ()

Default constructor.

• Defect (double x, double y, double z)

Constructor specifying the position.

• Defect (double *p)

Constructor specifying the position.

void setPosition (double *a)

Sets the position of the defect.

• void setPosition (double x, double y, double z)

Sets the position of the defect.

void setPosition (Vector3d a)

Sets the position of the defect.

void setX (double x)

Sets the X-coordinate of the defect.

void setY (double y)

Sets the Y-coordinate of the defect.

void setZ (double z)

Sets the Z-coordinate of the defect.

double * getPosition ()

Returns in an array the position.

• void getPosition (double *a)

Returns the array position in a pre-allocated array.

Vector3d getPosition ()

Returns the position vector of the defect.

· double getX ()

Returns the X-coordinate of the defect.

· double getY ()

Returns the Y-coordinate of the defect.

double getZ ()

Returns the Z-coordinate of the defect.

• virtual Stress stressField (Vector3d p, double mu, double nu)

Virtual function for calculating the stress field.

Protected Attributes

· Vector3d pos

Position vector of the defect in 2D space.

5.1.1 Detailed Description

Class Defect representing a generic defect in a material.

Defines the Defect class representing an defect in the simulation. This is simply a generic description class with virtual functions. Later classes like dislocations, precipitates, boundaries etc will inherit from this class.

Definition at line 20 of file defect.h.

5.1.2 Constructor & Destructor Documentation

5.1.2.1 Defect::Defect ()

Default constructor.

Creates the object with position (0.0, 0.0, 0.0).

Definition at line 17 of file defect.cpp.

```
18 {
19    for (int i=0; i<3; i++)
20     {
21        this->pos.setValue(i, 0.0);
22    }
23 }
```

5.1.2.2 Defect::Defect (double x, double y, double z)

Constructor specifying the position.

The object is initialized with the position specified by the arguments (x, y, z).

Parameters

X	X-coordinate of the defect.
У	Y-coordinate of the defect
Z	Z-coordinate of the defect.

Definition at line 32 of file defect.cpp.

```
33 {
34     this->pos.setValue (0, x);
35     this->pos.setValue (1, y);
36     this->pos.setValue (2, z);
37 }
```

5.1.2.3 Defect::Defect (double * p)

Constructor specifying the position.

The object is initialized with the position specified in the array pointed to by the argument.

Parameters

```
p Pointer to the array containing the coordinates of the defect.
```

Definition at line 44 of file defect.cpp.

```
45 {
46 this->pos.setValue (p);
```

5.1.3 Member Function Documentation

5.1.3.1 Vector3d Defect::getPosition ()

Returns in an array the position.

Returns the position vector of the defect.

The position of the defect is saved in an array and a pointer to its first term is returned.

Returns

Pointer to the first term of the array containing the position of the defect.

The position vector of the defect, in a variable of type Vector3d.

Definition at line 119 of file defect.cpp.

```
120 {
121    return (this->pos.getVector ());
122 }
```

5.1.3.2 void Defect::getPosition (double * a)

Returns the array position in a pre-allocated array.

Returns in the array provided in the argument the position of the defect. The array must be pre-allocated.

Parameters

a Pointer to the location where the defect coordinates are to be populated.

Definition at line 129 of file defect.cpp.

```
130 {
131    a = this->pos.getVector ();
132 }
```

5.1.3.3 Vector3d Defect::getPosition ()

Returns the position vector of the defect.

Returns

The position vector of the defect, in a variable of type Vector3d.

5.1.3.4 double Defect::getX ()

Returns the X-coordinate of the defect.

Returns

X-coordinate of the defect.

Definition at line 147 of file defect.cpp.

```
148 {
149    return (this->getValue (0));
150 }
```

5.1.3.5 double Defect::getY()

Returns the Y-coordinate of the defect.

5.1 Defect Class Reference 13

Returns

Y-coordinate of the defect.

Definition at line 156 of file defect.cpp.

```
157 {
158     return (this->pos.getValue (1));
159 }
```

5.1.3.6 double Defect::getZ()

Returns the Z-coordinate of the defect.

Returns

Z-coordinate of the defect.

Definition at line 165 of file defect.cpp.

```
166 {
167    return (this->pos.getValue (2));
168 }
```

5.1.3.7 void Defect::setPosition (double * a)

Sets the position of the defect.

The position of the defect is set to the co-ordinates present in the array pointed to by the argument. Sets the position of the defect as the values in the array pointed to by the argument.

Parameters

```
a Pointer to the array containing the coordinates of the defect.
```

Definition at line 56 of file defect.cpp.

```
57 {
58   this->pos.setVector (a);
59 }
```

5.1.3.8 void Defect::setPosition (double x, double y, double z)

Sets the position of the defect.

The position of the defect is set to the co-ordinates specified by the arguments (x, y, z). Sets the position of the defect as the coordinates provided as arguments.

Parameters

X	X-coordinate of the defect.
У	Y-coordinate of the defect.
Z	Z-coordinate of the defect.

Definition at line 69 of file defect.cpp.

```
70 {
71 this->pos.setValue (0, x);
```

```
72 this->pos.setValue (1, y);
73 this->pos.setValue (2, z);
74 }
```

5.1.3.9 void Defect::setPosition (Vector3d a)

Sets the position of the defect.

The position of the defect is set to the position vector fiven by the argument a.

Parameters

```
a Position vector of the defect.
```

Definition at line 81 of file defect.cpp.

```
82 {
83    this->position = a;
84 }
```

5.1.3.10 void Defect::setX (double x)

Sets the X-coordinate of the defect.

Parameters

```
x X-coordinate of the defect.
```

Definition at line 90 of file defect.cpp.

```
91 {
92   this->pos.setValue (0, x);
93 }
```

5.1.3.11 void Defect::setY (double y)

Sets the Y-coordinate of the defect.

Parameters

```
y | Y-coordinate of the defect.
```

Definition at line 99 of file defect.cpp.

```
100 {
101    this->pos.setValue (1, y);
102 }
```

5.1.3.12 void Defect::setZ (double z)

Sets the Z-coordinate of the defect.

Parameters

```
z Z-coordinate of the defect.
```

Definition at line 108 of file defect.cpp.

```
109 {
110   this->pos.setValue (2, z);
111 }
```

5.1.3.13 virtual Stress Defect::stressField (Vector3d p, double mu, double nu) [inline], [virtual]

Virtual function for calculating the stress field.

Returns the value of the stress field of the given defect at the position given by the argument. This is a virtual function and always returns a zero matrix. Classes which inherit this function should have their own implementations of this function to override its behaviour.

Parameters

р	Position vector of the the point where the stress field is to be calculated.
mu	Shear modulus in Pascals.
nu	Poisson's ratio.

Returns

Stress field value at the position p.

Reimplemented in Dislocation.

Definition at line 142 of file defect.h.

5.1.4 Field Documentation

```
5.1.4.1 Vector3d Defect::pos [protected]
```

Position vector of the defect in 2D space.

Definition at line 26 of file defect.h.

The documentation for this class was generated from the following files:

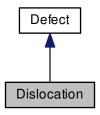
- · defect.h
- · defect.cpp

5.2 Dislocation Class Reference

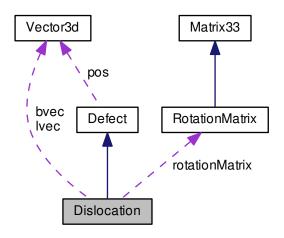
Dislocation class representing a dislocation in the simulation.

```
#include <dislocation.h>
```

Inheritance diagram for Dislocation:



Collaboration diagram for Dislocation:



Public Member Functions

• Dislocation ()

Default constructor.

• Dislocation (Vector3d burgers, Vector3d line, Vector3d position, double bm, bool m)

Constructor that explicitly specifies all parameters.

• void setBurgers (Vector3d burgers)

Sets the Burgers vector of the dislocation.

• void setLineVector (Vector3d line)

Sets the line vector of the dislocation.

• void setMobile ()

Sets the dislocation as mobile.

• void setPinned ()

Sets the dislocation as pinned.

· Vector3d getBurgers ()

Gets the Burgers vector of the dislocation.

Vector3d getLineVector ()

Gets the line vector of the dislocation.

· bool isMobile ()

Returns whether the dislocation is mobile or pinned.

void calculateRotationMatrix ()

Calculate the roation matrix.

• Stress stressField (Vector3d p, double mu, double nu)

Calculates the stress field due to this dislocation at the position given as argument.

• Stress stressFieldLocal (Vector3d p, double mu, double nu)

Calculates the stress field due to the dislocation in the local co-ordinate system.

Vector3d forcePeachKoehler (Stress sigma, double tau_crss)

Calculate the Peach-Koehler force acting on the dislocation due the stress.

double idealTimeIncrement (Vector3d v0, double minDistance, Defect d, Vector3d v1)

Returns the ideal time increment for the dislocation.

void setPosition (double *a)

Sets the position of the defect.

• void setPosition (double x, double y, double z)

Sets the position of the defect.

• void setPosition (Vector3d a)

Sets the position of the defect.

void setX (double x)

Sets the X-coordinate of the defect.

void setY (double y)

Sets the Y-coordinate of the defect.

void setZ (double z)

Sets the Z-coordinate of the defect.

double * getPosition ()

Returns in an array the position.

void getPosition (double *a)

Returns the array position in a pre-allocated array.

Vector3d getPosition ()

Returns the position vector of the defect.

• double getX ()

Returns the X-coordinate of the defect.

· double getY ()

Returns the Y-coordinate of the defect.

double getZ ()

Returns the Z-coordinate of the defect.

Protected Attributes

Vector3d bvec

Burgers vector of the dislocation.

Vector3d Ivec

Line vector if the dislocation.

· bool mobile

Boolean term indicating mobility.

double bmag

Magnitude of the Burgers vector in metres.

· RotationMatrix rotationMatrix

The rotation matrix for rotating from the global to the local co-ordinate system and vice-versa.

· Vector3d pos

Position vector of the defect in 2D space.

5.2.1 Detailed Description

Dislocation class representing a dislocation in the simulation.

The Dislocation class represents a dislocation in the simulation. The class inherits from the Defect class. A dislocation has several properties like a Burgers vector, line vector, etc. which will all be declared here.

Definition at line 21 of file dislocation.h.

5.2.2 Constructor & Destructor Documentation

```
5.2.2.1 Dislocation::Dislocation ( )
```

Default constructor.

Initializes the dislocation with the following default parameters: Position: (0.0, 0.0, 0.0) Burgers vector: Default value set in defaults file. Line vector: Default value set in defaults file. Burgers vector magnitude: Default value set in the defaults file. Mobile: true.

Initializes the dislocation with the following default parameters: Position: (0.0, 0.0, 0.0) Burgers vector: Default value set in defaults file. Line vector: Default value set in defaults file. Burgers vector magnitude: Default value set in teh defaults file. Mobile: true.

Definition at line 21 of file dislocation.cpp.

5.2.2.2 Dislocation::Dislocation (Vector3d burgers, Vector3d line, Vector3d position, double bm, bool m)

Constructor that explicitly specifies all parameters.

All parameters: Burgers vector, line vector, position, are specified.

Parameters

burgers	Burgers vector.
line	Line vector.
position	Position of the dislocation.
bm	Magnitude of the Burgers vector in metres.
m	Mobility (true/false).

Definition at line 40 of file dislocation.cpp.

```
41 {
42 this->bvec = burgers;
43 this->lvec = line;
```

```
44 this->pos = position;

45 this->mobile = m;

46 this->bmag = bm;

47 this->calculateRotationMatrix ();

48 }
```

5.2.3 Member Function Documentation

5.2.3.1 void Dislocation::calculateRotationMatrix ()

Calculate the roation matrix.

This function calculates the rotation matrix for this dislocation using the global and local co-ordinate systems. The matrix rotationMatrix is for rotation from the old (unprimed, global) to the new (primed, dislocation) system.

Definition at line 118 of file dislocation.cpp.

```
119 {
       Vector3d globalSystem[3];
                                            // Global co-ordinate systems
120
                                            // Dislocation co-ordinate system
121
       Vector3d localSystem[3];
122
       // Vectors of the global co-ordinate system
       globalSystem[0] = Vector3d (1.0, 0.0, 0.0);
globalSystem[1] = Vector3d (0.0, 1.0, 0.0);
124
125
126
       globalSystem[2] = Vector3d (0.0, 0.0, 1.0);
127
       // Vectors of the dislocation co-ordinate system
128
       localSystem[0] = bvec.normalize ();
localSystem[2] = lvec.normalize ();
129
130
131
       localSystem[1] = (lvec ^ bvec).normalize ();
132
      // Calculate rotation matrix
this->rotationMatrix = RotationMatrix (globalSystem, localSystem);
133
134
```

5.2.3.2 Vector3d Dislocation::forcePeachKoehler (Stress sigma, double tau_crss)

Calculate the Peach-Koehler force acting on the dislocation due the stress.

This function calculates the Peach-Koehler force in the dislocation due to the stress (expressed in the global coordinate system) provided as argument. The force returned is also in the global co-ordinate system. This function checks if the xy component of the stress tensorm expressed in the dislocation's local co-ordinate system, is greater than tau_crss. If it is, the force is calculated using the Peach-Koehler equation, otherwise, the force on the dislocation is zero.

Parameters

sigma	The stress tensor, expressed in the global co-ordinate system.
tau_crss	Critical Resolved Shear Stress in Pa.

Returns

The Peach-Koehler force on the dislocation, expressed in the global co-ordinate system.

Definition at line 201 of file dislocation.cpp.

```
202 {
      // Stress in the local co-ordinate system
203
204
     Stress sigmaLocal = (this->rotationMatrix) * (sigma) * (this->
      rotationMatrix)^;
205
      Vector3d force;
206
207
      // Check for CRSS condition
208
      if (sigmaLocal.getValue(0,1) >= tau_crss)
209
210
          Vector3d force = sigma * ((this->bvec)^(this->lvec));
211
```

```
213 return (force);
```

5.2.3.3 Vector3d Dislocation::getBurgers ()

Gets the Burgers vector of the dislocation.

Returns

Burgers vector in a variable of type Vector3d.

Definition at line 90 of file dislocation.cpp.

```
91 {
92    return ( this->bvec );
93 }
```

5.2.3.4 Vector3d Dislocation::getLineVector()

Gets the line vector of the dislocation.

Returns

Line vector in a variable of type Vector3d.

Definition at line 99 of file dislocation.cpp.

```
100 {
101    return ( this->lvec );
102 }
```

5.2.3.5 Vector3d Defect::getPosition() [inherited]

Returns in an array the position.

Returns the position vector of the defect.

The position of the defect is saved in an array and a pointer to its first term is returned.

Returns

Pointer to the first term of the array containing the position of the defect.

The position vector of the defect, in a variable of type Vector3d.

Definition at line 119 of file defect.cpp.

```
120 {
121    return (this->pos.getVector ());
122 }
```

5.2.3.6 void Defect::getPosition (double * a) [inherited]

Returns the array position in a pre-allocated array.

Returns in the array provided in the argument the position of the defect. The array must be pre-allocated.

Parameters

a Pointer to the location where the defect coordinates are to be populated.

Definition at line 129 of file defect.cpp.

```
130 {
131    a = this->pos.getVector ();
132 }
```

5.2.3.7 Vector3d Defect::getPosition() [inherited]

Returns the position vector of the defect.

Returns

The position vector of the defect, in a variable of type Vector3d.

```
5.2.3.8 double Defect::getX( ) [inherited]
```

Returns the X-coordinate of the defect.

Returns

X-coordinate of the defect.

Definition at line 147 of file defect.cpp.

```
148 {
149    return (this->getValue (0));
150 }
```

```
5.2.3.9 double Defect::getY( ) [inherited]
```

Returns the Y-coordinate of the defect.

Returns

Y-coordinate of the defect.

Definition at line 156 of file defect.cpp.

```
157 {
158    return (this->pos.getValue (1));
159 }
```

```
5.2.3.10 double Defect::getZ( ) [inherited]
```

Returns the Z-coordinate of the defect.

Returns

Z-coordinate of the defect.

Definition at line 165 of file defect.cpp.

```
166 {
167    return (this->pos.getValue (2));
168 }
```

5.2.3.11 double Dislocation::idealTimeIncrement (Vector3d v0, double minDistance, Defect d, Vector3d v1)

Returns the ideal time increment for the dislocation.

A dislocation is not allowed to approach another defect beyond a certain distance, specified by the argument min-Distance. This function calculates the ideal time increment for this dislocation to not collide with the defect.

Parameters

v0	Velocity of the dislocation.
minDistance	Minimum distance of approach to the defect.
d	The defect for which the present dislocation's time increment is to be calculated.
v1	Velocity of the other defect.

Returns

The ideal time increment for this dislocation.

Definition at line 225 of file dislocation.cpp.

```
226 {
       double norm_v0 = v0.magnitude();
if (norm_v0 == 0.0)
227
229
230
         // This dislocation is not moving
231
           return (1000.0);
        }
232
233
234
       // Positions
       Vector3d p0 = this->getPosition();
      Vector3d p1 = d.getPosition();
Vector3d p01 = p1 - p0;
236
237
238
      double norm_p01 = p01.magnitude();
239
240
       if (norm_p01 == 0.0)
241
242
           // The dislocation is lying on top of the obstacle - so it should not move
243
           return (0.0);
        }
244
245
       else
246
247
           // Find out if the dislocation is approaching the defect or not
248
249
           // Velocities
           Vector3d v01 = v1 - v0;
250
           double norm_v01 = v01.magnitude();
2.51
           double dotProduct = v01 * p01;
252
253
           double cosine = dotProduct/(norm_v01 * norm_p01);
254
           if (cosine < 0.0)</pre>
255
                // The dislocation is approaching the other defect return ( (norm_p01 - minDistance)/norm_v01 );
256
2.57
258
259
           else
260
             {
261
               // They are diverging
                // They are diverging
// So any time increment will do
return (1000.0);
2.62
263
264
         }
265
266 }
```

5.2.3.12 bool Dislocation::isMobile ()

Returns whether the dislocation is mobile or pinned.

Returns

Returns true if the dislocation is mobile, false if pinned.

Definition at line 108 of file dislocation.cpp.

```
109 {
110    return (this->mobile);
111 }
```

5.2.3.13 void Dislocation::setBurgers (Vector3d burgers)

Sets the Burgers vector of the dislocation.

Parameters

burgers	Bergers vector of the dislocation.

Definition at line 54 of file dislocation.cpp.

```
55 {
56   this->bvec = burgers;
57 }
```

5.2.3.14 void Dislocation::setLineVector (Vector3d line)

Sets the line vector of the dislocation.

Parameters

```
line Line vector of the dislocation.
```

Definition at line 62 of file dislocation.cpp.

```
63 {
64 this->lvec = line;
65 }
```

5.2.3.15 void Dislocation::setMobile ()

Sets the dislocation as mobile.

Sets the flag mobile to true.

Definition at line 71 of file dislocation.cpp.

```
72 {
73   this->mobile = true;
74 }
```

5.2.3.16 void Dislocation::setPinned ()

Sets the dislocation as pinned.

Sets the flag mobile to false.

Definition at line 80 of file dislocation.cpp.

```
81 {
82   this->mobile = false;
83 }
```

```
5.2.3.17 void Defect::setPosition ( double * a ) [inherited]
```

Sets the position of the defect.

The position of the defect is set to the co-ordinates present in the array pointed to by the argument. Sets the position of the defect as the values in the array pointed to by the argument.

Parameters

```
a Pointer to the array containing the coordinates of the defect.
```

Definition at line 56 of file defect.cpp.

```
57 {
58   this->pos.setVector (a);
59 }
```

```
5.2.3.18 void Defect::setPosition ( double x, double y, double z ) [inherited]
```

Sets the position of the defect.

The position of the defect is set to the co-ordinates specified by the arguments (x, y, z). Sets the position of the defect as the coordinates provided as arguments.

Parameters

X	X-coordinate of the defect.
у	Y-coordinate of the defect.
Z	Z-coordinate of the defect.

Definition at line 69 of file defect.cpp.

```
70 {
71     this->pos.setValue (0, x);
72     this->pos.setValue (1, y);
73     this->pos.setValue (2, z);
74 }
```

```
5.2.3.19 void Defect::setPosition( Vector3d a ) [inherited]
```

Sets the position of the defect.

The position of the defect is set to the position vector fiven by the argument a.

Parameters

```
a Position vector of the defect.
```

Definition at line 81 of file defect.cpp.

```
82 {
83 this->position = a;
```

```
5.2.3.20 void Defect::setX ( double x ) [inherited]
```

Sets the X-coordinate of the defect.

Parameters

X	X-coordinate of the defect.

Definition at line 90 of file defect.cpp.

```
91 {
92   this->pos.setValue (0, x);
93 }
```

5.2.3.21 void Defect::setY (double y) [inherited]

Sets the Y-coordinate of the defect.

Parameters

У	Y-coordinate of the defect.

Definition at line 99 of file defect.cpp.

```
100 {
101   this->pos.setValue (1, y);
102 }
```

5.2.3.22 void Defect::setZ(double z) [inherited]

Sets the Z-coordinate of the defect.

Parameters

```
z Z-coordinate of the defect.
```

Definition at line 108 of file defect.cpp.

```
109 {
110   this->pos.setValue (2, z);
111 }
```

5.2.3.23 Stress Dislocation::stressField (Vector3d p, double mu, double nu) [virtual]

Calculates the stress field due to this dislocation at the position given as argument.

The stress field of the dislocation is calculated at the position indicated by the argument.

Parameters

р	Position vector of the point where the stress field is to be calculated.
mu	Shear modulus in Pascals.
nu	Poisson's ratio.

Returns

Stress tensor, expressed in the global co-ordinate system, giving the value of the stress field at position p.

Reimplemented from Defect.

Definition at line 146 of file dislocation.cpp.

```
147 {
      double principalStresses[3];
148
149
      double shearStresses[3];
150
      {\tt Vector3d}\ r; // {\tt Vector}\ {\tt joining}\ {\tt the}\ {\tt present}\ {\tt dislocation}\ {\tt to}\ {\tt the}\ {\tt point}\ {\tt p}
1.5.1
      r = p - this->pos; // Still in global coordinate system
152
      Vector3d rLocal = this->rotationMatrix * r;
153
                                                           // Rotated to local co-ordinate
154
155
      \ensuremath{//} Calculate the stress field in the local co-ordinate system
      Stress sLocal = this->stressFieldLocal (rLocal, mu, nu);
156
157
      // Calculate the stress field in the global co-ordinate system
158
      Stress sGlobal = (this->rotationMatrix) * sLocal * (^(this->
      rotationMatrix));
160
161
      return (sGlobal);
162 }
```

5.2.3.24 Stress Dislocation::stressFieldLocal (Vector3d p, double mu, double nu)

Calculates the stress field due to the dislocation in the local co-ordinate system.

The stress field due to the dislocation is calculated at the position indicated by the argument. The stress tensor is expressed in the dislocation's local co-ordinate system.

Parameters

р	Position vector of the point where the stress field is to be calculated. This position vector is
	calculated in the local co-ordinate system, taking the dislocation as the origin.
mu	Shear modulus in Pascals.
nu	Poisson's ratio.

Returns

Stress tensor, expressed in the dislocation's local co-ordinate system.

Definition at line 172 of file dislocation.cpp.

```
173 {
174
    double D = ( mu * this - > bm ) / ( 2.0 * PI * ( 1.0 - nu ) ); // Constant for all components of the
      stress tensor
175
176
                              // Terms that appear repeatedly in the stress tensor
    double x, y, denominator;
177
178
     x = p.getValue (0);
     y = p.getValue (1);
179
180
    denominator = pow ( ((x*x) + (y*y)), 2);
181
    182
183
    principalStresses[2] = nu * ( principalStresses[0] + principalStresses[1] );
185
186
     shearStresses[0] = D * x * ( (x*x) - (y*y) ) / denominator;
     shearStresses[1] = 0.0;
187
188
     shearStresses[2] = 0.0;
189
     return (Stress(principalStresses, shearStresses));
191 }
```

5.2.4 Field Documentation

5.2.4.1 double Dislocation::bmag [protected]

Magnitude of the Burgers vector in metres.

The magnitude of the Burgers vector is useful for several calculations such as stress field around the dislocation. Definition at line 44 of file dislocation.h.

5.2.4.2 Vector3d Dislocation::bvec [protected]

Burgers vector of the dislocation.

Definition at line 27 of file dislocation.h.

5.2.4.3 Vector3d Dislocation::lvec [protected]

Line vector if the dislocation.

Definition at line 32 of file dislocation.h.

5.2.4.4 bool Dislocation::mobile [protected]

Boolean term indicating mobility.

For mobile dislocations this term is true and for pinned dislocations it is false.

Definition at line 38 of file dislocation.h.

5.2.4.5 **Vector3d Defect::pos** [protected], [inherited]

Position vector of the defect in 2D space.

Definition at line 26 of file defect.h.

5.2.4.6 RotationMatrix Dislocation::rotationMatrix [protected]

The rotation matrix for rotating from the global to the local co-ordinate system and vice-versa.

This is the rotation matrix that represents the relationship between the global and local co-ordinate systems. It is used to convert tensors and vectors between the two systems. The rotation matrix needs to be calculated once and may be refreshed periodically if lattice rotation is implemented. In the absence of lattice rotation, the matrix will remain invariant.

Definition at line 50 of file dislocation.h.

The documentation for this class was generated from the following files:

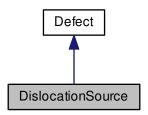
- · dislocation.h
- · dislocation.cpp

5.3 DislocationSource Class Reference

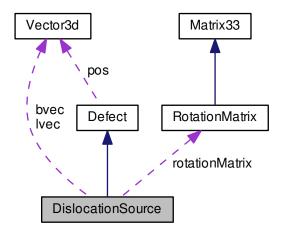
DislocationSource class representing a source of dislocations in the simulation.

#include <dislocationSource.h>

Inheritance diagram for DislocationSource:



Collaboration diagram for DislocationSource:



Public Member Functions

- DislocationSource ()
 - Default constructor.
- DislocationSource (Vector3d burgers, Vector3d line, Vector3d position, double bm, double tau, int nlter) Constructor that explicitly specifies all parameters.
- void setBurgers (Vector3d burgers)

Sets the Burgers vector of the dislocation.

- void setLineVector (Vector3d line)
 - Sets the line vector of the dislocation.
- void setBurgersMagnitude (double bm)
 - Set the magnitude of the Burgers vector.
- void setTauCritical (double tauC)

Set the critical shear stres for dipole emission.

void setNumIterations (int nIter)

Set the number of iterations before a dipole is emitted.

void resetIterationCounter ()

Sets the iteration counter to zero.

Vector3d getBurgers ()

Returns the Burgers vector of the dislocations in the dipole.

Vector3d getLineVector ()

Returns the line vector of the dislocations in the dipole.

double getBurgersMag ()

Returns the magnitude of the Burgers vector.

double getTauCritical ()

Returns the critical shear stress value for dipole emission.

• int getNumIterations ()

Returns the number if iterations that the dislocation source must spend experiencing a shear stress greater than the critical value before it can emit a dislocation dipole.

• int getIterationCount ()

Get the count of the iterations spent at higher than critical shear stress.

• double dipoleNucleationLength (double tau, double mu, double nu)

The nucleation length of the dipole.

void incrementIterationCount ()

Increments the variable countIterations by 1.

• bool ifEmitDipole ()

Checks if the dislocation source has experienced higher than critical shear stress for long enough to emit a dipole.

void setPosition (double *a)

Sets the position of the defect.

void setPosition (double x, double y, double z)

Sets the position of the defect.

void setPosition (Vector3d a)

Sets the position of the defect.

void setX (double x)

Sets the X-coordinate of the defect.

void setY (double y)

Sets the Y-coordinate of the defect.

void setZ (double z)

Sets the Z-coordinate of the defect.

double * getPosition ()

Returns in an array the position.

void getPosition (double *a)

Returns the array position in a pre-allocated array.

• Vector3d getPosition ()

Returns the position vector of the defect.

double getX ()

Returns the X-coordinate of the defect.

• double getY ()

Returns the Y-coordinate of the defect.

• double getZ ()

Returns the Z-coordinate of the defect.

• virtual Stress stressField (Vector3d p, double mu, double nu)

Virtual function for calculating the stress field.

Protected Attributes

· Vector3d bvec

Burgers vector of the dislocation.

Vector3d Ivec

Line vector if the dislocation.

· bool mobile

Boolean term indicating mobility.

· double bmag

Magnitude of the Burgers vector in metres.

· RotationMatrix rotationMatrix

The rotation matrix for rotating from the global to the local co-ordinate system and vice-versa.

· double tauCritical

Critical stress for the emission of a dislocation dipole.

· int nlterations

Number of iterations before a dipole is emitted.

· int countIterations

Counter variable for the number of consecutive iterations the dislocation source has experienced a shear stress greater than its critical value.

· Vector3d pos

Position vector of the defect in 2D space.

5.3.1 Detailed Description

DislocationSource class representing a source of dislocations in the simulation.

This class inherits from the Defect class. This object is basically the representation of a Frank-Read source emitting dislocation dipoles. When the dislocation source experiences a shear stress greater than a critical value for a certain amount of time (or number of iterations), it emits a dislocation dipole with a length that is a function of the applied stress. The properties of this class and the member functions will be declared here.

Definition at line 22 of file dislocationSource.h.

5.3.2 Constructor & Destructor Documentation

5.3.2.1 DislocationSource::DislocationSource ()

Default constructor.

Initializes the dislocation with the default parameters provided in the files dislocationDefaults.h and dislocationSourceDefaults.h.

Definition at line 17 of file dislocationSource.cpp.

5.3.2.2 DislocationSource::DislocationSource (Vector3d burgers, Vector3d line, Vector3d position, double bm, double tau, int nlter)

Constructor that explicitly specifies all parameters.

All parameters: Burgers vector, line vector, position, are specified.

Parameters

burgers	Burgers vector.
line	Line vector.
position	Position of the dislocation source.
bm	Magnitude of the Burgers vector in metres.
tau	Critical shear stress value.
nlter	Number of iterations of experiencing critical stress before a dipole is emitted.

All parameters: Burgers vector, line vector, position, are specified.

Parameters

burgers	Burgers vector.
line	Line vector.
position	Position of the dislocation.
bm	Magnitude of the Burgers vector in metres.
tau	Critical shear stress value.
nlter	Number of iterations of experiencing critical stress before a dipole is emitted.

Definition at line 38 of file dislocationSource.cpp.

```
39 {
40    this->bvec = burgers;
41    this->lvec = line;
42    this->pos = position;
43    this->bmag = bm;
44    this->tauCritical = tau;
45    this->nIterations = nIter;
46    this->countIterations = 0;
```

5.3.3 Member Function Documentation

5.3.3.1 double DislocationSource::dipoleNucleationLength (double tau, double mu, double nu)

The nucleation length of the dipole.

When a dislocation source has experienced a shear stress greater than the critical value for a certain amount of time, it emits a dislocation dipole. In three dimensions, this is equivalent to a dislocation loop emitted by a Frank-Read source. The length of the dipole (or diameter of the loop in 3D) is such that the interaction force between the two dislocations (or line tension in 3D) balances out the applied shear stress.

Parameters

tau	The shear stress experienced by the dislocation source.
mu	Shear modulus of the material, in Pa.
nu	Poisson's ratio.

Returns

The length of the dislocation dipole.

Definition at line 167 of file dislocationSource.cpp.

5.3.3.2 Vector3d DislocationSource::getBurgers ()

Returns the Burgers vector of the dislocations in the dipole.

Returns

The Burgers vector of the dislocations in the dipole.

Definition at line 108 of file dislocationSource.cpp.

```
109 {
110    return (this->bvec);
111 }
```

5.3.3.3 double DislocationSource::getBurgersMag ()

Returns the magnitude of the Burgers vector.

Returns

The magnitude of the Burgers vector.

Definition at line 126 of file dislocationSource.cpp.

```
127 {
128    return (this->bmag);
129 }
```

5.3.3.4 int DislocationSource::getIterationCount ()

Get the count of the iterations spent at higher than critical shear stress.

Returns

Number of iterations spent at higher than critical shear stress.

Definition at line 153 of file dislocationSource.cpp.

```
154 {
155   return (this->countIterations);
156 }
```

5.3.3.5 Vector3d DislocationSource::getLineVector ()

Returns the line vector of the dislocations in the dipole.

Returns

The line vector of the dislocations in the dipole.

Definition at line 117 of file dislocationSource.cpp.

```
118 {
119    return (this->lvec);
120 }
```

5.3.3.6 int DislocationSource::getNumIterations ()

Returns the number if iterations that the dislocation source must spend experiencing a shear stress greater than the critical value before it can emit a dislocation dipole.

Returns

The number if iterations that the dislocation source must spend experiencing a shear stress greater than the critical value before it can emit a dislocation dipole.

Definition at line 144 of file dislocationSource.cpp.

```
145 {
146    return (this->nIterations);
147 }
```

5.3.3.7 Vector3d Defect::getPosition() [inherited]

Returns in an array the position.

Returns the position vector of the defect.

The position of the defect is saved in an array and a pointer to its first term is returned.

Returns

Pointer to the first term of the array containing the position of the defect.

The position vector of the defect, in a variable of type Vector3d.

Definition at line 119 of file defect.cpp.

```
120 {
121    return (this->pos.getVector ());
122 }
```

5.3.3.8 void Defect::getPosition (double * a) [inherited]

Returns the array position in a pre-allocated array.

Returns in the array provided in the argument the position of the defect. The array must be pre-allocated.

Parameters

a Pointer to the location where the defect coordinates are to be populated.

Definition at line 129 of file defect.cpp.

```
130 {
131    a = this->pos.getVector ();
```

```
132 }
```

```
5.3.3.9 Vector3d Defect::getPosition() [inherited]
```

Returns the position vector of the defect.

Returns

The position vector of the defect, in a variable of type Vector3d.

```
5.3.3.10 double DislocationSource::getTauCritical()
```

Returns the critical shear stress value for dipole emission.

Returns

The critical shear stress value for dipole emission.

Definition at line 135 of file dislocationSource.cpp.

```
136 {
137   return (this->tauCritical);
138 }
```

5.3.3.11 double Defect::getX() [inherited]

Returns the X-coordinate of the defect.

Returns

X-coordinate of the defect.

Definition at line 147 of file defect.cpp.

```
148 {
149         return (this->getValue (0));
150 }
```

5.3.3.12 double Defect::getY() [inherited]

Returns the Y-coordinate of the defect.

Returns

Y-coordinate of the defect.

Definition at line 156 of file defect.cpp.

```
157 {
158    return (this->pos.getValue (1));
159 }
```

```
5.3.3.13 double Defect::getZ( ) [inherited]
```

Returns the Z-coordinate of the defect.

Returns

Z-coordinate of the defect.

Definition at line 165 of file defect.cpp.

```
166 {
167    return (this->pos.getValue (2));
168 }
```

```
5.3.3.14 bool DislocationSource::ifEmitDipole ( )
```

Checks if the dislocation source has experienced higher than critical shear stress for long enough to emit a dipole.

The number of iterations for which the dislocation source must experience a shear stress higher than the critical value is given in the member nlterations. When the counter variable countlterations reaches this value, the source is ready to emit a dipole, so a true value is returned. In other cases, false is returned.

Returns

The boolean result of whether the count of iterations is greater than the limiting number of iterations provided at input.

Definition at line 192 of file dislocationSource.cpp.

```
193 {
194    return ( this->countIterations >= this->nIterations );
195 }
```

5.3.3.15 void DislocationSource::incrementIterationCount ()

Increments the variable countIterations by 1.

Definition at line 182 of file dislocationSource.cpp.

```
183 {
184   this->countIterations++;
185 }
```

5.3.3.16 void DislocationSource::resetIterationCounter ()

Sets the iteration counter to zero.

Definition at line 98 of file dislocationSource.cpp.

```
99 {
100 this->countIterations = 0;
101 }
```

5.3.3.17 void DislocationSource::setBurgers (Vector3d burgers)

Sets the Burgers vector of the dislocation.

Parameters

burgers | Burgers vector of the dislocation.

Definition at line 54 of file dislocationSource.cpp.

```
55 {
56   this->bvec = burgers;
57 }
```

5.3.3.18 void DislocationSource::setBurgersMagnitude (double bm)

Set the magnitude of the Burgers vector.

Parameters

bm	Magnitude of the Burgers vector.
-	1 10 1111 1 1 1 0 1 1 1 1 1 1 1 1 1 1 1

Definition at line 72 of file dislocationSource.cpp.

```
73 {
74 this->bmag = bm;
75 }
```

5.3.3.19 void DislocationSource::setLineVector (Vector3d line)

Sets the line vector of the dislocation.

Parameters

```
line Line vector of the dislocation.
```

Definition at line 63 of file dislocationSource.cpp.

```
64 {
65 this->lvec = line;
66 }
```

5.3.3.20 void DislocationSource::setNumIterations (int nlter)

Set the number of iterations before a dipole is emitted.

Parameters

nlter Number of iterations spent at a high shear stress value before a dislocation dipole is emitted.

Definition at line 90 of file dislocationSource.cpp.

```
91 {
92  this->nIterations = nIter;
93 }
```

5.3.3.21 void Defect::setPosition (double * a) [inherited]

Sets the position of the defect.

The position of the defect is set to the co-ordinates present in the array pointed to by the argument. Sets the position of the defect as the values in the array pointed to by the argument.

Parameters

```
a Pointer to the array containing the coordinates of the defect.
```

Definition at line 56 of file defect.cpp.

```
57 {
58   this->pos.setVector (a);
59 }
```

5.3.3.22 void Defect::setPosition (double x, double y, double z) [inherited]

Sets the position of the defect.

The position of the defect is set to the co-ordinates specified by the arguments (x, y, z). Sets the position of the defect as the coordinates provided as arguments.

Parameters

X	X-coordinate of the defect.
У	Y-coordinate of the defect.
Z	Z-coordinate of the defect.

Definition at line 69 of file defect.cpp.

```
70 {
71    this->pos.setValue (0, x);
72    this->pos.setValue (1, y);
73    this->pos.setValue (2, z);
74 }
```

5.3.3.23 void Defect::setPosition (Vector3d a) [inherited]

Sets the position of the defect.

The position of the defect is set to the position vector fiven by the argument a.

Parameters

```
a Position vector of the defect.
```

Definition at line 81 of file defect.cpp.

```
82 {
83   this->position = a;
84 }
```

5.3.3.24 void DislocationSource::setTauCritical (double tauC)

Set the critical shear stres for dipole emission.

Parameters

$\mathit{tauC} \mid$ Critical shear stress for dipole emission.

Definition at line 81 of file dislocationSource.cpp.

```
82 {
83  this->tauCritical = tauC;
84 }
```

```
5.3.3.25 void Defect::setX ( double x ) [inherited]
```

Sets the X-coordinate of the defect.

Parameters

```
x X-coordinate of the defect.
```

Definition at line 90 of file defect.cpp.

```
91 {
92   this->pos.setValue (0, x);
93 }
```

```
5.3.3.26 void Defect::setY ( double y ) [inherited]
```

Sets the Y-coordinate of the defect.

Parameters

```
y Y-coordinate of the defect.
```

Definition at line 99 of file defect.cpp.

```
100 {
101   this->pos.setValue (1, y);
102 }
```

```
5.3.3.27 void Defect::setZ ( double z ) [inherited]
```

Sets the Z-coordinate of the defect.

Parameters

```
z Z-coordinate of the defect.
```

Definition at line 108 of file defect.cpp.

```
109 {
110   this->pos.setValue (2, z);
111 }
```

Virtual function for calculating the stress field.

Returns the value of the stress field of the given defect at the position given by the argument. This is a virtual function and always returns a zero matrix. Classes which inherit this function should have their own implementations of this function to override its behaviour.

Parameters

р	Position vector of the the point where the stress field is to be calculated.
mu	Shear modulus in Pascals.
nu	Poisson's ratio.

Returns

Stress field value at the position p.

Reimplemented in Dislocation.

Definition at line 142 of file defect.h.

5.3.4 Field Documentation

5.3.4.1 double DislocationSource::bmag [protected]

Magnitude of the Burgers vector in metres.

The magnitude of the Burgers vector is useful for several calculations such as stress field around the dislocation.

Definition at line 45 of file dislocationSource.h.

```
5.3.4.2 Vector3d DislocationSource::bvec [protected]
```

Burgers vector of the dislocation.

Definition at line 28 of file dislocationSource.h.

```
5.3.4.3 int DislocationSource::countIterations [protected]
```

Counter variable for the number of consecutive iterations the dislocation source has experienced a shear stress greater than its critical value.

A dislocation source needs to experience a shear stress higher than a critical value, given by tauCritical, for a certain amount of time before it is triggered and it emits a dislocation dipole. This limiting number of iterations is given by the variable nlterations, and this variable countlterations is a counter variable. Once this limit is reached, a dipole is emitted and this counter variable is set to zero.

Definition at line 69 of file dislocationSource.h.

```
5.3.4.4 Vector3d DislocationSource::lvec [protected]
```

Line vector if the dislocation.

Definition at line 33 of file dislocationSource.h.

5.3.4.5 bool DislocationSource::mobile [protected]

Boolean term indicating mobility.

For mobile dislocations this term is true and for pinned dislocations it is false.

Definition at line 39 of file dislocationSource.h.

5.3.4.6 int DislocationSource::nlterations [protected]

Number of iterations before a dipole is emitted.

A dislocation dipole source needs to experience a certain critical level of shear stress for a certain amount of time before it can emit a dipole. The amount of time is represented instead by a number of iterations nlterations.

Definition at line 63 of file dislocationSource.h.

5.3.4.7 Vector3d Defect::pos [protected], [inherited]

Position vector of the defect in 2D space.

Definition at line 26 of file defect.h.

5.3.4.8 RotationMatrix DislocationSource::rotationMatrix [protected]

The rotation matrix for rotating from the global to the local co-ordinate system and vice-versa.

This is the rotation matrix that represents the relationship between the global and local co-ordinate systems. It is used to convert tensors and vectors between the two systems. The rotation matrix needs to be calculated once and may be refreshed periodically if lattice rotation is implemented. In the absence of lattice rotation, the matrix will remain invariant.

Definition at line 51 of file dislocationSource.h.

5.3.4.9 double DislocationSource::tauCritical [protected]

Critical stress for the emission of a dislocation dipole.

A dislocation dipole source needs to experience a certain critical level of shear stress for a certain amount of time before it can emit a dipole. This critical stress is given by tauCritical.

Definition at line 57 of file dislocationSource.h.

The documentation for this class was generated from the following files:

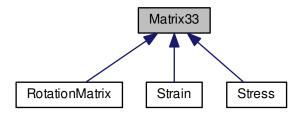
- · dislocationSource.h
- dislocationSource.cpp

5.4 Matrix33 Class Reference

Matrix33 class representing a 3x3 square matrix.

#include <matrix33.h>

Inheritance diagram for Matrix33:



Public Member Functions

• Matrix33 ()

Default constructor.

Matrix33 (double **a)

Constructor with the values provided in a 3x3 matrix.

Matrix33 (Vector3d a)

Constructor to create the matrix from the dyadic product of a vector with itself.

• Matrix33 (Vector3d a, Vector3d b)

Constructor with the vectors, the product of which will result in the matrix.

void setValue (int row, int column, double value)

Function to set the value of an element indicated by its position.

• double getValue (int row, int column)

Returns the value of the element located by the row and column indices provided.

• Matrix33 adjugate ()

Returns the adjugate matrix of the present matrix.

• Matrix33 operator+ (const Matrix33 &) const

Operator for addition of two matrices.

void operator+= (const Matrix33 &)

Operator for reflexive addition of two matrices.

• Matrix33 operator- (const Matrix33 &) const

Operator for the subtraction of two matrices.

• void operator-= (const Matrix33 &)

Operator for reflexive subtraction of two matrices.

Matrix33 operator* (const double &) const

Operator for scaling the matrix by a scalar.

void operator*= (const double &)

Operator for reflexive scaling of the matrix by a scalar.

• Matrix33 operator* (const Matrix33 &) const

Operator for the multiplication of two matrices.

• void operator*= (const Matrix33 &)

Operator for reflexive multiplication of two matrices.

Vector3d operator* (const Vector3d &) const

Operator for the multiplication of a matrix with a vector.

Matrix33 operator[∧] () const

Transpose.

• double operator \sim () const

Determinant.

• Matrix33 operator! () const

Inverse.

Protected Attributes

• double x [3][3]

Array containing the elements of the matrix.

5.4.1 Detailed Description

Matrix33 class representing a 3x3 square matrix.

This class represents a 3x3 square matrix. The member functions and operators define various operations that may be carried out on the matrix.

Definition at line 20 of file matrix33.h.

5.4.2 Constructor & Destructor Documentation

```
5.4.2.1 Matrix33::Matrix33 ( )
```

Default constructor.

Initializes the matrix with all elements equal to 0.0.

Definition at line 17 of file matrix33.cpp.

```
18 {
19    int i, j;
20
21    for (i=0; i<3; i++)
22    {
23        for (j=0; j<3; j++)
24        {
25             this->x[i][j] = 0.0;
26        }
27    }
28 }
```

5.4.2.2 Matrix33::Matrix33 (double ** a)

Constructor with the values provided in a 3x3 matrix.

Populated the mstrix with data present in corresponding elements of the provided 3x3 array.

Parameters

```
a Pointer to the two-dimensional 3x3 array.
```

Definition at line 35 of file matrix33.cpp.

```
36 {
37   int i, j;
38
39   for (i=0; i<3; i++)
40   {
41     for (j=0; j<3; j++)
42     {
43         this->x[i][j] = a[i][j];
```

```
44
45 }
46 }
```

5.4.2.3 Matrix33::Matrix33 (Vector3d a)

Constructor to create the matrix from the dyadic product of a vector with itself.

The matrix is created by performing the dyadic product of the provided vector with itself.

Parameters

a The vector whose dyadic product results in the matrix.

Definition at line 53 of file matrix33.cpp.

```
54 {
55   int i, j;
56
57   for (i=0; i<3; i++)
58   {
59      for (j=0; j<3; j++)
60      {
61          this->x[i][j] = a.x[i] * a.x[j];
62      }
63   }
64 }
```

5.4.2.4 Matrix33::Matrix33 (Vector3d a, Vector3d b)

Constructor with the vectors, the product of which will result in the matrix.

The matrix is created from the product the first vector with the second.

Parameters

а	First vector.
b	Second vector.

Definition at line 72 of file matrix33.cpp.

5.4.3 Member Function Documentation

5.4.3.1 Matrix33 Matrix33::adjugate ()

Returns the adjugate matrix of the present matrix.

The adjugate matrix of the present matrix is returned. The adjugate matrix is calculated by evaluating the determinant of the cofactor matrix of each element, and then replacing the corresponding element position by the value of the determinant. This operation is useful in calculating the inverse of a matrix.

Returns

The adjugate matrix of the present matrix.

Definition at line 129 of file matrix33.cpp.

```
130 {
              Matrix33 adj;
131
132
              adj.x[0][0] = (this->x[1][1]*this->x[2][2]) - (this->x[1][2]*this->x[2][1]);
adj.x[0][1] = (this->x[1][2]*this->x[2][0]) - (this->x[1][0]*this->x[2][2]);
adj.x[0][2] = (this->x[1][0]*this->x[2][1]) - (this->x[1][1]*this->x[2][0]);
133
134
135
136
              adj.x[1][0] = (this->x[2][1]*this->x[0][2]) - (this->x[0][1]*this->x[2][2]);
adj.x[1][1] = (this->x[2][2]*this->x[0][0]) - (this->x[2][0]*this->x[0][2]);
adj.x[1][2] = (this->x[2][0]*this->x[0][1]) - (this->x[2][1]*this->x[0][0]);
137
138
139
140
             adj.x[2][0] = (this->x[0][1]*this->x[1][2]) - (this->x[0][2]*this->x[1][1]);
adj.x[2][1] = (this->x[0][2]*this->x[1][0]) - (this->x[0][0]*this->x[1][2]);
adj.x[2][2] = (this->x[0][0]*this->x[1][1]) - (this->x[1][0]*this->x[0][1]);
141
142
143
144
145
             return (adj);
```

5.4.3.2 double Matrix33::getValue (int row, int column)

Returns the value of the element located by the row and column indices provided.

The value of the element indicated by the arguments row and column is returned. The values of row and column must correspond to array indices, and thus can be one of 0, 1 and 2. In any other case 0.0 is returned.

Parameters

row	Row index of the element.
column	Column index of the element.

Returns

Value of the element located at the given position.

Definition at line 111 of file matrix33.cpp.

```
112 {
113     if (row>=0 && row<3)
114     {
115          if (column>=0 && column<3)
116          {
117                return (this->x[row][column]);
118          }
119     }
120     return (0.0);
121     return (0.0);
```

5.4.3.3 Matrix33 Matrix33::operator! () const

Inverse.

Returns in a new matrix the inverse of the current matrix. If the current matrix is non-invertible, a zero matrix is returned.

Returns

Matrix with the inverse of the current matrix. If the current matrix is non-invertible, a zero matrix is returned.

Definition at line 370 of file matrix33.cpp.

```
372
     Matrix33 r; // Result matrix
373
374
     double determinant = ~(*this);
375
376
     if (determinant == 0.0)
377
378
          \ensuremath{//} The matrix is non-invertible
379
         return (r); // Zero matrix
380
381
     // If we are still here, the matrix is invertible
382
383
     // Transpose
384
385
     Matrix33 tr = ^(*this);
386
     // Find Adjugate matrix
387
388
     Matrix33 adj = tr.adjugate();
389
390
     // Calculate the inverse by dividing the adjugate matrix by the determinant
391
     r = adj * (1.0/determinant);
392
393
     return (r);
394 }
```

5.4.3.4 Matrix33 Matrix33::operator* (const double & p) const

Operator for scaling the matrix by a scalar.

Scales the current matrix by the scalar provided and returns the result in a third matrix.

Returns

Matrix containing the result of scaling the current matrix by the scalar provided as argument.

Definition at line 233 of file matrix33.cpp.

```
235
      int i, j;
      Matrix33 r;
236
237
238
      for (i=0; i<3; i++)</pre>
239
          for (j=0; j<3; j++)</pre>
240
241
               r.x[i][j] = this->x[i][j] * p;
2.42
243
244
245
246
     return (r);
247 }
```

5.4.3.5 Matrix33 Matrix33::operator* (const Matrix33 & p) const

Operator for the multiplication of two matrices.

Multiplies the current matrix with another 3x3 matrix and returns the result in a new matrix.

Returns

The result of the multiplication of the current matrix with the one provided as argument.

Definition at line 271 of file matrix33.cpp.

```
272 {
273    int i, j, k;
274    Matrix33 r;
275
276    for (i=0; i<3; i++)
277    {
278         for (j=0; j<3; j++)
```

5.4.3.6 Vector3d Matrix33::operator* (const Vector3d & v) const

Operator for the multiplication of a matrix with a vector.

Returns in a vector the result of the multiplication of the current matrix with the provided vector.

Returns

The vector resulting from the multiplication of the current matrix with a vector.

Definition at line 311 of file matrix33.cpp.

```
312 {
      Vector3d r(0.0, 0.0, 0.0);
313
314
     int i, j;
316
     for (i=0; i<3; i++)</pre>
317
        for (j=0; j<3; j++)
318
319
             r[i] += this -> x[i][j] * v.x[j];
320
321
      }
323
324
     return (r);
325 }
```

5.4.3.7 void Matrix33::operator*= (const double & p)

Operator for reflexive scaling of the matrix by a scalar.

Scales the current matrix by the scalar provided and populates the current matrix elements with the result.

Definition at line 253 of file matrix33.cpp.

```
254 {
255   int i, j;
256
257   for (i=0; i<3; i++)
258   {
259     for (j=0; j<3; j++)
260     {
261         this->x[i][j] *= p;
262     }
263   }
264 }
```

5.4.3.8 void Matrix33::operator*= (const Matrix33 & p)

Operator for reflexive multiplication of two matrices.

Multiplies the current matrix with another 3x3 matrix and populates the elements of the current matrix with the result. Definition at line 295 of file matrix33.cpp.

```
296 {
297     Matrix33* r = new Matrix33;
298
299     *r = (*this) * p;
300     *this = *r;
301
302     delete(r);
303     r = NULL;
304 }
```

5.4.3.9 Matrix33 Matrix33::operator+ (const Matrix33 & p) const

Operator for addition of two matrices.

Adds the current matrix to the provided matrix and returns a third matrix with the result.

Returns

Matrix containing the sum of the present matrix and the one provided.

Definition at line 155 of file matrix33.cpp.

```
156 {
      int i, j;
Matrix33 r;
157
159
160
       for (i=0; i<3; i++)</pre>
161
           for (j=0; j<3; j++)</pre>
162
163
                r.x[i][j] = this->x[i][j] + p.x[i][j];
164
166
       }
168 return (r);
169 }
167
```

5.4.3.10 void Matrix33::operator+= (const Matrix33 & p)

Operator for reflexive addition of two matrices.

Adds the current matrix to the provided matrix and populates the current matrix elements with the result.

Definition at line 175 of file matrix33.cpp.

5.4.3.11 Matrix33 Matrix33::operator-(const Matrix33 & p) const

Operator for the subtraction of two matrices.

Subtracts the given matrix from the current matrix and returns the result in a new matrix.

Returns

Matrix containing the result of subtracting the provided matrix from the current matrix.

Definition at line 194 of file matrix33.cpp.

```
195 {
     int i, j;
Matrix33 r;
196
197
198
      for (i=0; i<3; i++)
200
          for (j=0; j<3; j++)
201
202
              r.x[i][j] = this->x[i][j] - p.x[i][j];
203
204
205
206
207
     return (r);
208 1
```

5.4.3.12 void Matrix33::operator-= (const Matrix33 & p)

Operator for reflexive subtraction of two matrices.

Subtracts the given matrix from the current matrix and populates the current matrix with the result.

Definition at line 214 of file matrix33.cpp.

```
215 {
216    int i, j;
217
218    for (i=0; i<3; i++)
219    {
220         for (j=0; j<3; j++)
221         {
222             this->x[i][j] -= p.x[i][j];
223         }
224     }
225 }
```

5.4.3.13 Matrix33 Matrix33::operator () const

Transpose.

Performs the transpose of the current matrix.

Returns

A new matrix with the transpose of the current matrix.

Definition at line 333 of file matrix33.cpp.

```
334 {
     Matrix33 r;
335
336
      int i, j;
337
      for (i=0; i<3; i++)</pre>
338
339
340
          for (j=0; j<3; j++)</pre>
341
               r.x[i][j] = this->x[j][i];
342
343
345
346
      return (r);
347 }
```

5.4.3.14 double Matrix33::operator \sim () const

Determinant.

Calculates the determinant of the current matrix.

Returns

Returns the determinant of the current matrix.

Definition at line 354 of file matrix33.cpp.

```
356
                                                                            double d = 0.0;
357
                                                                         358
                                                                              x[1][2]));
359
                                                                       d += this.x[0][1] * ( (this->x[1][2]*this->x[2][0]) - (this->x[1][0]*this-> (this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x
                                                                            x[2][2]));
360
                                                                                                                                            this.x[0][2] * ( (this->x[1][0]*this->x[2][1]) - (this->x[2][0]*this->x[2][0] + (this->x[2][0]) + (this-x[2][0]) + (this-x[2]
                                                                            x[1][1]));
361
362
                                                                       return (d);
363 }
```

5.4.3.15 void Matrix33::setValue (int row, int column, double value)

Function to set the value of an element indicated by its position.

The element indicated by the arguments row and column is set to the value provided. The values of row and column must correspond to array indices, and thus can be one of 0, 1 and 2. In any other case 0.0 is returned.

Parameters

rov	Row index of the element.
columi	Column index of the element.
value	Value that the element is to be set to.

Definition at line 93 of file matrix33.cpp.

5.4.4 Field Documentation

```
5.4.4.1 double Matrix33::x[3][3] [protected]
```

Array containing the elements of the matrix.

Definition at line 26 of file matrix33.h.

The documentation for this class was generated from the following files:

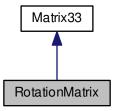
- matrix33.h
- · matrix33.cpp

5.5 RotationMatrix Class Reference

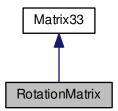
RotationMatrix class to represent a rotation matrix.

#include <rotationMatrix.h>

Inheritance diagram for RotationMatrix:



Collaboration diagram for RotationMatrix:



Public Member Functions

• RotationMatrix ()

Default constructor.

RotationMatrix (Vector3d *unPrimed, Vector3d *primed)

Defines the rotation matrix based on two co-ordinate systems.

• void setValue (int row, int column, double value)

Function to set the value of an element indicated by its position.

double getValue (int row, int column)

Returns the value of the element located by the row and column indices provided.

• Matrix33 adjugate ()

Returns the adjugate matrix of the present matrix.

Matrix33 operator+ (const Matrix33 &) const

Operator for addition of two matrices.

• void operator+= (const Matrix33 &)

Operator for reflexive addition of two matrices.

• Matrix33 operator- (const Matrix33 &) const

Operator for the subtraction of two matrices.

void operator-= (const Matrix33 &)

Operator for reflexive subtraction of two matrices.

• Matrix33 operator* (const double &) const

Operator for scaling the matrix by a scalar.

• Matrix33 operator* (const Matrix33 &) const

Operator for the multiplication of two matrices.

Vector3d operator* (const Vector3d &) const

Operator for the multiplication of a matrix with a vector.

void operator*= (const double &)

Operator for reflexive scaling of the matrix by a scalar.

void operator*= (const Matrix33 &)

Operator for reflexive multiplication of two matrices.

Matrix33 operator[∧] () const

Transpose.

Determinant.

· Matrix33 operator! () const

Inverse.

Protected Attributes

• double x [3][3]

Array containing the elements of the matrix.

5.5.1 Detailed Description

RotationMatrix class to represent a rotation matrix.

The member functions of this class create a rotation matrix for carrying out rotations in 3D and transformation of axes.

Definition at line 19 of file rotationMatrix.h.

5.5.2 Constructor & Destructor Documentation

5.5.2.1 RotationMatrix::RotationMatrix ()

Default constructor.

Initializes the rotation matrix with a unit matrix.

Definition at line 14 of file rotationMatrix.cpp.

```
15 {
16
     int i, j;
17
     18
19
               this->setValue ( i, j, 1.0 );
23
           else {
               this->setValue ( i, j, 0.0 );
24
25
26
        }
     }
28 }
```

5.5.2.2 RotationMatrix::RotationMatrix (Vector3d * unPrimed, Vector3d * primed)

Defines the rotation matrix based on two co-ordinate systems.

The rotation matrix is created using the axes of the two co-ordinate systems provided as arguments. The vectors must be normalized to be unit vectors.

Parameters

unPrimed	Pointer to the array containing the three axes vectors of the unprimed (old) system.
primed	Pointer to the array containing the three axes vectors of the primed (new) system.

Definition at line 36 of file rotationMatrix.cpp.

```
37 {
38     int i, j;
39
40     for ( i=0; i<3; i++ ) {
41          for ( j=0; j<3; j++ ) {
42                this->setValue ( i, j, primed[i]*unPrimed[j] );
43          }
44     }
45 }
```

5.5.3 Member Function Documentation

5.5.3.1 Matrix33 Matrix33::adjugate() [inherited]

Returns the adjugate matrix of the present matrix.

The adjugate matrix of the present matrix is returned. The adjugate matrix is calculated by evaluating the determinant of the cofactor matrix of each element, and then replacing the corresponding element position by the value of the determinant. This operation is useful in calculating the inverse of a matrix.

Returns

The adjugate matrix of the present matrix.

Definition at line 129 of file matrix33.cpp.

```
130 {
131
       Matrix33 adi:
133
       {\tt adj.x[0][0] = (this->x[1][1]*this->x[2][2]) - (this->x[1][2]*this->x[2][1]);}
       adj.x[0][1] = (this->x[1][2]*this->x[2][0]) - (this->x[1][0]*this->x[2][2]);
134
       adj.x[0][2] = (this->x[1][0]*this->x[2][1]) - (this->x[1][1]*this->x[2][0]);
135
136
137
       adj.x[1][0] = (this->x[2][1]*this->x[0][2]) - (this->x[0][1]*this->x[2][2]);
       adj.x[1][0] (this->x[2][2]*this->x[0][0]) - (this->x[2][0]*this->x[0][2]);
adj.x[1][2] = (this->x[2][0]*this->x[0][1]) - (this->x[2][1]*this->x[0][0]);
138
139
140
141
       adj.x[2][0] = (this->x[0][1]*this->x[1][2]) - (this->x[0][2]*this->x[1][1]);
       adj.x[2][1] = (this->x[0][2]*this->x[1][0]) - (this->x[0][0]*this->x[1][2]);
adj.x[2][2] = (this->x[0][0]*this->x[1][1]) - (this->x[1][0]*this->x[0][1]);
142
143
144
145
       return (adj);
146 }
```

5.5.3.2 double Matrix33::getValue (int row, int column) [inherited]

Returns the value of the element located by the row and column indices provided.

The value of the element indicated by the arguments row and column is returned. The values of row and column must correspond to array indices, and thus can be one of 0, 1 and 2. In any other case 0.0 is returned.

Parameters

row	Row index of the element.
column	Column index of the element.

Returns

Value of the element located at the given position.

Definition at line 111 of file matrix33.cpp.

5.5.3.3 Matrix33 Matrix33::operator! () const [inherited]

Inverse.

Returns in a new matrix the inverse of the current matrix. If the current matrix is non-invertible, a zero matrix is returned

Returns

Matrix with the inverse of the current matrix. If the current matrix is non-invertible, a zero matrix is returned.

Definition at line 370 of file matrix33.cpp.

```
372
     Matrix33 r; // Result matrix
373
374
     double determinant = \sim(*this);
375
376
     if (determinant == 0.0)
377
378
         // The matrix is non-invertible
379
         return (r);
                         // Zero matrix
380
381
     // If we are still here, the matrix is invertible
382
383
     // Transpose
384
385
     Matrix33 tr = ^(*this);
386
     // Find Adjugate matrix
387
388
     Matrix33 adj = tr.adjugate();
389
     // Calculate the inverse by dividing the adjugate matrix by the determinant
391
     r = adj * (1.0/determinant);
392
393
     return (r);
394 }
```

5.5.3.4 Matrix33 Matrix33::operator* (const double & p) const [inherited]

Operator for scaling the matrix by a scalar.

Scales the current matrix by the scalar provided and returns the result in a third matrix.

Returns

Matrix containing the result of scaling the current matrix by the scalar provided as argument.

Definition at line 233 of file matrix33.cpp.

```
234 {
      int i, j;
Matrix33 r;
235
236
237
      for (i=0; i<3; i++)</pre>
2.38
239
240
          for (j=0; j<3; j++)
242
               r.x[i][j] = this->x[i][j] * p;
             }
243
244
       }
245
246
      return (r);
247 }
```

5.5.3.5 Matrix33 Matrix33::operator* (const Matrix33 & p) const [inherited]

Operator for the multiplication of two matrices.

Multiplies the current matrix with another 3x3 matrix and returns the result in a new matrix.

Returns

The result of the multiplication of the current matrix with the one provided as argument.

Definition at line 271 of file matrix33.cpp.

```
int i, j, k;
Matrix33 r;
274
275
276
      for (i=0; i<3; i++)</pre>
277
278
           for (j=0; j<3; j++)</pre>
279
280
               r.x[i][j] = 0.0;
281
              for (k=0; k<3; k++)
282
                    r.x[i][j] += this->x[i][k] * p.x[k][j];
283
284
285
             }
286
       }
287
288
     return (r);
289 }
```

5.5.3.6 Vector3d Matrix33::operator*(const Vector3d & v) const [inherited]

Operator for the multiplication of a matrix with a vector.

Returns in a vector the result of the multiplication of the current matrix with the provided vector.

Returns

The vector resulting from the multiplication of the current matrix with a vector.

Definition at line 311 of file matrix33.cpp.

5.5.3.7 void Matrix33::operator*=(const double & p) [inherited]

Operator for reflexive scaling of the matrix by a scalar.

Scales the current matrix by the scalar provided and populates the current matrix elements with the result.

Definition at line 253 of file matrix33.cpp.

5.5.3.8 void Matrix33::operator*=(const Matrix33 & p) [inherited]

Operator for reflexive multiplication of two matrices.

Multiplies the current matrix with another 3x3 matrix and populates the elements of the current matrix with the result. Definition at line 295 of file matrix33.cpp.

```
296 {
297    Matrix33* r = new Matrix33;
298
299    *r = (*this) * p;
300    *this = *r;
301
302    delete(r);
303    r = NULL;
304 }
```

5.5.3.9 Matrix33 Matrix33::operator+(const Matrix33 & p) const [inherited]

Operator for addition of two matrices.

Adds the current matrix to the provided matrix and returns a third matrix with the result.

Returns

Matrix containing the sum of the present matrix and the one provided.

Definition at line 155 of file matrix33.cpp.

```
156 {
157    int i, j;
158    Matrix33 r;
159
160    for (i=0; i<3; i++)
161    {
162         for (j=0; j<3; j++)
163         {
```

5.5.3.10 void Matrix33::operator+= (const Matrix33 & p) [inherited]

Operator for reflexive addition of two matrices.

Adds the current matrix to the provided matrix and populates the current matrix elements with the result.

Definition at line 175 of file matrix33.cpp.

5.5.3.11 Matrix33 Matrix33::operator-(const Matrix33 & p) const [inherited]

Operator for the subtraction of two matrices.

Subtracts the given matrix from the current matrix and returns the result in a new matrix.

Returns

Matrix containing the result of subtracting the provided matrix from the current matrix.

Definition at line 194 of file matrix33.cpp.

```
195 {
196
      int i, j;
      Matrix33 r;
198
199
      for (i=0; i<3; i++)</pre>
200
          for (j=0; j<3; j++)</pre>
201
202
              r.x[i][j] = this->x[i][j] - p.x[i][j];
204
205
      }
206
207
     return (r);
208 }
```

5.5.3.12 void Matrix33::operator-= (const Matrix33 & p) [inherited]

Operator for reflexive subtraction of two matrices.

Subtracts the given matrix from the current matrix and populates the current matrix with the result.

Definition at line 214 of file matrix33.cpp.

```
215 {
216    int i, j;
217
218    for (i=0; i<3; i++)
219    {
220         for (j=0; j<3; j++)
```

5.5.3.13 Matrix33 Matrix33::operator^() const [inherited]

Transpose.

Performs the transpose of the current matrix.

Returns

A new matrix with the transpose of the current matrix.

Definition at line 333 of file matrix33.cpp.

```
334 {
335
      Matrix33 r;
336
      int i, j;
337
      for (i=0; i<3; i++)</pre>
338
339
340
           for (j=0; j<3; j++)</pre>
341
342
               r.x[i][j] = this->x[j][i];
343
344
        }
345
346
      return (r);
```

5.5.3.14 double Matrix33::operator ∼ () const [inherited]

Determinant.

Calculates the determinant of the current matrix.

Returns

Returns the determinant of the current matrix.

Definition at line 354 of file matrix33.cpp.

```
355 {
356          double d = 0.0;
357
358          d += this.x[0][0] * ( (this->x[1][1]*this->x[2][2]) - (this->x[2][1]*this->
          x[1][2]) );
359          d += this.x[0][1] * ( (this->x[1][2]*this->x[2][0]) - (this->x[1][0]*this->
          x[2][2]) );
360          d += this.x[0][2] * ( (this->x[1][0]*this->x[2][1]) - (this->x[2][0]*this->
          x[1][1]) );
361
362          return (d);
363 }
```

5.5.3.15 void Matrix33::setValue (int row, int column, double value) [inherited]

Function to set the value of an element indicated by its position.

The element indicated by the arguments row and column is set to the value provided. The values of row and column must correspond to array indices, and thus can be one of 0, 1 and 2. In any other case 0.0 is returned.

Parameters

row	Row index of the element.
column	Column index of the element.
value	Value that the element is to be set to.

Definition at line 93 of file matrix33.cpp.

5.5.4 Field Documentation

5.5.4.1 double Matrix33::x[3][3] [protected], [inherited]

Array containing the elements of the matrix.

Definition at line 26 of file matrix33.h.

The documentation for this class was generated from the following files:

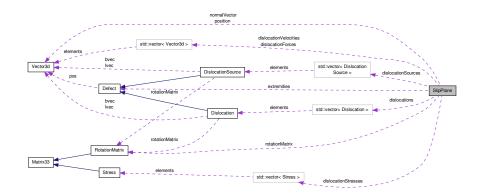
- rotationMatrix.h
- rotationMatrix.cpp

5.6 SlipPlane Class Reference

SlipPlane class representing a slip plane in the simulation.

```
#include <slipPlane.h>
```

Collaboration diagram for SlipPlane:



Public Member Functions

• SlipPlane ()

Default constructor.

• SlipPlane (Vector3d *ends, Vector3d normal, Vector3d pos, std::vector< Dislocation > dislocationList, std::vector< DislocationSource > dislocationSourceList)

Constructor that specifies all members explicitly.

void setExtremities (Vector3d *ends)

Set the extremities of the slip plane.

void setNormal (Vector3d normal)

Set the normal vector of the slip plane.

void setPosition (Vector3d pos)

Set the position of the slip plane.

void setDislocationList (std::vector< Dislocation > dislocationList)

Set the list of dislocations of the slip plane.

void setDislocationSourceList (std::vector < DislocationSource > dislocationSourceList)

Set the list of dislocation sources on the slip plane.

Vector3d getExtremity (int i)

Get the position vector of the extremity whose index is provided as argument.

Defect * getExtremities ()

Get the position vectors of the extremities of the slip plane.

Vector3d getNormal ()

Get the normal vector of the slip plane.

• Vector3d getPosition ()

Get the position vector of the slip plane.

bool getDislocation (int i, Dislocation *d)

Get the dislocation on the slip plane indicated by the index provided as argument.

std::vector< Dislocation > getDislocationList ()

Get the entire vector container which holds the dislocations lying on this slip plane.

int getNumDislocations ()

Get the number of dislocations.

bool getDislocationSource (int i, DislocationSource *dSource)

Get the dislocation source on the slip plane indicated by the index provided as argument.

int getNumDislocationSources ()

Get the number of dislocation sources.

std::vector< DislocationSource > getDislocationSourceList ()

Get the entire vector container which holds the dislocation sources lying on this slip plane.

• RotationMatrix getRotationMatrix ()

Get the rotation matrix for this slip plane.

Vector3d getAxis (int i)

Get the axis (expressed in the global co-ordinate system) of the slip plane's local co-ordinate system, as indicated by the argument. (0, 1, 2)=(x, y, z).

void calculateRotationMatrix ()

Calculates the rotation matrix for this slip plane.

• void calculateDislocationStresses (Stress appliedStress, double mu, double nu)

Calculates the total stress field experienced by each dislocation and stored it in the STL vector container dislocation-Stresses.

void calculateDislocationForces (double tau_crss)

This function populates the STL vector container dislocationForces with the Peach-Koehler force experienced by each dislocation.

void calculateVelocities (double B)

Calculates the velocities of dislocations and stores them in the std::vector container velocities.

• void calculateTimeIncrement (double minDistance, double minDt)

Calculate the time increment based on the velocities of the dislocations.

void moveDislocations ()

Displaces the dislocations according to their velocities and the time increment.

double distanceFromExtremity (Vector3d pos, int n)

The distance of the point pos from the n^{\wedge} th extremity is returned.

void sortDislocations ()

Sorts the dislocations present on the slip plane in the ascending order of distance from the first extremity.

Protected Attributes

• Defect extremities [2]

The extremities of the slip plane.

Vector3d normalVector

The normal vector to the slip plane.

· Vector3d position

The position vector of the slip plane.

• std::vector< Dislocation > dislocations

STL vector container with dislocations.

std::vector < Stress > dislocationStresses

STL vector container with the stress fields of dislocations.

std::vector< Vector3d > dislocationForces

The Peach-Koehler force experienced by each dislocation.

std::vector< Vector3d > dislocationVelocities

STL vector container with dislocation velocities.

std::vector < DislocationSource > dislocationSources

STL vector container with dislocation sources.

double dt

Time increment for the slip plane.

RotationMatrix rotationMatrix

Rotation matrix for co-ordinate system transformations.

5.6.1 Detailed Description

SlipPlane class representing a slip plane in the simulation.

This is the definition of the class SlipPlane. It represents a slip plane in the simulation. A slip plane is considered to be a collection of defects, such as dislocations and dislocation sources. In these simulations in two dimensions, the slip plane becomes a straight line. Its attributes are: position vectors of the extremities, normal vector (since we are concerned with the cubic system here, the normal vector's indices are the same as those of the plane), and the collection of defects.

Definition at line 29 of file slipPlane.h.

5.6.2 Constructor & Destructor Documentation

```
5.6.2.1 SlipPlane::SlipPlane ( )
```

Default constructor.

The slip plane is initialized with default parameters specified in the file slipPlaneDefaults.h.

Definition at line 17 of file slipPlane.cpp.

```
18 {
    // Initialize the default variables.
19
    Vector3d pos(DEFAULT_SLIPPLANE_POSITION_0,
20
                DEFAULT_SLIPPLANE_POSITION_1
21
                DEFAULT_SLIPPLANE_POSITION_2);
23
    Vector3d normal(DEFAULT_SLIPPLANE_NORMALVECTOR_0,
                   DEFAULT_SLIPPLANE_NORMALVECTOR_1,
24
                   DEFAULT SLIPPLANE NORMALVECTOR 2);
25
    Vector3d ends[2];
27
    ends[0] = Vector3d(DEFAULT_SLIPPLANE_EXTREMITY1_0,
28
                      DEFAULT_SLIPPLANE_EXTREMITY1_1,
29
                      DEFAULT_SLIPPLANE_EXTREMITY1_2);
   30
31
                      DEFAULT_SLIPPLANE_EXTREMITY2_2);
32
    std::vector<Dislocation> dislocationList(1, Dislocation());
```

```
34    std::vector<DislocationSource> dislocationSourceList(1, DislocationSource());
35
    *this = SlipPlane(ends, normal, pos, dislocationList, dislocationSourceList);
37 }
```

5.6.2.2 SlipPlane::SlipPlane (Vector3d * ends, Vector3d normal, Vector3d pos, std::vector< Dislocation > dislocationList, std::vector< DislocationSource > dislocationSourceList)

Constructor that specifies all members explicitly.

The slip plane is initialized with parameters specified in the arguments.

Parameters

ends	Pointer to an array of type Vector3d, containing the position vectors of the extremities of the
	slip plane in consecutive locations.
normal	The normal vector of the slip plane.
pos	The position vector of the slip plane. (This parameter is useful for locating the slip plane within
	a slip system)
dislocationList	A vector container of type Dislocation containing the dislocations lying on this slip plane.
dislocation-	A vector container of type DislocationSource containing the dislocation sources lying on this
SourceList	slip plane.

Definition at line 48 of file slipPlane.cpp.

```
49 {
50
    this->setExtremities (ends);
51
    this->setNormal (normal);
52
    this->setPosition (pos);
    this->setDislocationList (dislocationList);
53
    this->setDislocationSourceList (dislocationSourceList);
54
    // Fill the vectors and stresses with zero vectors and stresses
    int nDisl = this->getNumDislocations ();
58
    this->dislocationStresses.resize(nDisl, Stress ());
    this->dislocationVelocities.resize(nDisl, Vector3d());
59
60
    this->dislocationForces.resize(nDisl, Vector3d());
61
     // Time increment
63
    this->dt = 0;
64
6.5
    this->calculateRotationMatrix ();
66 }
```

5.6.3 Member Function Documentation

5.6.3.1 void SlipPlane::calculateDislocationForces (double tau_crss)

This function populates the STL vector container dislocationForces with the Peach-Koehler force experienced by each dislocation.

This function calculates the Peach-Koehler force experienced by each dislocation using the function Dislocation::forcePeachKoehler and the STL vector SlipPlane::dislocationStresses. The argument tau_crss is the Critical Resolved Shear Stress in Pa.

Parameters

```
tau_crss | Critical Resolved Shear Stress in Pa.
```

Definition at line 354 of file slipPlane.cpp.

```
355 {
356 std::vector<Dislocation>::iterator d; // Iterator for dislocations
357 std::vector<Vector3d>::iterator f; // Iterator for forces
358 std::vector<Stress>::iterator s; // Iterator for stresses
```

```
359
360
       s = this->dislocationStresses.begin();
361
       f = this->dislocationForces.begin();
362
363
       for (d = this->dislocations.begin(); d!=this->dislocations.end(); d++)
364
           f = d->forcePeachKoehler (*s, tau_crss);
365
366
367
          f++;
368
369 }
```

5.6.3.2 void SlipPlane::calculateDislocationStresses (Stress appliedStress, double mu, double nu)

Calculates the total stress field experienced by each dislocation and stored it in the STL vector container dislocation-Stresses.

The total stress field is calculated as a superposition of the applied stress field and the stress fields experienced by each dislocation due to every other dislocation in the simulation.

Parameters

appliedStress	The stress applied externally.
mu	Shear modulus of the material.
nu	Poisson's ratio.

Definition at line 322 of file slipPlane.cpp.

```
323
      std::vector<Dislocation>::iterator dl;  // Iterator for each dislocation
std::vector<Dislocation>::iterator d2;  // Nested iterator
324
325
326
                                              // Iterator for the Stress
      std::vector<Stress>::iterator s;
327
328
                                              // Position vector
329
330
      s = this->dislocationStresses.begin();
      331
332
333
           *s = appliedStress;
334
          p = d1->getPosition();
335
           for (d2 = this->dislocations.begin(); d2!=this->dislocations.end(); d2++)
336
337
              if (d1==d2)
338
                {
339
                  continue;
              else
341
342
               {
343
                  *s = *s + d2 -> stressField(p, mu, nu);
344
345
        }
347 }
```

5.6.3.3 void SlipPlane::calculateRotationMatrix ()

Calculates the rotation matrix for this slip plane.

The slip plane has a local co-ordinate system whose axes are the following: z-axis||normal vector and x-axis||slip plane vector (vector joining the extremities). The rotation matrix is calculated in order to carry out transformations between the global and local co-ordinate systems.

Definition at line 289 of file slipPlane.cpp.

```
290 {
291    Vector3d *unPrimed = new Vector3d[3]; // Old system (global)
292    Vector3d *primed = new Vector3d[3]; // New system (local)
293
294    int i, j;
295
```

```
296
      // Prepare the global and local systems
297
      for (i=0; i<3; i++)
298
299
        for (j=0; j<3; j++)</pre>
300
          unPrimed[i].setValue(j, (double)(i==j));
301
302
303
       primed[i] = this->getAxis(i);
304
305
306
      // Calculate the rotationMatrix
307
308
      this->rotationMatrix = RotationMatrix(unPrimed, primed);
309
310
311
      delete(unPrimed);
                            unPrimed = NULL;
312
     delete(primed);
                            primed = NULL;
313 }
```

5.6.3.4 void SlipPlane::calculateTimeIncrement (double minDistance, double minDt)

Calculate the time increment based on the velocities of the dislocations.

In order to avoid the collision of dislocations with similar sign of Burgers vector, it is important to specify a minimum distance of approach between dislocations. When a dislocation reaches this limit, it is pinned. The velocities of the dislocations all being different, a time increment needs to be evaluated, which will limit the distance traveled by the dislocations in a given iteration.

Parameters

minDistance	Minimum distance of approach between dislocations having Burgers vectors of the same sign.
minDt	The smallest time step permissible. Dislocations having time steps smaller than this are made
	immobile for the present iteration.

Definition at line 408 of file slipPlane.cpp.

```
409
410
       // Get the number of dislocations
411
       int nDisl = this->dislocations.size();
412
413
       // Vector of time increments
414
       std::vector<double> timeIncrement(nDisl, 1000.0);
415
416
       // Position vectors
417
       Vector3d p0, p1;
418
      double norm_p01;
419
420
       // Velocity vectors
421
       Vector3d v0. v1:
422
      double norm v01;
423
424
                      // Counter for the loop
425
       double t1, t2;
426
       double dtMin; // Minimum time increment
427
428
       // For the first dislocation, the time increment has to be calculated
      // for approach to both a dislocation and the slip plane extremity.
429
430
       // Time for slip plane extremity
431
       t1 = this->dislocations[0].idealTimeIncrement(this->
      dislocationVelocities[0],
432
                                                       minDistance,
                                                       this->extremity[0],
433
                                                       Vector3d(0.0, 0.0, 0.0));
434
       t2 = this->dislocations[0].idealTimeIncrement(this->
435
      dislocationVelocities[0],
436
                                                       minDistance,
437
                                                       this->dislocations[1],
                                                       this->dislocationVelocities[1]);
438
       \ensuremath{//} Choose the smaller of the two
439
       timeIncrement[0] = t1 < t2 ? t1:t2;
440
441
       if (timeIncrement[0] < minDt)</pre>
442
443
           // This dislocation should not move in this iteration because it might collide with the next defect
444
           timeIncrement[0] = minDt;
445
           this->dislocationVelocities[0] = Vector3d(0.0, 0.0, 0.0);
446
           // The other defect is a slip plane extremity
```

```
// This dislocation will not move any more
           this->dislocations[0].setPinned();
449
450
451
452
       for (i=1; i<(nDisl-1); i++)</pre>
453
           t1 = this->dislocations[i].idealTimeIncrement(this->
454
      dislocationVelocities[i],
                                                           minDistance,
455
456
                                                           this->dislocations[i-1],
                                                           this->dislcoationVelocities[i-1]);
457
           t2 = this->dislocations[i].idealTimeIncrement(this->
458
      dislocationVelocities[i],
459
460
                                                           this->dislocations[i+1],
461
                                                           this->dislcoationVelocities[i+1]);
           timeIncrement[i] = t1 < t2 ? t1 t2:
462
463
464
           if (timeIncrement[i] < minDt)</pre>
465
             {
               // This dislocation should not move in this iteration because it might collide with the next
       defect
467
               timeIncrement[i] = minDt;
               this->dislocationVelocities[i] = Vector3d(0.0, 0.0, 0.0);
468
             }
469
470
       }
471
472
       // For the last dislocation, the time increment has to be calculated
473
       // for approach to both a dislocation and the slip plane extremity.
       // Time for slip plane extremity
474
475
       i=nDisl-1;
476
       t1 = this->dislocations[i].idealTimeIncrement(this->
      dislocationVelocities[i],
477
                                                       minDistance,
478
                                                       this->extremity[1],
                                                       Vector3d(0.0, 0.0, 0.0));
479
       t2 = this->dislocations[i].idealTimeIncrement(this->
480
      dislocationVelocities[i],
481
                                                       minDistance,
482
                                                       this->dislocations[i-1],
483
                                                       this->dislocationVelocities[i-1]);
       // Choose the smaller of the two
484
       timeIncrement[i] = t1 < t2 ? t1:t2;</pre>
485
486
487
       if (timeIncrement[i] < minDt)</pre>
488
489
           // This dislocation should not move in this iteration because it might collide with the next defect
490
           timeIncrement[i] = minDt;
           this->dislocationVelocities[i] = Vector3d(0.0, 0.0, 0.0);
491
492
493
           // The other defect is a slip plane extremity
494
           // This dislocation will not move any more
495
           this->dislocations[i].setPinned();
496
497
498
       dtMin = 1000;
       for (i=0; i<nDisl; i++)</pre>
499
500
501
           if (timeIncrement[i] < dtMin)</pre>
502
503
               dtMin = timeIncrement[i];
504
505
506
507
       this->dt = dtMin;
508 }
```

5.6.3.5 void SlipPlane::calculateVelocities (double B)

Calculates the velocities of dislocations and stores them in the std::vector container velocities.

The velocities of the dislocations are calculated and stored in the std::vector container called velocities. The velocities are calculated using the proportionality law between them and the Peach-Koehler force, using the drag coefficient B as the constant of proportionality. param B The drag coefficient.

Definition at line 376 of file slipPlane.cpp.

```
381
382
       d = this->dislocations.begin();
383
       f = this->dislocationForces.begin();
384
      v = this->dislocationVelocities.begin();
385
386
       while (v != this->dislocationVelocities.end())
387
388
           if (d->isMobile())
389
               *v = (*f)/B;
390
            }
391
392
           else
393
394
              *v = Vector3d(0.0, 0.0, 0.0);
395
396
          d++;
397
           f++;
398
          v++;
399
400 }
```

5.6.3.6 double SlipPlane::distanceFromExtremity (Vector3d pos, int n)

The distance of the point pos from the n^{\wedge} th extremity is returned.

Parameters

pos	Position vector of the point whose distance is to be calculated.
n	Index of the extremity. Can be only 0 or 1. In all other cases 0.0 is returned.

Returns

Distance of the point pos from the n^{\wedge} th extremity of the slip plane.

Definition at line 539 of file slipPlane.cpp.

5.6.3.7 Vector3d SlipPlane::getAxis (int i)

Get the axis (expressed in the global co-ordinate system) of the slip plane's local co-ordinate system, as indicated by the argument. (0, 1, 2)=(x, y, z).

Parameters

```
i Index of the axis that is to be returned. (0, 1, 2)=(x, y, z).
```

Returns

The desired axis of the slip plane's local co-ordinate system, expressed in the global co-ordinate system. In case of invalid argument, a zero vector is returned.

Definition at line 251 of file slipPlane.cpp.

```
255
      if (i==2)
256
      {
        // Z-axis
257
258
       axis = this->normalVector;
259
260
261
      if (i==0)
262
      // X-axis
Vector3d *el = new Vector3d;
263
264
       Vector3d *e2 = new Vector3d;
265
266
267
        *e1 = this->extremities[0].getPosition();
268
       *e2 = this->extremities[1].getPosition();
269
       axis = ((*e2) - (*e1));
270
       delete(e1); e1 = NULL;
delete(e2); e2 = NULL;
271
272
273
274
275
276
      // Y-axis = Z x X
2.77
       axis = this->getAxis(2) ^ this->getAxis(0);
278
279
281
      return ( axis.normalize() );
282 }
```

5.6.3.8 bool SlipPlane::getDislocation (int i, Dislocation * d)

Get the dislocation on the slip plane indicated by the index provided as argument.

The slip plane contains several dislocations that are stored in a vector container. This function returns the dislocation in that vector that corresponds to the index provided as argument.

Parameters

i	Index of the required dislocation in the vector. This value should be greater than or equal to 0
	and less than the number of dislocations on the slip plane.
d	Pointer to the memory location where the required dislocation is to be stored. Space in memory
	must be pre-allocated.

Returns

True if the provided index is greater than or equal to 0 and less than the number of dislocations on the slip plane (the memory location pointed to by d is populated with the Dislocation data). Otherwise, the return value is false.

Definition at line 168 of file slipPlane.cpp.

```
169 {
170    if (i>=0 && i<this->dislocations.size ())
171    {
172        *d = this->dislocations[i];
173        return (true);
174    }
175    else
176    {
177        return (false);
178    }
179 }
```

5.6.3.9 std::vector < Dislocation > SlipPlane::getDislocationList ()

Get the entire vector container which holds the dislocations lying on this slip plane.

Returns

The vector of dislocations lying on this slip plane.

Definition at line 185 of file slipPlane.cpp.

```
186 {
187    return (this->dislocations);
188 }
```

5.6.3.10 bool SlipPlane::getDislocationSource (int i, DislocationSource * dSource)

Get the dislocation source on the slip plane indicated by the index provided as argument.

The slip plane contains several dislocation sources that are stored in a vector container. This function returns the dislocation source in that vector that corresponds to the index provided as argument.

Parameters

i	Index of the required dislocation source in the vector. This value should be greater than or
	equal to 0 and less than the number of dislocation sources on the slip plane.
dSource	Pointer to the memory location where the required dislocation source is to be stored. Space
	in memory must be pre-allocated.

Returns

True if the provided index is greater than or equal to 0 and less than the number of dislocation sources on the slip plane (the memory location pointed to by d is populated with the DislocationSource data). Otherwise, the return value is false.

Definition at line 206 of file slipPlane.cpp.

```
207 {
208    if (i>=0 && i<this->dislocationSources.size ())
209    {
210       *dSource = this->dislocationSources[i];
211       return (true);
212    }
213    else
214    {
215       return (false);
216    }
217 }
```

$5.6.3.11 \quad std:: vector < \textbf{DislocationSource} > SlipPlane:: getDislocationSourceList (\ \)$

Get the entire vector container which holds the dislocation sources lying on this slip plane.

Returns

The vector of dislocation sources lying on this slip plane.

Definition at line 223 of file slipPlane.cpp.

```
224 {
225    return (this->dislocationSources);
226 }
```

5.6.3.12 Defect * SlipPlane::getExtremities ()

Get the position vectors of the extremities of the slip plane.

Returns

Pointer to an array containing the two extremities of the slip plane, variables of type Defect.

Pointer to an array containing the position vectors of the two extremities of the slip plane, variables of type

Vector3d.

Definition at line 137 of file slipPlane.cpp.

```
138 {
139   return (this->extremities);
140 }
```

5.6.3.13 Vector3d SlipPlane::getExtremity (int i)

Get the position vector of the extremity whose index is provided as argument.

Parameters

```
i Index of the extremity. Possible values: 0, 1
```

Returns

Position vector of the extremity indicated by the argument, returned as a variable of type Vector3d.

Definition at line 121 of file slipPlane.cpp.

```
122 {
123    if (i==0 || i==1)
124    {
125        return (this->extremities[i].getPosition());
126    }
127    else
128    {
129        return (Vector3d());
130    }
131    }
```

5.6.3.14 Vector3d SlipPlane::getNormal ()

Get the normal vector of the slip plane.

Returns

The normal vector of the slip plane, in a variable of type Vector3d.

Definition at line 146 of file slipPlane.cpp.

```
147 {
148    return (this->normalVector);
149 }
```

5.6.3.15 int SlipPlane::getNumDislocations ()

Get the number of dislocations.

Returns

The number of dislocations on the slip plane.

Definition at line 194 of file slipPlane.cpp.

```
195 {
196    return (this->dislocations.size ());
197  }
```

5.6.3.16 int SlipPlane::getNumDislocationSources ()

Get the number of dislocation sources.

Returns

The number of dislocation sources on the slip plane.

Definition at line 232 of file slipPlane.cpp.

```
233 {
234    return (this->dislocationSources.size ());
235 }
```

5.6.3.17 Vector3d SlipPlane::getPosition ()

Get the position vector of the slip plane.

This function returns the position vector of the slip plane. The position vector is redundant because the slip plane is completely defined by its extremities and the normal vector. Nevertheless, this value can be useful to locate the slip plane within a slip system.

Returns

Position vector of the slip plane, in a variable of type Vector3d.

Definition at line 156 of file slipPlane.cpp.

```
157 {
158    return (this->position);
159 }
```

5.6.3.18 RotationMatrix SlipPlane::getRotationMatrix ()

Get the rotation matrix for this slip plane.

Returns

The rotation matrix of this slip plane, in a variable of type RotationMatrix.

Definition at line 241 of file slipPlane.cpp.

```
242 {
243   return (this->rotationMatrix);
244 }
```

5.6.3.19 void SlipPlane::moveDislocations ()

Displaces the dislocations according to their velocities and the time increment.

Definition at line 513 of file slipPlane.cpp.

```
514 {
     std::vector<Dislocation>::iterator d;
515
516
     std::vector<Vector3d>::iterator v;
     Vector3d p;
518
519
     d = this->dislocations.begin();
520
     v = this->dislocationVelocities.begin();
521
     while (d != this->dislocations.end())
522
523
524
         p = d->getPosition();
525
         p += (*v) * (this->dt);
526
         d->setPosition(p);
527
528
         d++;
         v++;
530
531 }
```

5.6.3.20 void SlipPlane::setDislocationList (std::vector< Dislocation > dislocationList)

Set the list of dislocations of the slip plane.

Parameters

dislocationList | A vector container of type Dislocation containing the dislocations lying on this slip plane.

Definition at line 101 of file slipPlane.cpp.

```
102 {
103   this->dislocations = dislocationList;
104 }
```

5.6.3.21 void SlipPlane::setDislocationSourceList (std::vector < DislocationSource > dislocationSourceList)

Set the list of dislocation sources on the slip plane.

Parameters

dislocation-SourceList A vector container of type DislocationSource containing the dislocation sources lying on this

Definition at line 110 of file slipPlane.cpp.

```
111 {
112   this->dislocationSources = dislocationSourceList;
113 }
```

5.6.3.22 void SlipPlane::setExtremities (Vector3d * ends)

Set the extremities of the slip plane.

Parameters

ends Pointer to an array of type Vector3d, containing the position vectors of the extremities of the slip plane in consecutive locations.

Definition at line 73 of file slipPlane.cpp.

```
74 {
75    this->extremities[0] = Defect(ends);
76    this->extremities[1] = Defect(ends+1);
77 }
```

5.6.3.23 void SlipPlane::setNormal (Vector3d normal)

Set the normal vector of the slip plane.

Parameters

```
normal | The normal vector of the slip plane.
```

Definition at line 83 of file slipPlane.cpp.

```
84 {
85  this->normalVector = normal;
86 }
```

5.6.3.24 void SlipPlane::setPosition (Vector3d pos)

Set the position of the slip plane.

Parameters

pos	The position vector of the slip plane. (This parameter is useful for locating the slip plane within	1
	a slip system)	

Definition at line 92 of file slipPlane.cpp.

```
93 {
94    this->position = pos;
95 }
```

5.6.3.25 void SlipPlane::sortDislocations ()

Sorts the dislocations present on the slip plane in the ascending order of distance from the first extremity.

The dislocations present on the slip plane are sorted in ascending order of distance from the first extremity of the slip plane.

Definition at line 554 of file slipPlane.cpp.

```
555 {
       int nDisl = this->dislocations.size();
556
557
       int i, j;
double di, dj;
558
       Vector pi, pj;
Dislocation temp;
559
561
       for (i=0; i<nDisl-1; i++)</pre>
562
563
            for (j=i+1; j<nDisl; j++)</pre>
564
565
                 pi = this->dislocations[i].getPosition();
567
                  di = this->distanceFromExtremity(pi, 0);
568
                  pj = this->dislocations[j].getPosition();
dj = this->distanceFromExtremity(pj, 0);
569
570
571
                  if (dj < di)</pre>
```

5.6.4 Field Documentation

5.6.4.1 std::vector< Vector3d > SlipPlane::dislocationForces [protected]

The Peach-Koehler force experienced by each dislocation.

This vector container stores the Peah-Koehler force experienced by each dislocation. They are calculated in each iteration by thefunction calculateDislocationForces(tau_crss).

Definition at line 66 of file slipPlane.h.

```
5.6.4.2 std::vector<Dislocation> SlipPlane::dislocations [protected]
```

STL vector container with dislocations.

A slip plane may contain several dislocations. These are stored in this vector container dislocations.

Definition at line 54 of file slipPlane.h.

```
5.6.4.3 std::vector < DislocationSource > SlipPlane::dislocationSources [protected]
```

STL vector container with dislocation sources.

A slip plane may contain several dislocation sources. These are stored in this vector container dislocationSources. Definition at line 78 of file slipPlane.h.

```
5.6.4.4 std::vector<Stress> SlipPlane::dislocationStresses [protected]
```

STL vector container with the stress fields of dislocations.

The stress fields experienced by the dislocations, expressed in the global co-ordinate system, are stored in this vector with positions corresponding to the positions of dislocations in the vector dislocations.

Definition at line 60 of file slipPlane.h.

```
5.6.4.5 std::vector< Vector3d> SlipPlane::dislocationVelocities [protected]
```

STL vector container with dislocation velocities.

The dislocations on this slip plane will have a velocity associated with them. These velocity vectors are stored in this container. The order is the same as the order of the dislocations.

Definition at line 72 of file slipPlane.h.

```
5.6.4.6 double SlipPlane::dt [protected]
```

Time increment for the slip plane.

A time increment is calculated for each slip plane based on the distances traveled by the dislocations.

Definition at line 84 of file slipPlane.h.

5.7 Strain Class Reference 73

5.6.4.7 Defect SlipPlane::extremities[2] [protected]

The extremities of the slip plane.

The slip plane is represented as a straight line in these two dimensional simulations. The position vectors of the two ends are given here.

Definition at line 36 of file slipPlane.h.

5.6.4.8 Vector3d SlipPlane::normalVector [protected]

The normal vector to the slip plane.

This is the vector normal to the slip plane. Since we are concerned with the cubic system here, the indices of the normal vector are the same as those of the slip plane.

Definition at line 42 of file slipPlane.h.

5.6.4.9 Vector3d SlipPlane::position [protected]

The position vector of the slip plane.

This position vector is redundant because the combination of the position vectors of the extremities and the normal vector define the slip plane completely. However, this vector, position, is useful to locate the slip plane in a given slip system.

Definition at line 48 of file slipPlane.h.

5.6.4.10 RotationMatrix SlipPlane::rotationMatrix [protected]

Rotation matrix for co-ordinate system transformations.

The slip plane's local co-ordinate system is defined as follows: z-axis||NormalVector; x-axis||slipPlane line. The rotation matrix is created using this convention.

Definition at line 90 of file slipPlane.h.

The documentation for this class was generated from the following files:

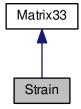
- slipPlane.h
- · slipPlane.cpp

5.7 Strain Class Reference

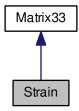
Strain class to represent the strain tensor.

#include <strain.h>

Inheritance diagram for Strain:



Collaboration diagram for Strain:



Public Member Functions

• Strain ()

Default constructor.

• Strain (double *principal, double *shear)

Constructor specifying the principal and shear strains.

• void populateMatrix ()

Construct the strain tensor from the principal and shear strains.

• double * getPrincipalStrains ()

Get the principal strains.

double * getShearStrains ()

Get the shear strains.

• Strain rotate (RotationMatrix alpha)

Rotate the strain tensor from one coordinate system to another.

• void setValue (int row, int column, double value)

Function to set the value of an element indicated by its position.

• double getValue (int row, int column)

Returns the value of the element located by the row and column indices provided.

• Matrix33 adjugate ()

Returns the adjugate matrix of the present matrix.

5.7 Strain Class Reference 75

Matrix33 operator+ (const Matrix33 &) const

Operator for addition of two matrices.

void operator+= (const Matrix33 &)

Operator for reflexive addition of two matrices.

• Matrix33 operator- (const Matrix33 &) const

Operator for the subtraction of two matrices.

• void operator-= (const Matrix33 &)

Operator for reflexive subtraction of two matrices.

Matrix33 operator* (const double &) const

Operator for scaling the matrix by a scalar.

Matrix33 operator* (const Matrix33 &) const

Operator for the multiplication of two matrices.

Vector3d operator* (const Vector3d &) const

Operator for the multiplication of a matrix with a vector.

void operator*= (const double &)

Operator for reflexive scaling of the matrix by a scalar.

void operator*= (const Matrix33 &)

Operator for reflexive multiplication of two matrices.

Matrix33 operator[∧] () const

Transpose.

• double operator \sim () const

Determinant.

Matrix33 operator! () const

Inverse.

Protected Attributes

- double principalStrains [3]
- double shearStrains [3]
- double x [3][3]

Array containing the elements of the matrix.

5.7.1 Detailed Description

Strain class to represent the strain tensor.

The member functions of this class construct the symmetric strain tensor and operate on it.

Definition at line 21 of file strain.h.

5.7.2 Constructor & Destructor Documentation

5.7.2.1 Strain::Strain()

Default constructor.

Initializes the strain tensor with zeros.

Definition at line 16 of file strain.cpp.

```
17 {
18    int i, j;
19
20    for (i=0; i<3; i++)
21    {
22        principalStrains [i] = 0.0;
23        shearStrains [i] = 0.0;
24    }
25
    this->populateMatrix ();
27 }
```

5.7.2.2 Strain::Strain (double * principal, double * shear)

Constructor specifying the principal and shear strains.

The principal and shear strains are provided in the arguments and the symmetrical strain tensor is contstructed using them.

Parameters

principal	Pointer to the array containing principal strains.
shear	Pointer to the array containing shear strains.

Definition at line 35 of file strain.cpp.

```
36 {
37    int i;
38
39    for (i=0; i<3; i++)
40    {
41         this->principalStrains [i] = principal [i];
42         this->shearStrains [i] = shear [i];
43    }
44    this->populateMatrix ();
46 }
```

5.7.3 Member Function Documentation

5.7.3.1 Matrix33 Matrix33::adjugate() [inherited]

Returns the adjugate matrix of the present matrix.

The adjugate matrix of the present matrix is returned. The adjugate matrix is calculated by evaluating the determinant of the cofactor matrix of each element, and then replacing the corresponding element position by the value of the determinant. This operation is useful in calculating the inverse of a matrix.

Returns

The adjugate matrix of the present matrix.

Definition at line 129 of file matrix33.cpp.

```
130 {
           Matrix33 adj;
131
132
           adj.x[0][0] = (this->x[1][1]*this->x[2][2]) - (this->x[1][2]*this->x[2][1]);
adj.x[0][1] = (this->x[1][2]*this->x[2][0]) - (this->x[1][0]*this->x[2][2]);
adj.x[0][2] = (this->x[1][0]*this->x[2][1]) - (this->x[1][1]*this->x[2][0]);
133
134
135
136
           adj.x[1][0] = (this->x[2][1]*this->x[0][2]) - (this->x[0][1]*this->x[2][2]);
adj.x[1][1] = (this->x[2][2]*this->x[0][0]) - (this->x[2][0]*this->x[0][2]);
137
138
            adj.x[1][2] = (this->x[2][0]*this->x[0][1]) - (this->x[2][1]*this->x[0][0]);
139
140
           adj.x[2][0] = (this->x[0][1]*this->x[1][2]) - (this->x[0][2]*this->x[1][1]);
adj.x[2][1] = (this->x[0][2]*this->x[1][0]) - (this->x[0][0]*this->x[1][2]);
adj.x[2][2] = (this->x[0][0]*this->x[1][1]) - (this->x[1][0]*this->x[0][1]);
141
142
143
144
145
           return (adj);
146 }
```

5.7 Strain Class Reference 77

```
5.7.3.2 double * Strain::getPrincipalStrains ( )
```

Get the principal strains.

Returns a 3-member array with the principal strains: s11 s22 s33.

Returns

3-member array with the principal strains.

Definition at line 68 of file strain.cpp.

```
69 {
70    double p[3];
71    int i;
72
73    for (i=0; i<3; i++)
74    {
75         p[i] = this->principalStrains[i];
76    }
77    return (p);
79 }
```

5.7.3.3 double * Strain::getShearStrains ()

Get the shear strains.

Returns a 3-member array with the shear strains: s12 s13 s23.

Returns

3-member array with the shear strains.

Definition at line 86 of file strain.cpp.

```
87 {
88     double s[3];
89     int i;
90
91     for (i=0; i<3; i++)
92     {
93         s[i] = this->shearStrains[i];
94     }
95
96     return (s);
97 }
```

5.7.3.4 double Matrix33::getValue (int row, int column) [inherited]

Returns the value of the element located by the row and column indices provided.

The value of the element indicated by the arguments row and column is returned. The values of row and column must correspond to array indices, and thus can be one of 0, 1 and 2. In any other case 0.0 is returned.

Parameters

row	Row index of the element.
column	Column index of the element.

Returns

Value of the element located at the given position.

Definition at line 111 of file matrix33.cpp.

```
112 {
113     if (row>=0 && row<3)
114     {
115         if (column>=0 && column<3)
116         {
117             return (this->x[row][column]);
118         }
119     }
120     return (0.0);
121     return (0.0);
```

5.7.3.5 Matrix33 Matrix33::operator! () const [inherited]

Inverse.

Returns in a new matrix the inverse of the current matrix. If the current matrix is non-invertible, a zero matrix is returned.

Returns

Matrix with the inverse of the current matrix. If the current matrix is non-invertible, a zero matrix is returned.

Definition at line 370 of file matrix33.cpp.

```
371 {
     Matrix33 r; // Result matrix
372
373
374
     double determinant = ~(*this);
375
376
     if (determinant == 0.0)
377
378
       // The matrix is non-invertible
379
         return (r);  // Zero matrix
380
381
382
     // If we are still here, the matrix is invertible
383
     // Transpose
384
385
     Matrix33 tr = ^(*this);
386
387
     // Find Adjugate matrix
388 Matrix33 adj = tr.adjugate();
389
390
     // Calculate the inverse by dividing the adjugate matrix by the determinant
391
     r = adj * (1.0/determinant);
392
393
     return (r);
394 }
```

5.7.3.6 Matrix33 Matrix33::operator* (const double & p) const [inherited]

Operator for scaling the matrix by a scalar.

Scales the current matrix by the scalar provided and returns the result in a third matrix.

Returns

Matrix containing the result of scaling the current matrix by the scalar provided as argument.

Definition at line 233 of file matrix33.cpp.

5.7 Strain Class Reference 79

```
234 {
      int i, j;
Matrix33 r;
235
236
237
      for (i=0; i<3; i++)</pre>
238
239
         for (j=0; j<3; j++)
241
242
               r.x[i][j] = this->x[i][j] * p;
243
       }
244
245
246
      return (r);
```

5.7.3.7 Matrix33 Matrix33::operator* (const Matrix33 & p) const [inherited]

Operator for the multiplication of two matrices.

Multiplies the current matrix with another 3x3 matrix and returns the result in a new matrix.

Returns

The result of the multiplication of the current matrix with the one provided as argument.

Definition at line 271 of file matrix33.cpp.

```
272 {
      int i, j, k;
Matrix33 r;
273
274
275
276
      for (i=0; i<3; i++)</pre>
277
           for (j=0; j<3; j++)</pre>
278
279
               r.x[i][j] = 0.0;
281
               for (k=0; k<3; k++)
282
283
                    r.x[i][j] += this -> x[i][k] * p.x[k][j];
284
285
             }
286
       }
288
      return (r);
289 }
```

5.7.3.8 **Vector3d Matrix33::operator* (const Vector3d & v) const** [inherited]

Operator for the multiplication of a matrix with a vector.

Returns in a vector the result of the multiplication of the current matrix with the provided vector.

Returns

The vector resulting from the multiplication of the current matrix with a vector.

Definition at line 311 of file matrix33.cpp.

```
312 {
313
      Vector3d r(0.0, 0.0, 0.0);
314
     int i, j;
315
316
      for (i=0; i<3; i++)</pre>
317
318
        for (j=0; j<3; j++)
320
              r[i] += this -> x[i][j] * v.x[j];
321
322
      }
323
324
     return (r);
325 }
```

```
5.7.3.9 void Matrix33::operator*=(const double & p) [inherited]
```

Operator for reflexive scaling of the matrix by a scalar.

Scales the current matrix by the scalar provided and populates the current matrix elements with the result.

Definition at line 253 of file matrix33.cpp.

5.7.3.10 void Matrix33::operator*=(const Matrix33 & p) [inherited]

Operator for reflexive multiplication of two matrices.

Multiplies the current matrix with another 3x3 matrix and populates the elements of the current matrix with the result. Definition at line 295 of file matrix33.cpp.

```
296 {
297    Matrix33* r = new Matrix33;
298
299    *r = (*this) * p;
300    *this = *r;
301
302    delete(r);
303    r = NULL;
304 }
```

5.7.3.11 Matrix33 Matrix33::operator+(const Matrix33 & p) const [inherited]

Operator for addition of two matrices.

Adds the current matrix to the provided matrix and returns a third matrix with the result.

Returns

Matrix containing the sum of the present matrix and the one provided.

Definition at line 155 of file matrix33.cpp.

```
156 {
157
      int i, j;
      Matrix33 r;
158
159
      for (i=0; i<3; i++)</pre>
160
161
162
          for (j=0; j<3; j++)
163
               r.x[i][j] = this->x[i][j] + p.x[i][j];
164
165
        1
166
167
      return (r);
```

5.7 Strain Class Reference 81

```
5.7.3.12 void Matrix33::operator+=(const Matrix33 & p) [inherited]
```

Operator for reflexive addition of two matrices.

Adds the current matrix to the provided matrix and populates the current matrix elements with the result.

Definition at line 175 of file matrix33.cpp.

5.7.3.13 Matrix33 Matrix33::operator-(const Matrix33 & p) const [inherited]

Operator for the subtraction of two matrices.

Subtracts the given matrix from the current matrix and returns the result in a new matrix.

Returns

Matrix containing the result of subtracting the provided matrix from the current matrix.

Definition at line 194 of file matrix33.cpp.

```
int i, j;
Matrix33 r;
196
197
198
      for (i=0; i<3; i++)</pre>
199
200
          for (j=0; j<3; j++)</pre>
201
202
203
               r.x[i][j] = this->x[i][j] - p.x[i][j];
204
205
        }
206
207
      return (r);
208 }
```

5.7.3.14 void Matrix33::operator=(const Matrix33 & p) [inherited]

Operator for reflexive subtraction of two matrices.

Subtracts the given matrix from the current matrix and populates the current matrix with the result.

Definition at line 214 of file matrix33.cpp.

```
215 {
216    int i, j;
217
218    for (i=0; i<3; i++)
219    {
220         for (j=0; j<3; j++)
221         {
222             this->x[i][j] -= p.x[i][j];
223         }
224    }
225 }
```

```
5.7.3.15 Matrix33 Matrix33::operator ( ) const [inherited]
```

Transpose.

Performs the transpose of the current matrix.

Returns

A new matrix with the transpose of the current matrix.

Definition at line 333 of file matrix33.cpp.

```
334 {
      Matrix33 r;
336
      int i, j;
337
      for (i=0; i<3; i++)</pre>
338
339
340
           for (j=0; j<3; j++)</pre>
341
342
                r.x[i][j] = this \rightarrow x[j][i];
343
       }
344
345
346
      return (r);
347 }
```

```
5.7.3.16 double Matrix33::operator\sim ( ) const [inherited]
```

Determinant.

Calculates the determinant of the current matrix.

Returns

Returns the determinant of the current matrix.

Definition at line 354 of file matrix33.cpp.

5.7.3.17 void Strain::populateMatrix ()

Construct the strain tensor from the principal and shear strains.

Takes the values in principalStrains and shearStrains and constructs the symmetrical strain matrix.

Definition at line 52 of file strain.cpp.

```
53 {
54     this->x[0][0] = this->principalStrains [0];
55     this->x[1][1] = this->principalStrains [1];
56     this->x[2][2] = this->principalStrains [2];
57
58     this->x[0][1] = this->x[1][0] = this->shearStrains [0];
59     this->x[0][2] = this->x[2][0] = this->shearStrains [1];
60     this->x[1][2] = this->x[2][1] = this->shearStrains [2];
61 }
```

5.7 Strain Class Reference 83

5.7.3.18 Strain Strain::rotate (RotationMatrix alpha)

Rotate the strain tensor from one coordinate system to another.

Rotates the present strain matrix from one coordinate system to another using the rotation matrix supplied. The result is returned in a new Strain matrix.

Parameters

```
alpha Rotation matrix.
```

Returns

Rotated strain tensor.

Definition at line 105 of file strain.cpp.

5.7.3.19 void Matrix33::setValue (int row, int column, double value) [inherited]

Function to set the value of an element indicated by its position.

The element indicated by the arguments row and column is set to the value provided. The values of row and column must correspond to array indices, and thus can be one of 0, 1 and 2. In any other case 0.0 is returned.

Parameters

row	Row index of the element.
column	Column index of the element.
value	Value that the element is to be set to.

Definition at line 93 of file matrix33.cpp.

5.7.4 Field Documentation

5.7.4.1 double Strain::principalStrains[3] [protected]

The three principal strains: s11, s22, s33.

Definition at line 27 of file strain.h.

5.7.4.2 double Strain::shearStrains[3] [protected]

The three shear strains: s12, s13, s23,

Definition at line 31 of file strain.h.

5.7.4.3 double Matrix33::x[3][3] [protected], [inherited]

Array containing the elements of the matrix.

Definition at line 26 of file matrix33.h.

The documentation for this class was generated from the following files:

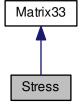
- strain.h
- strain.cpp

5.8 Stress Class Reference

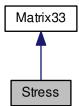
Stress class to represent the stress tensor.

#include <stress.h>

Inheritance diagram for Stress:



Collaboration diagram for Stress:



Public Member Functions

• Stress ()

Default constructor.

• Stress (double *principal, double *shear)

Constructor specifying the principal and shear stresses.

void populateMatrix ()

Construct the stress tensor from the principal and shear stresses.

double * getPrincipalStresses ()

Get the principal stresses.

double * getShearStresses ()

Get the shear stresses.

• Stress rotate (RotationMatrix alpha)

Rotate the stress tensor from one coordinate system to another.

void setValue (int row, int column, double value)

Function to set the value of an element indicated by its position.

double getValue (int row, int column)

Returns the value of the element located by the row and column indices provided.

• Matrix33 adjugate ()

Returns the adjugate matrix of the present matrix.

• Matrix33 operator+ (const Matrix33 &) const

Operator for addition of two matrices.

• void operator+= (const Matrix33 &)

Operator for reflexive addition of two matrices.

Matrix33 operator- (const Matrix33 &) const

Operator for the subtraction of two matrices.

void operator-= (const Matrix33 &)

Operator for reflexive subtraction of two matrices.

• Matrix33 operator* (const double &) const

Operator for scaling the matrix by a scalar.

• Matrix33 operator* (const Matrix33 &) const

Operator for the multiplication of two matrices.

Vector3d operator* (const Vector3d &) const

Operator for the multiplication of a matrix with a vector.

• void operator*= (const double &)

Operator for reflexive scaling of the matrix by a scalar.

void operator*= (const Matrix33 &)

Operator for reflexive multiplication of two matrices.

Matrix33 operator[∧] () const

Transpose.

• double operator \sim () const

Determinant.

Matrix33 operator! () const

Inverse.

Protected Attributes

- · double principalStresses [3]
- double shearStresses [3]
- double x [3][3]

Array containing the elements of the matrix.

5.8.1 Detailed Description

Stress class to represent the stress tensor.

The member functions of this class construct the symmetric stress tensor and operate on it.

Definition at line 21 of file stress.h.

5.8.2 Constructor & Destructor Documentation

```
5.8.2.1 Stress::Stress()
```

Default constructor.

Initializes the stress tensor with zeros.

Definition at line 16 of file stress.cpp.

```
17 {
18   int i, j;
19
20   for (i=0; i<3; i++)
21    {
22      principalStresses [i] = 0.0;
23      shearStresses [i] = 0.0;
24   }
25
26   this->populateMatrix ();
27 }
```

5.8.2.2 Stress::Stress (double * principal, double * shear)

Constructor specifying the principal and shear stresses.

The principal and shear stresses are provided in the arguments and the symmetrical stress tensor is contstructed using them.

Parameters

princip	oal	Pointer to the array containing principal stresses.
she	ear	Pointer to the array containing shear stresses.

Definition at line 35 of file stress.cpp.

```
36 {
37    int i;
38
39    for (i=0; i<3; i++)
40    {
41         this->principalStresses [i] = principal [i];
42         this->shearStresses [i] = shear [i];
43    }
44
45    this->populateMatrix ();
46 }
```

5.8.3 Member Function Documentation

5.8.3.1 Matrix33 Matrix33::adjugate() [inherited]

Returns the adjugate matrix of the present matrix.

The adjugate matrix of the present matrix is returned. The adjugate matrix is calculated by evaluating the determinant of the cofactor matrix of each element, and then replacing the corresponding element position by the value of the determinant. This operation is useful in calculating the inverse of a matrix.

Returns

The adjugate matrix of the present matrix.

Definition at line 129 of file matrix33.cpp.

```
130 {
          Matrix33 adj;
131
132
          adj.x[0][0] = (this->x[1][1]*this->x[2][2]) - (this->x[1][2]*this->x[2][1]);
adj.x[0][1] = (this->x[1][2]*this->x[2][0]) - (this->x[1][0]*this->x[2][2]);
adj.x[0][2] = (this->x[1][0]*this->x[2][1]) - (this->x[1][1]*this->x[2][0]);
133
134
135
136
          137
138
139
         adj.x[2][0] = (this->x[0][1]*this->x[1][2]) - (this->x[0][2]*this->x[1][1]);
adj.x[2][1] = (this->x[0][2]*this->x[1][0]) - (this->x[0][0]*this->x[1][2]);
adj.x[2][2] = (this->x[0][0]*this->x[1][1]) - (this->x[1][0]*this->x[0][1]);
141
142
143
144
145
          return (adj);
146 }
```

5.8.3.2 double * Stress::getPrincipalStresses ()

Get the principal stresses.

Returns a 3-member array with the principal stresses: s11 s22 s33.

Returns

3-member array with the principal stresses.

Definition at line 68 of file stress.cpp.

```
69 {
70    double p[3];
71    int i;
72
73    for (i=0; i<3; i++)
74    {
75       p[i] = this->principalStresses[i];
76    }
77
78    return (p);
79 }
```

5.8.3.3 double * Stress::getShearStresses ()

Get the shear stresses.

Returns a 3-member array with the shear stresses: s12 s13 s23.

Returns

3-member array with the shear stresses.

Definition at line 86 of file stress.cpp.

```
87 {
88     double s[3];
89     int i;
90
91     for (i=0; i<3; i++)
92     {
93          s[i] = this->shearStresses[i];
94     }
95
96     return (s);
97 }
```

5.8.3.4 double Matrix33::getValue (int row, int column) [inherited]

Returns the value of the element located by the row and column indices provided.

The value of the element indicated by the arguments row and column is returned. The values of row and column must correspond to array indices, and thus can be one of 0, 1 and 2. In any other case 0.0 is returned.

Parameters

row	Row index of the element.
column	Column index of the element.

Returns

Value of the element located at the given position.

Definition at line 111 of file matrix33.cpp.

5.8.3.5 Matrix33 Matrix33::operator! () const [inherited]

Inverse.

Returns in a new matrix the inverse of the current matrix. If the current matrix is non-invertible, a zero matrix is returned.

Returns

Matrix with the inverse of the current matrix. If the current matrix is non-invertible, a zero matrix is returned.

Definition at line 370 of file matrix33.cpp.

```
371 {
372
      Matrix33 r; // Result matrix
373
374
      double determinant = ~(*this);
375
376
      if (determinant == 0.0)
377
378
          // The matrix is non-invertible
379
                           // Zero matrix
          return (r);
380
381
382
     \ensuremath{//} If we are still here, the matrix is invertible
383
      // Transpose
384
     Matrix33 tr = ^(*this);
385
386
387
      // Find Adjugate matrix
388
     Matrix33 adj = tr.adjugate();
389
      \ensuremath{//} Calculate the inverse by dividing the adjugate matrix by the determinant
390
391
     r = adj * (1.0/determinant);
393
     return (r);
394 }
```

5.8 Stress Class Reference 89

5.8.3.6 Matrix33 Matrix33::operator* (const double & p) const [inherited]

Operator for scaling the matrix by a scalar.

Scales the current matrix by the scalar provided and returns the result in a third matrix.

Returns

Matrix containing the result of scaling the current matrix by the scalar provided as argument.

Definition at line 233 of file matrix33.cpp.

```
234 {
      int i, j;
235
      Matrix33 r;
236
237
238
      for (i=0; i<3; i++)</pre>
239
240
          for (j=0; j<3; j++)</pre>
241
242
               r.x[i][j] = this->x[i][j] * p;
243
244
245
246
      return (r);
247 }
```

5.8.3.7 Matrix33 Matrix33::operator*(const Matrix33 & p) const [inherited]

Operator for the multiplication of two matrices.

Multiplies the current matrix with another 3x3 matrix and returns the result in a new matrix.

Returns

The result of the multiplication of the current matrix with the one provided as argument.

Definition at line 271 of file matrix33.cpp.

```
273
      int i, j, k;
      Matrix33 r;
274
275
276
      for (i=0; i<3; i++)</pre>
277
          for (j=0; j<3; j++)</pre>
279
280
              r.x[i][j] = 0.0;
281
              for (k=0; k<3; k++)
282
                   r.x[i][j] += this->x[i][k] * p.x[k][j];
283
284
285
            }
286
       }
287
288
     return (r);
289 }
```

5.8.3.8 Vector3d Matrix33::operator*(const Vector3d & v) const [inherited]

Operator for the multiplication of a matrix with a vector.

Returns in a vector the result of the multiplication of the current matrix with the provided vector.

Returns

The vector resulting from the multiplication of the current matrix with a vector.

Definition at line 311 of file matrix33.cpp.

```
312 {
      Vector3d r(0.0, 0.0, 0.0);
313
      int i, j;
315
316
      for (i=0; i<3; i++)</pre>
317
         for (j=0; j<3; j++)
318
319
              r[i] += this -> x[i][j] * v.x[j];
320
322
      }
323
324
     return (r);
325 }
```

5.8.3.9 void Matrix33::operator*=(const double & p) [inherited]

Operator for reflexive scaling of the matrix by a scalar.

Scales the current matrix by the scalar provided and populates the current matrix elements with the result.

Definition at line 253 of file matrix33.cpp.

```
254 {
255   int i, j;
256
257   for (i=0; i<3; i++)
258   {
259     for (j=0; j<3; j++)
260     {
261         this->x[i][j] *= p;
262     }
263   }
264 }
```

5.8.3.10 void Matrix33::operator*=(const Matrix33 & p) [inherited]

Operator for reflexive multiplication of two matrices.

Multiplies the current matrix with another 3x3 matrix and populates the elements of the current matrix with the result. Definition at line 295 of file matrix33.cpp.

```
296 {
297     Matrix33* r = new Matrix33;
298
299     *r = (*this) * p;
300     *this = *r;
301
302     delete(r);
303     r = NULL;
```

5.8.3.11 Matrix33 Matrix33::operator+(const Matrix33 & p) const [inherited]

Operator for addition of two matrices.

Adds the current matrix to the provided matrix and returns a third matrix with the result.

5.8 Stress Class Reference 91

Returns

Matrix containing the sum of the present matrix and the one provided.

Definition at line 155 of file matrix33.cpp.

```
156 {
      int i, j;
Matrix33 r;
157
158
159
160
      for (i=0; i<3; i++)
161
          for (j=0; j<3; j++)</pre>
162
163
               r.x[i][j] = this->x[i][j] + p.x[i][j];
164
165
166
167
168 return (r);
169 }
```

5.8.3.12 void Matrix33::operator+= (const Matrix33 & p) [inherited]

Operator for reflexive addition of two matrices.

Adds the current matrix to the provided matrix and populates the current matrix elements with the result.

Definition at line 175 of file matrix33.cpp.

```
176 {
177
      int i, j;
178
179
      for (i=0; i<3; i++)</pre>
180
         for (j=0; j<3; j++)
181
182
183
              this->x[i][j] += p.x[i][j];
184
       }
185
186 }
```

5.8.3.13 Matrix33 Matrix33::operator-(const Matrix33 & p) const [inherited]

Operator for the subtraction of two matrices.

Subtracts the given matrix from the current matrix and returns the result in a new matrix.

Returns

Matrix containing the result of subtracting the provided matrix from the current matrix.

Definition at line 194 of file matrix33.cpp.

```
195 {
      int i, j;
196
      Matrix33 r;
197
198
      for (i=0; i<3; i++)</pre>
199
200
201
          for (j=0; j<3; j++)</pre>
202
               r.x[i][j] = this->x[i][j] - p.x[i][j];
203
204
206
207
      return (r);
208 }
```

```
5.8.3.14 void Matrix33::operator=( const Matrix33 & p ) [inherited]
```

Operator for reflexive subtraction of two matrices.

Subtracts the given matrix from the current matrix and populates the current matrix with the result.

Definition at line 214 of file matrix33.cpp.

5.8.3.15 Matrix33 Matrix33::operator^() const [inherited]

Transpose.

Performs the transpose of the current matrix.

Returns

A new matrix with the transpose of the current matrix.

Definition at line 333 of file matrix33.cpp.

```
334 {
335
      Matrix33 r;
336
      int i, j;
337
338
      for (i=0; i<3; i++)</pre>
339
          for (j=0; j<3; j++)</pre>
340
341
342
               r.x[i][j] = this->x[j][i];
343
344
345
346
      return (r);
347 }
```

5.8.3.16 double Matrix33::operator \sim () const [inherited]

Determinant.

Calculates the determinant of the current matrix.

Returns

Returns the determinant of the current matrix.

Definition at line 354 of file matrix33.cpp.

```
355 {
356
                                      double d = 0.0;
357
                                      358
                                       x[1][2]));
359
                                    d += this.x[0][1] * ( (this->x[1][2]*this->x[2][0]) - (this->x[1][0]*this-> (this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x[1][0]*this->x
                                      x[2][2]));
360
                                                                    x[1][1]));
361
                                     return (d);
362
363 }
```

5.8 Stress Class Reference 93

5.8.3.17 void Stress::populateMatrix ()

Construct the stress tensor from the principal and shear stresses.

Takes the values in principalStresses and shearStresses and constructs the symmetrical stress matrix.

Definition at line 52 of file stress.cpp.

```
53 {
54     this->x[0][0] = this->principalStresses [0];
55     this->x[1][1] = this->principalStresses [1];
56     this->x[2][2] = this->principalStresses [2];
57
58     this->x[0][1] = this->x[1][0] = this->shearStresses [0];
59     this->x[0][2] = this->x[2][0] = this->shearStresses [1];
60     this->x[1][2] = this->x[2][1] = this->shearStresses [2];
61 }
```

5.8.3.18 Stress Stress::rotate (RotationMatrix alpha)

Rotate the stress tensor from one coordinate system to another.

Rotates the present stress matrix from one coordinate system to another using the rotation matrix supplied. The result is returned in a new Stress matrix.

Parameters

```
alpha Rotation matrix.
```

Returns

Rotated stress tensor.

Definition at line 105 of file stress.cpp.

```
106 {
107    Matrix33 alphaT = ^alpha;  // Transpose
108    Stress sNew;
109
110    sNew = alpha * (*this) * alphaT;  // Rotate the stress matrix
111
112    return (sNew);
113 }
```

5.8.3.19 void Matrix33::setValue (int row, int column, double value) [inherited]

Function to set the value of an element indicated by its position.

The element indicated by the arguments row and column is set to the value provided. The values of row and column must correspond to array indices, and thus can be one of 0, 1 and 2. In any other case 0.0 is returned.

Parameters

row	Row index of the element.
column	Column index of the element.
value	Value that the element is to be set to.

Definition at line 93 of file matrix33.cpp.

5.8.4 Field Documentation

5.8.4.1 double Stress::principalStresses[3] [protected]

The three principal stresses: s11, s22, s33.

Definition at line 27 of file stress.h.

5.8.4.2 double Stress::shearStresses[3] [protected]

The three shear stresses: s12, s13, s23,

Definition at line 31 of file stress.h.

5.8.4.3 double Matrix33::x[3][3] [protected], [inherited]

Array containing the elements of the matrix.

Definition at line 26 of file matrix33.h.

The documentation for this class was generated from the following files:

- · stress.h
- · stress.cpp

5.9 Vector3d Class Reference

Vector3d class representing a single 3-dimensional vector in the simulation.

```
#include <vector3d.h>
```

Public Member Functions

· Vector3d ()

Default constructor.

• Vector3d (double *a)

Constructor with values provided in an array.

• Vector3d (double a1, double a2, double a3)

Constructor with values provided explicitly.

• void setValue (int index, double value)

Function to set the value of an element of the vector.

void setVector (double *a)

Function to set the value of the entire vector using an array.

• double getValue (int index)

Function to get the value of an element of the vector.

double * getVector ()

Function to get the values of the elements of the vector in an array.

• double sum ()

Computes the sum of the elements of the vector.

• double magnitude ()

Computes the magnitude of the vector.

• Vector3d normalize ()

Returns the vector normalized to be a unit vector.

Vector3d operator+ (const Vector3d &) const

Operator for addition of two vectors.

void operator+= (const Vector3d &)

Operator for reflexive addition of two vectors.

Vector3d operator- (const Vector3d &) const

Operator for the subtraction of two vectors.

void operator-= (const Vector3d &)

Operator for reflexive subtraction of two vectors.

• Vector3d operator* (const double &) const

Operator for scaling the vector by a scalar.

void operator*= (const double &)

Operator for reflexive scaling of the vector by a scalar.

• double operator* (const Vector3d &) const

Operator for the scalar product of two vectors.

Vector3d operator[∧] (const Vector3d &) const

Operator for the vector product of two vectors.

void operator[^]= (const Vector3d &)

Operator for reflexive vector product of two vectors.

Protected Attributes

double x [3]

The elements of the vector.

5.9.1 Detailed Description

Vector3d class representing a single 3-dimensional vector in the simulation.

This class represents a vector in 3D space. The member functions and operators define various operations on the vector and its interactions with other data types.

Definition at line 20 of file vector3d.h.

5.9.2 Constructor & Destructor Documentation

```
5.9.2.1 Vector3d::Vector3d()
```

Default constructor.

Initializes the vector with all elements equal to 0.0.

Definition at line 16 of file vector3d.cpp.

```
17 {
18    this->x[0] = 0.0;
19    this->x[1] = 0.0;
20    this->x[2] = 0.0;
21 }
```

5.9.2.2 Vector3d::Vector3d (double * a)

Constructor with values provided in an array.

Initializes the vector with the values provided in the array.

Parameters

```
a Pointer to the array containing the elements of the vector
```

Definition at line 28 of file vector3d.cpp.

```
29 {
30    this->x[0] = a[0];
31    this->x[1] = a[1];
32    this->x[2] = a[2];
33 }
```

5.9.2.3 Vector3d::Vector3d (double a1, double a2, double a3)

Constructor with values provided explicitly.

Initializes the vector with the three values provided as arguments.

Parameters

a1	Value of the first element of the vector.
a2	Value of the second element of the vector.
аЗ	Value of the third element of the vector.

Definition at line 42 of file vector3d.cpp.

```
43 {
44    this->x[0] = al;
45    this->x[1] = a2;
46    this->x[2] = a3;
```

5.9.3 Member Function Documentation

5.9.3.1 double Vector3d::getValue (int index)

Function to get the value of an element of the vector.

Returns the value of the element at the position indicated by the argument index.

Parameters

```
index Index of the element whose value is to be got.
```

Returns

The value of the element of the vector at the position

Definition at line 83 of file vector3d.cpp.

```
84 {
85    if (index>=0 && index<3)
86    {
87       return (this->x[index]);
88    }
89    else
```

```
90 {
91     return (0);
92     }
93 }
```

5.9.3.2 double * Vector3d::getVector()

Function to get the values of the elements of the vector in an array.

The vector is returned in an array.

Returns

Pointer to the first term of an array containing the elements of the vector.

Definition at line 100 of file vector3d.cpp.

```
101 {
102     double* a = new double[3];
103
104     a[0] = this->x[0];
105     a[1] = this->x[1];
106     a[2] = this->x[2];
107
108     return (a);
109 }
```

5.9.3.3 double Vector3d::magnitude ()

Computes the magnitude of the vector.

Computes the magnitude of the vector. Basically the square root of the sum of the squares of the vector elements.

Returns

The magnitude of the vector.

Definition at line 134 of file vector3d.cpp.

5.9.3.4 Vector3d Vector3d::normalize ()

Returns the vector normalized to be a unit vector.

This function normalizes a vector by dividing its elements by the magnitude. In case the magnitude is zero, a zero vector is returned.

Returns

Normalized vector.

Definition at line 152 of file vector3d.cpp.

```
153 {
     double m = this->magnitude ();
154
155
156
     if (m==0.0)
157
    return (Vector3d ());
}
158
159
160
    else
162
       return ((*this) * (1.0/m));
163
164 }
```

5.9.3.5 Vector3d Vector3d::operator* (const double & p) const

Operator for scaling the vector by a scalar.

Scales the current vector by the scalar provided and returns the result in a third vector.

Returns

Vector containing the result of scaling the current vector by the scala provided as argument.

Definition at line 239 of file vector3d.cpp.

5.9.3.6 double Vector3d::operator* (const Vector3d & p) const

Operator for the scalar product of two vectors.

Performs the scalar product or dot product of the current vector with the one provided as argument and returns the result.

Returns

Scalar value of the scalar product of dot product of the current vector with the one provided as argument.

Definition at line 271 of file vector3d.cpp.

5.9.3.7 void Vector3d::operator*= (const double & p)

Operator for reflexive scaling of the vector by a scalar.

Scales the current vector by the scalar provided and populates the current vector elements with the result.

Definition at line 256 of file vector3d.cpp.

```
257 {
258    int i;
259
260    for (i=0; i<3; i++)
261    {
262        this->x[i] *= p;
263    }
264 }
```

5.9.3.8 Vector3d Vector3d::operator+ (const Vector3d & p) const

Operator for addition of two vectors.

Adds the current vector to the provided vector and returns a third vector with the result.

Returns

Vector containing the sum of the current vector with the one provided as argument.

Definition at line 173 of file vector3d.cpp.

5.9.3.9 void Vector3d::operator+= (const Vector3d & p)

Operator for reflexive addition of two vectors.

Adds the current vector to the provided vector and populates the current vector elements with the result.

Definition at line 190 of file vector3d.cpp.

```
191 {
192    int i;
193
194    for (i=0; i<3; i++)
195     {
196         this->x[i] += p.x[i];
197    }
198 }
```

5.9.3.10 Vector3d Vector3d::operator-(const Vector3d & p) const

Operator for the subtraction of two vectors.

Subtracts the given vector from the current vector and returns the result in a new vector.

Returns

Vector containing the result of subtracting the vector provided as argument from the current vector.

Definition at line 206 of file vector3d.cpp.

5.9.3.11 void Vector3d::operator== (const Vector3d & p)

Operator for reflexive subtraction of two vectors.

Subtracts the given vector from the current vector and populates the current vector with the result.

Definition at line 223 of file vector3d.cpp.

```
224 {
225    int i;
226
227    for (i=0; i<3; i++)
228    {
229        this->x[i] -= p.x[i];
230    }
231 }
```

5.9.3.12 Vector3d Vector3d::operator (const Vector3d & p) const

Operator for the vector product of two vectors.

Evaluates the vector product of the current vector with the provided vector and returns the result in a third vector.

Returns

Vector containing the result of the vector product of the current vector with the one provided as argument.

Definition at line 289 of file vector3d.cpp.

```
290 {
291    Vector3d r(0.0, 0.0, 0.0);
292
293    r.x[0] = (this->x[1] * p.x[2]) - (this->x[2] * p.x[1]);
294    r.x[1] = (this->x[2] * p.x[0]) - (this->x[0] * p.x[2]);
295    r.x[2] = (this->x[0] * p.x[1]) - (this->x[1] * p.x[0]);
296
297    return (r);
298 }
```

5.9.3.13 void Vector3d::operator $^{\wedge}$ = (const Vector3d & p)

Operator for reflexive vector product of two vectors.

Evaluates the vector product of the current vector and the one provided, and populates the result in the current vector.

Definition at line 304 of file vector3d.cpp.

5.9.3.14 void Vector3d::setValue (int index, double value)

Function to set the value of an element of the vector.

Sets the value of the element indicated by the index argument.

Parameters

index	Index of the element whose value is to be set.
value	Value that is to be given to the element.

Definition at line 56 of file vector3d.cpp.

```
57 {
58    if (index>=0 && index <3)
59    {
60        this->x[index] = value;
61    }
62 }
```

5.9.3.15 void Vector3d::setVector (double * a)

Function to set the value of the entire vector using an array.

Sets the values of the elements if the vector to values in the array pointed to by the argument a.

Parameters

```
a Pointer ot the array containing the values of the elements of the vector.
```

Definition at line 69 of file vector3d.cpp.

```
70 {
71    this->x[0] = a[0];
72    this->x[1] = a[1];
73    this->x[2] = a[2];
```

5.9.3.16 double Vector3d::sum ()

Computes the sum of the elements of the vector.

Sums the elements of the vector and returns the result.

Returns

The sum of the elements of the vector.

Definition at line 116 of file vector3d.cpp.

5.9.4 Field Documentation

5.9.4.1 double Vector3d::x[3] [protected]

The elements of the vector.

Definition at line 26 of file vector3d.h.

The documentation for this class was generated from the following files:

- · vector3d.h
- vector3d.cpp

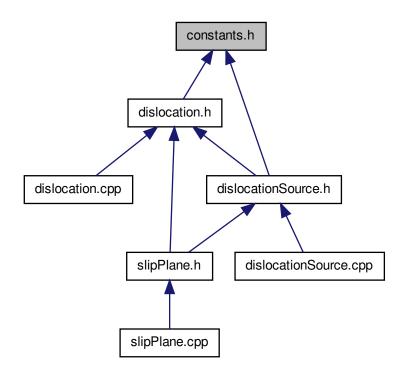
Chapter 6

File Documentation

6.1 constants.h File Reference

Definition of constants used in the program.

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



Macros

• #define PI 3.141592654

The irrational number pi.

• #define SQRT2 1.414213562

The square root of 2.

• #define SQRT3 1.732050808

The square root of 3.

#define SQRT5 2.236067978

The square root of 5.

6.1.1 Detailed Description

Definition of constants used in the program.

Author

Adhish Majumdar

Version

0.0

Date

26/04/2013

This file defines the values of various constants used in the program.

Definition in file constants.h.

6.1.2 Macro Definition Documentation

6.1.2.1 #define PI 3.141592654

The irrational number pi.

Definition at line 16 of file constants.h.

6.1.2.2 #define SQRT2 1.414213562

The square root of 2.

Definition at line 21 of file constants.h.

6.1.2.3 #define SQRT3 1.732050808

The square root of 3.

Definition at line 26 of file constants.h.

6.1.2.4 #define SQRT5 2.236067978

The square root of 5.

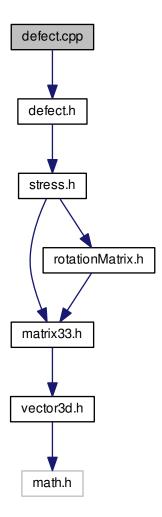
Definition at line 31 of file constants.h.

6.2 defect.cpp File Reference

Definition of member functions of the Defect class.

#include "defect.h"

Include dependency graph for defect.cpp:



6.2.1 Detailed Description

Definition of member functions of the Defect class.

Author

Adhish Majumdar

Version

0.0

Date

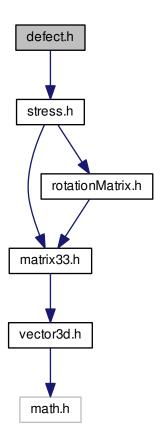
03/06/2013

This file defines the member functions of the Defect class representing a single defect in the simulation. Definition in file defect.cpp.

6.3 defect.h File Reference

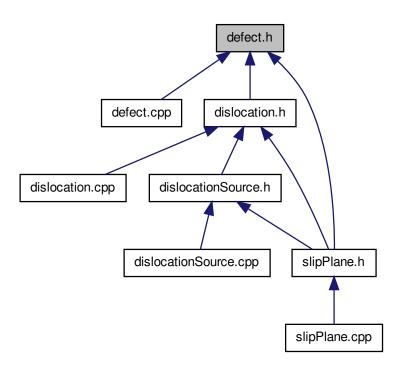
Definition of the **Defect** class.

#include "stress.h"
Include dependency graph for defect.h:



6.3 defect.h File Reference 107

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



Data Structures

class Defect

Class Defect representing a generic defect in a material.

6.3.1 Detailed Description

Definition of the **Defect** class.

Author

Adhish Majumdar

Version

0.0

Date

03/06/2013

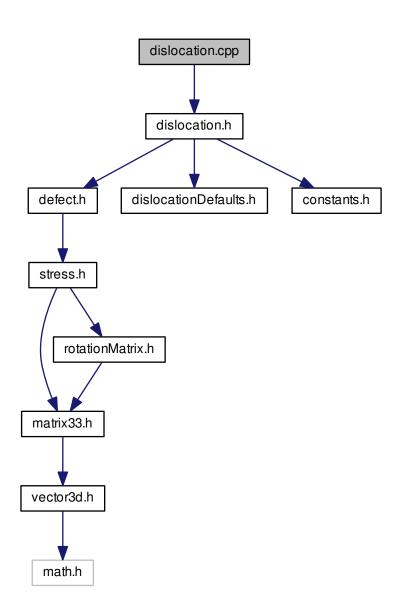
This file defines the Defect class representing an defect in the simulation. This is simply a generic description class with virtual functions. Later classes like dislocations, precipitates, boundaries etc will inherit from this class.

Definition in file defect.h.

6.4 dislocation.cpp File Reference

Definition of constructors and member functions of the Dislocation class.

#include "dislocation.h"
Include dependency graph for dislocation.cpp:



6.4.1 Detailed Description

Definition of constructors and member functions of the Dislocation class.

Author

Adhish Majumdar

Version

0.0

Date

03/06/2013

This file defines the constructors and member functions of the Dislocation class. This class inherits from the Defect class.

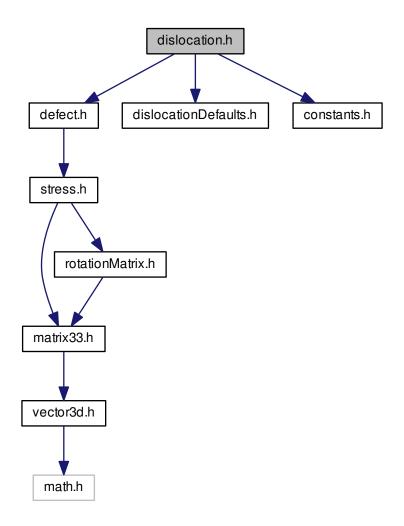
Definition in file dislocation.cpp.

6.5 dislocation.h File Reference

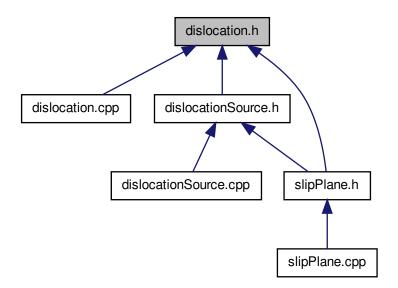
Definition of the Dislocation class.

```
#include "defect.h"
#include "dislocationDefaults.h"
#include "constants.h"
```

Include dependency graph for dislocation.h:



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



Data Structures

class Dislocation

Dislocation class representing a dislocation in the simulation.

6.5.1 Detailed Description

Definition of the Dislocation class.

Author

Adhish Majumdar

Version

0.0

Date

03/06/2013

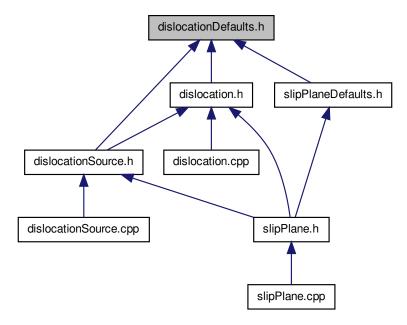
This file defines the Dislocation class representing a dislocation in the simulation. This class inherits from the Defect class

Definition in file dislocation.h.

6.6 dislocationDefaults.h File Reference

Definition of certain default values for members of the Dislocation class.

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



Macros

- #define DEFAULT_POSITION_0 0.0
 - Default value of the position vector x-coordinate.
- #define DEFAULT_POSITION_1 0.0

Default value of the position vector y-coordinate.

• #define DEFAULT_POSITION_2 0.0

Default value of the position vector z-coordinate.

• #define DEFAULT_BURGERS_MAGNITUDE 5.0e-09

Default value of the magnitude of the Burgers vector.

• #define DEFAULT_BURGERS_0 1.0

Default value of the Burgers vector x-coordinate.

• #define DEFAULT_BURGERS_1 1.0

Default value of the Burgers vector y-coordinate.

• #define DEFAULT_BURGERS_2 0.0

Default value of the Burgers vector z-coordinate.

• #define DEFAULT_LINEVECTOR_0 1.0

Default value of the line vector x-coordinate.

• #define DEFAULT_LINEVECTOR_1 -1.0

Default value of the line vector y-coordinate.

• #define DEFAULT LINEVECTOR 2 -2.0

Default value of the line vector z-coordinate.

6.6.1 Detailed Description

Definition of certain default values for members of the Dislocation class.

Author

Adhish Majumdar

Version

0.0

Date

26/04/2013

This file defines some default values for members of the Dislocation class representing a dislocation in the simulation.

Definition in file dislocationDefaults.h.

6.6.2 Macro Definition Documentation

6.6.2.1 #define DEFAULT_BURGERS_0 1.0

Default value of the Burgers vector x-coordinate.

Definition at line 34 of file dislocationDefaults.h.

6.6.2.2 #define DEFAULT_BURGERS_1 1.0

Default value of the Burgers vector y-coordinate.

Definition at line 38 of file dislocationDefaults.h.

6.6.2.3 #define DEFAULT_BURGERS_2 0.0

Default value of the Burgers vector z-coordinate.

Definition at line 42 of file dislocationDefaults.h.

6.6.2.4 #define DEFAULT_BURGERS_MAGNITUDE 5.0e-09

Default value of the magnitude of the Burgers vector.

Definition at line 29 of file dislocationDefaults.h.

6.6.2.5 #define DEFAULT_LINEVECTOR_0 1.0

Default value of the line vector x-coordinate.

Definition at line 47 of file dislocationDefaults.h.

6.6.2.6 #define DEFAULT_LINEVECTOR_1 -1.0

Default value of the line vector y-coordinate.

Definition at line 51 of file dislocationDefaults.h.

6.6.2.7	#define DEFAULT_LINEVECTOR_2	-2.0

Default value of the line vector z-coordinate.

Definition at line 55 of file dislocationDefaults.h.

6.6.2.8 #define DEFAULT_POSITION_0 0.0

Default value of the position vector x-coordinate.

Definition at line 16 of file dislocationDefaults.h.

6.6.2.9 #define DEFAULT_POSITION_1 0.0

Default value of the position vector y-coordinate.

Definition at line 20 of file dislocationDefaults.h.

6.6.2.10 #define DEFAULT_POSITION_2 0.0

Default value of the position vector z-coordinate.

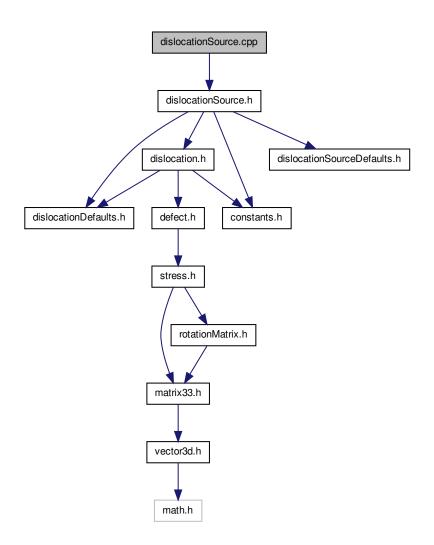
Definition at line 24 of file dislocationDefaults.h.

6.7 dislocationSource.cpp File Reference

Definition of the member functions of the DislocationSource class.

#include "dislocationSource.h"

Include dependency graph for dislocationSource.cpp:



6.7.1 Detailed Description

Definition of the member functions of the DislocationSource class.

Author

Adhish Majumdar

Version

0.0

Date

27/05/2013

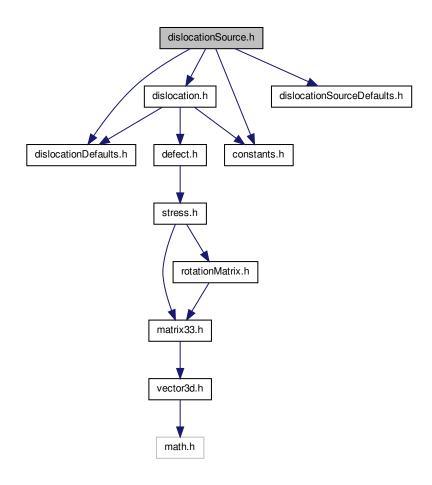
This file defines the member functions of the DislocationSource class representing a source of dislocations in the simulation. This class inherits from the Defect class. This object is basically the representation of a Frank-Read source emitting dislocation dipoles. When the dislocation source experiences a shear stress greater than a critical value for a certain amount of time (or number of iterations), it emits a dislocation dipole with a length that is a function of the applied stress.

Definition in file dislocationSource.cpp.

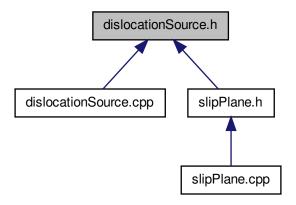
6.8 dislocationSource.h File Reference

Definition of the DislocationSource class.

```
#include "dislocation.h"
#include "constants.h"
#include "dislocationDefaults.h"
#include "dislocationSourceDefaults.h"
Include dependency graph for dislocationSource.h:
```



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



Data Structures

· class DislocationSource

DislocationSource class representing a source of dislocations in the simulation.

6.8.1 Detailed Description

Definition of the DislocationSource class.

Author

Adhish Majumdar

Version

0.0

Date

27/05/2013

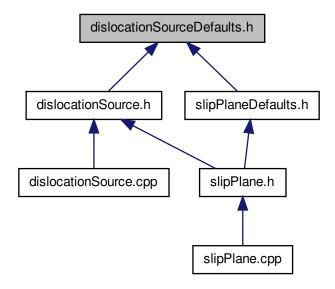
This file defines the DislocationSource class representing a source of dislocations in the simulation. This class inherits from the Defect class. This object is basically the representation of a Frank-Read source emitting dislocation dipoles. When the dislocation source experiences a shear stress greater than a critical value for a certain amount of time (or number of iterations), it emits a dislocation dipole with a length that is a function of the applied stress.

Definition in file dislocationSource.h.

6.9 dislocationSourceDefaults.h File Reference

Definition of certain default values for members of the DislocationSource class.

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



Macros

- #define DEFAULT_TAU_CRITICAL 1.0e09
 - Default value of the critical shear stress for a dislocation source to emit a dipole.
- #define DEFAULT_NITERATIONS 10

Default value of the number of iterations required for a dislocation source to emit a dipole.

6.9.1 Detailed Description

Definition of certain default values for members of the DislocationSource class.

Author

Adhish Majumdar

Version

0.0

Date

02/05/2013

This file defines some default values for members of the DislocationSource class representing a dislocation dipole source in the simulation.

Definition in file dislocationSourceDefaults.h.

6.9.2 Macro Definition Documentation

6.9.2.1 #define DEFAULT_NITERATIONS 10

Default value of the number of iterations required for a dislocation source to emit a dipole.

The dislocation source must experience a shear stress greater than the critical value in order to emit a dipole. This time is expressed in terms of the number of iterations here.

Definition at line 23 of file dislocationSourceDefaults.h.

6.9.2.2 #define DEFAULT_TAU_CRITICAL 1.0e09

Default value of the critical shear stress for a dislocation source to emit a dipole.

Default value of the critical shear stress for a dislocation source to emit a dipole. The number is expressed in Pa.

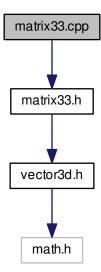
Definition at line 17 of file dislocationSourceDefaults.h.

6.10 mainpage.dox File Reference

6.11 matrix33.cpp File Reference

Definition of the member functions and operators of the Matrix33 class.

#include "matrix33.h"
Include dependency graph for matrix33.cpp:



6.11.1 Detailed Description

Definition of the member functions and operators of the Matrix33 class.

Author

Adhish Majumdar

Version

0.0

Date

22/04/2013

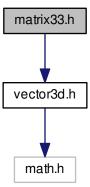
This file defines the member functions and operators of the Matrix33 class representing a 3x3 matrix in the simulation.

Definition in file matrix33.cpp.

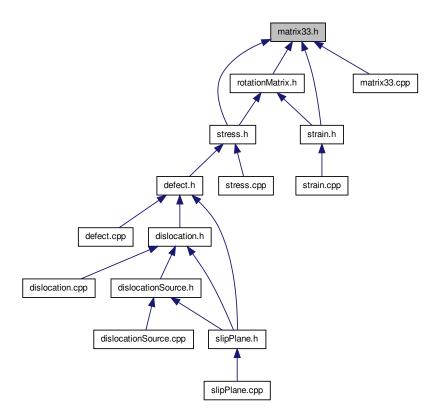
6.12 matrix33.h File Reference

Definition of the Matrix33 class.

#include "vector3d.h"
Include dependency graph for matrix33.h:



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



Data Structures

• class Matrix33

Matrix33 class representing a 3x3 square matrix.

6.12.1 Detailed Description

Definition of the Matrix33 class.

Author

Adhish Majumdar

Version

0.0

Date

22/04/2013

This file defines the ${\tt Matrix33}$ class representing a 3x3 matrix in the simulation.

Definition in file matrix33.h.

6.13 rotationMatrix.cpp File Reference

Definition of the RotationMatrix class member functions.

6.13.1 Detailed Description

Definition of the RotationMatrix class member functions.

Author

Adhish Majumdar

Version

0.0

Date

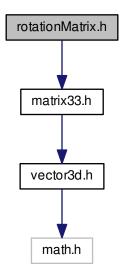
25/04/2013

This file defines member functions of the RotationMatrix class for carrying out 3D rotations and axes transformations. Definition in file rotationMatrix.cpp.

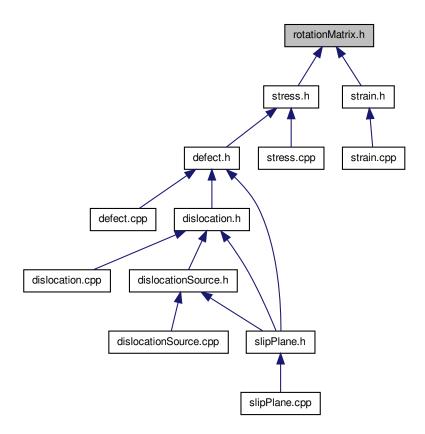
6.14 rotationMatrix.h File Reference

Definition of the RotationMatrix class.

```
#include "matrix33.h"
Include dependency graph for rotationMatrix.h:
```



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



Data Structures

• class RotationMatrix

RotationMatrix class to represent a rotation matrix.

6.14.1 Detailed Description

Definition of the RotationMatrix class.

Author

Adhish Majumdar

Version

0.0

Date

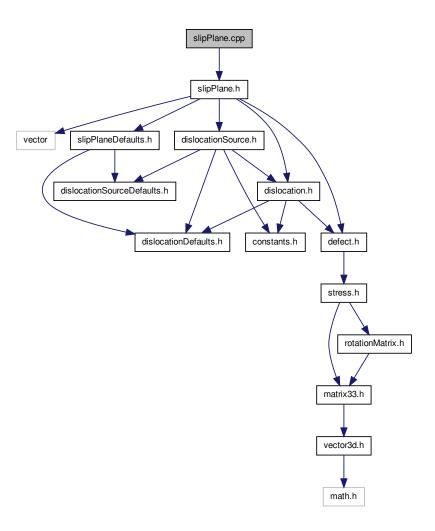
25/04/2013

This file defines the RotationMatrix class for carrying out 3D rotations and axes transformations. Definition in file rotationMatrix.h.

6.15 slipPlane.cpp File Reference

Definition of the member functions of the SlipPlane class.

#include "slipPlane.h"
Include dependency graph for slipPlane.cpp:



6.15.1 Detailed Description

Definition of the member functions of the SlipPlane class.

Author

Adhish Majumdar

Version

0.0

Date

03/06/2013

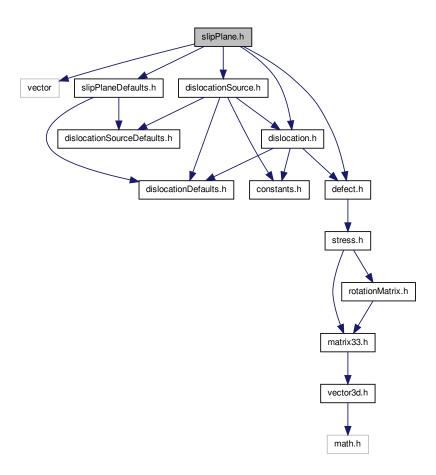
This file defines the member functions of the SlipPlane class.

Definition in file slipPlane.cpp.

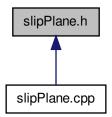
6.16 slipPlane.h File Reference

Definition of the SlipPlane class.

```
#include <vector>
#include "slipPlaneDefaults.h"
#include "defect.h"
#include "dislocation.h"
#include "dislocationSource.h"
Include dependency graph for slipPlane.h:
```



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



Data Structures

• class SlipPlane

SlipPlane class representing a slip plane in the simulation.

6.16.1 Detailed Description

Definition of the SlipPlane class.

Author

Adhish Majumdar

Version

0.0

Date

03/06/2013

This file defines the SlipPlane class representing a slip plane in the simulation.

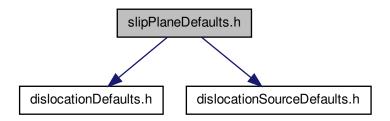
Definition in file slipPlane.h.

6.17 slipPlaneDefaults.h File Reference

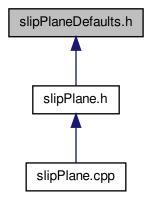
Definition of certain default values for members of the SlipPlane class.

```
#include "dislocationDefaults.h"
#include "dislocationSourceDefaults.h"
```

Include dependency graph for slipPlaneDefaults.h:



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



Macros

- #define DEFAULT_SLIPPLANE_POSITION_0 0.0
 - Default value of the position vector x-coordinate.
- #define DEFAULT_SLIPPLANE_POSITION_1 0.0
 - Default value of the position vector y-coordinate.
- #define DEFAULT_SLIPPLANE_POSITION_2 0.0
 - Default value of the position vector z-coordinate.
- #define DEFAULT_SLIPPLANE_NORMALVECTOR_0 1.0
 - Default value of the normal vector x-coordinate.
- #define DEFAULT_SLIPPLANE_NORMALVECTOR_1 1.0
 - Default value of the normal vector y-coordinate.
- #define DEFAULT_SLIPPLANE_NORMALVECTOR_2 1.0
 - Default value of the normal vector z-coordinate.
- #define DEFAULT_SLIPPLANE_EXTREMITY1_0 5.0e-06

Default value of the position vector of extremity 1 x-coordinate.

#define DEFAULT_SLIPPLANE_EXTREMITY1_1 0.0

Default value of the position vector of extremity 1 y-coordinate.

• #define DEFAULT_SLIPPLANE_EXTREMITY1_2 0.0

Default value of the position vector of extremity 1 z-coordinate.

• #define DEFAULT_SLIPPLANE_EXTREMITY2_0 0.0

Default value of the position vector of extremity 2 x-coordinate.

#define DEFAULT_SLIPPLANE_EXTREMITY2_1 5.0e-6

Default value of the position vector of extremity 2 y-coordinate.

#define DEFAULT_SLIPPLANE_EXTREMITY2_2 0.0

Default value of the position vector of extremity 2 z-coordinate.

6.17.1 Detailed Description

Definition of certain default values for members of the SlipPlane class.

Author

Adhish Majumdar

Version

0.0

Date

31/05/2013

This file defines some default values for members of the SlipPlane class representing a slip plane in the simulation. Definition in file slipPlaneDefaults.h.

6.17.2 Macro Definition Documentation

6.17.2.1 #define DEFAULT_SLIPPLANE_EXTREMITY1_0 5.0e-06

Default value of the position vector of extremity 1 x-coordinate.

Definition at line 50 of file slipPlaneDefaults.h.

6.17.2.2 #define DEFAULT_SLIPPLANE_EXTREMITY1_1 0.0

Default value of the position vector of extremity 1 y-coordinate.

Definition at line 55 of file slipPlaneDefaults.h.

6.17.2.3 #define DEFAULT_SLIPPLANE_EXTREMITY1_2 0.0

Default value of the position vector of extremity 1 z-coordinate.

Definition at line 60 of file slipPlaneDefaults.h.

6.17.2.4 #define DEFAULT_SLIPPLANE_EXTREMITY2_0 0.0

Default value of the position vector of extremity 2 x-coordinate.

Definition at line 65 of file slipPlaneDefaults.h.

6.17.2.5 #define DEFAULT_SLIPPLANE_EXTREMITY2_1 5.0e-6

Default value of the position vector of extremity 2 y-coordinate.

Definition at line 70 of file slipPlaneDefaults.h.

6.17.2.6 #define DEFAULT_SLIPPLANE_EXTREMITY2_2 0.0

Default value of the position vector of extremity 2 z-coordinate.

Definition at line 75 of file slipPlaneDefaults.h.

6.17.2.7 #define DEFAULT_SLIPPLANE_NORMALVECTOR_0 1.0

Default value of the normal vector x-coordinate.

Definition at line 35 of file slipPlaneDefaults.h.

6.17.2.8 #define DEFAULT_SLIPPLANE_NORMALVECTOR_1 1.0

Default value of the normal vector y-coordinate.

Definition at line 40 of file slipPlaneDefaults.h.

6.17.2.9 #define DEFAULT_SLIPPLANE_NORMALVECTOR_2 1.0

Default value of the normal vector z-coordinate.

Definition at line 45 of file slipPlaneDefaults.h.

6.17.2.10 #define DEFAULT_SLIPPLANE_POSITION_0 0.0

Default value of the position vector x-coordinate.

Definition at line 20 of file slipPlaneDefaults.h.

6.17.2.11 #define DEFAULT_SLIPPLANE_POSITION_1 0.0

Default value of the position vector y-coordinate.

Definition at line 25 of file slipPlaneDefaults.h.

6.17.2.12 #define DEFAULT_SLIPPLANE_POSITION_2 0.0

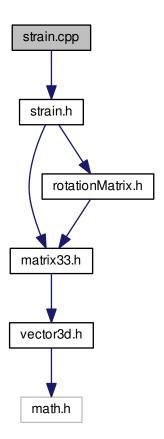
Default value of the position vector z-coordinate.

Definition at line 30 of file slipPlaneDefaults.h.

6.18 strain.cpp File Reference

Definition of the member functions if the Strain class.

#include "strain.h"
Include dependency graph for strain.cpp:



6.18.1 Detailed Description

Definition of the member functions if the Strain class.

Author

Adhish Majumdar

Version

0.0

Date

22/04/2013

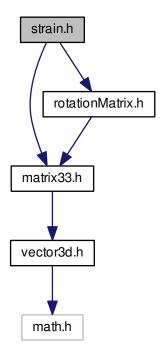
This file defines the member functions of the Strain class for the strain tensor.

Definition in file strain.cpp.

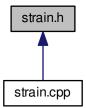
6.19 strain.h File Reference

Definition of the Strain class.

```
#include "matrix33.h"
#include "rotationMatrix.h"
Include dependency graph for strain.h:
```



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



Data Structures

• class Strain

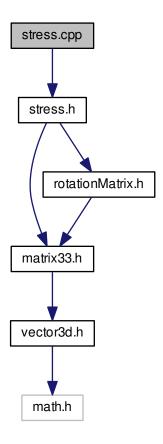
Strain class to represent the strain tensor.

6.19.1 Detailed Description		
Definition of the Strain class.		
Author Adhish Majumdar		
Version 0.0		
Date 25/04/2013		
This file defines the Strain class for the strain tensor. Definition in file strain.h.		

6.20 stress.cpp File Reference

Definition of the member functions if the Stress class.

#include "stress.h"
Include dependency graph for stress.cpp:



6.20.1 Detailed Description

Definition of the member functions if the Stress class.

Author

Adhish Majumdar

Version

0.0

Date

22/04/2013

This file defines the member functions of the Stress class for the stress tensor.

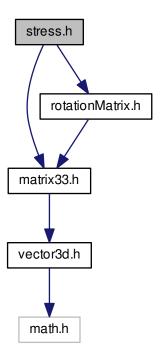
Definition in file stress.cpp.

6.21 stress.h File Reference

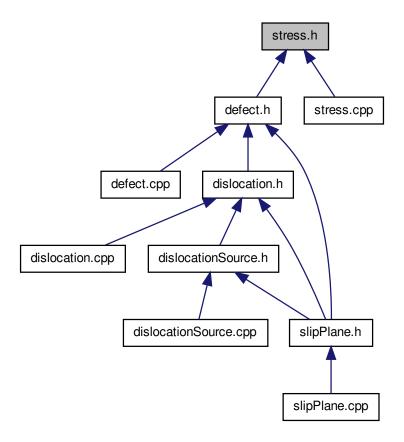
6.21 stress.h File Reference

Definition of the Stress class.

```
#include "matrix33.h"
#include "rotationMatrix.h"
Include dependency graph for stress.h:
```



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



Data Structures

• class Stress

Stress class to represent the stress tensor.

6.21.1 Detailed Description

Definition of the Stress class.

Author

Adhish Majumdar

Version

0.0

Date

22/04/2013

This file defines the Stress class for the stress tensor.

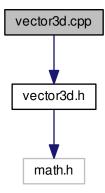
Definition in file stress.h.

6.22 vector3d.cpp File Reference

Definition of member functions and operators of the Vector3d class.

#include "vector3d.h"

Include dependency graph for vector3d.cpp:



6.22.1 Detailed Description

Definition of member functions and operators of the Vector3d class.

Author

Adhish Majumdar

Version

0.0

Date

29/04/2013

This file defines the member functions and operators of the Vector3d class representing a single 3-dimensional vector in the simulation.

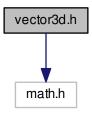
Definition in file vector3d.cpp.

6.23 vector3d.h File Reference

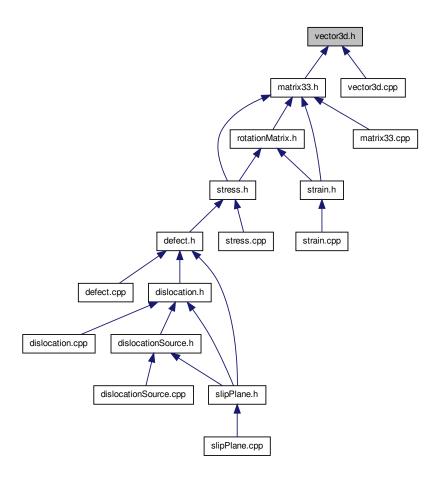
Definition of the Vector3d class.

#include <math.h>

Include dependency graph for vector3d.h:



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



Data Structures

class Vector3d

Vector3d class representing a single 3-dimensional vector in the simulation.

6.23.1 Detailed Description

Definition of the Vector3d class.

Author

Adhish Majumdar

Version

0.0

Date

29/04/2013

This file defines the Vector3d class representing a single 3-dimensional vector in the simulation.

Definition in file vector3d.h.

Index

adjugate	getY, 12
Matrix33, 43	getZ, 13
RotationMatrix, 52	pos, 15
Strain, 76	setPosition, 13, 14
Stress, 86	setX, 14
	setY, 14
bmag	setZ, 14
Dislocation, 26	stressField, 15
DislocationSource, 39	defect.cpp, 105
bvec	defect.h, 106
Dislocation, 26	dipoleNucleationLength
DislocationSource, 39	DislocationSource, 31
	Dislocation, 15
calculateDislocationForces	bmag, <mark>26</mark>
SlipPlane, 61	bvec, 26
calculateDislocationStresses	calculateRotationMatrix, 19
SlipPlane, 62	Dislocation, 18
calculateRotationMatrix	forcePeachKoehler, 19
Dislocation, 19	getBurgers, 20
SlipPlane, 62	getLineVector, 20
calculateTimeIncrement	getPosition, 20, 21
SlipPlane, 63	getX, 21
calculate Velocities	getY, 21
SlipPlane, 64	getZ, 21
constants.h, 103	idealTimeIncrement, 21
PI, 104	isMobile, 22
SQRT2, 104	lvec, 27
SQRT3, 104	mobile, 27
SQRT5, 104	pos, 27
countIterations	rotationMatrix, 27
DislocationSource, 39	setBurgers, 23
DEFAULT BURGERS 0	setLineVector, 23
dislocationDefaults.h, 112	setMobile, 23
DEFAULT BURGERS 1	setPinned, 23
dislocationDefaults.h, 112	setPosition, 23, 24
DEFAULT BURGERS 2	setX, 24
dislocationDefaults.h, 112	setY, 25
DEFAULT_NITERATIONS	setZ, 25
dislocationSourceDefaults.h, 118	stressField, 25
DEFAULT_POSITION_0	stressFieldLocal, 26
dislocationDefaults.h, 113	dislocation.cpp, 108
DEFAULT_POSITION_1	dislocation.h, 109
dislocationDefaults.h, 113	dislocationDefaults.h, 110
DEFAULT_POSITION_2	DEFAULT_BURGERS_0, 112
dislocationDefaults.h, 113	DEFAULT_BURGERS_1, 112
Defect, 9	DEFAULT BURGERS 2, 112
Defect, 11	DEFAULT POSITION 0, 113
getPosition, 11, 12	DEFAULT_POSITION_1, 113
getX, 12	DEFAULT_POSITION_2, 113
· ,	,

e 1 - e - -	
dislocationForces	getAxis
SlipPlane, 72	SlipPlane, 65
DislocationSource, 27	getBurgers
bmag, 39	Dislocation, 20
bvec, 39	DislocationSource, 32
countIterations, 39	getBurgersMag
dipoleNucleationLength, 31	DislocationSource, 32
DislocationSource, 30	getDislocation
DislocationSource, 30	SlipPlane, 66
getBurgers, 32	getDislocationList
getBurgersMag, 32	SlipPlane, 66
getIterationCount, 32	getDislocationSource
getLineVector, 32	SlipPlane, 67
getNumIterations, 33	getDislocationSourceList
getPosition, 33, 34	SlipPlane, 67
getTauCritical, 34	getExtremities
getX, 34	SlipPlane, 67
getY, 34	getExtremity
getZ, 34	SlipPlane, 68
ifEmitDipole, 35	getIterationCount
incrementIterationCount, 35	DislocationSource, 32
lvec, 39	getLineVector
mobile, 39	Dislocation, 20
nlterations, 39	DislocationSource, 32
pos, 40	getNormal
resetIterationCounter, 35	SlipPlane, 68
rotationMatrix, 40	getNumDislocationSources
setBurgers, 35	SlipPlane, 69
setBurgersMagnitude, 36	getNumDislocations
setLineVector, 36	SlipPlane, 68
setNumIterations, 36	getNumIterations
setPosition, 36, 37	DislocationSource, 33
setTauCritical, 37	getPosition
setX, 38	Defect, 11, 12
setY, 38	Dislocation, 20, 21
setZ, 38	DislocationSource, 33, 34
stressField, 38	SlipPlane, 69
tauCritical, 40	getPrincipalStrains
dislocationSource.cpp, 113	Strain, 77
dislocationSource.h, 115	getPrincipalStresses
dislocationSourceDefaults.h, 116	Stress, 87
dislocationSources	getRotationMatrix
SlipPlane, 72	SlipPlane, 69
dislocationStresses	getShearStrains
SlipPlane, 72	Strain, 77
dislocationVelocities	
SlipPlane, 72	getShearStresses
dislocations	Stress, 87
SlipPlane, 72	getTauCritical
distanceFromExtremity	DislocationSource, 34
SlipPlane, 65	getValue
dt	Matrix33, 44
SlipPlane, 72	RotationMatrix, 52
	Strain, 77
extremities	Stress, 87
SlipPlane, 72	Vector3d, 96
	getVector
forcePeachKoehler	Vector3d, 97
Dislocation, 19	getX

Defect, 12 Dislocation, 21 DislocationSource, 34	RotationMatrix, 53, 54 Strain, 78, 79 Stress, 88, 89
getY Defect, 12	Vector3d, 98 operator*=
Dislocation, 21 DislocationSource, 34	Matrix33, 46 RotationMatrix, 55
getZ Defect, 13	Strain, 79, 80 Stress, 90
Dislocation, 21 DislocationSource, 34	Vector3d, 98 operator∼
idealTimeIncrement	Matrix33, 48 RotationMatrix, 57
Dislocation, 21 ifEmitDipole	Strain, 82 Stress, 92
DislocationSource, 35	$operator^\wedge$
incrementIterationCount	Matrix33, 48
DislocationSource, 35	RotationMatrix, 57
isMobile	Strain, 81
Dislocation, 22	Stress, 92 Vector3d, 100
lvec	operator [∧] =
Dislocation, 27	Vector3d, 100
DislocationSource, 39	operator+
	Matrix33, 47
magnitude	RotationMatrix, 55
Vector3d, 97	Strain, 80
mainpage.dox, 118	Stress, 90
Matrix33, 40	Vector3d, 99
adjugate, 43	operator+=
getValue, 44	Matrix33, 47
Matrix33, 42, 43 operator*, 45, 46	RotationMatrix, 56
operator*=, 46	Strain, 80
operator~, 48	Stress, 91
operator [^] , 48	Vector3d, 99 operator-
operator+, 47	Matrix33, 47
operator+=, 47	RotationMatrix, 56
operator-, 47	Strain, 81
operator-=, 48	Stress, 91
setValue, 49	Vector3d, 99
x, 49	operator-=
matrix33.cpp, 118	Matrix33, 48
matrix33.h, 119	RotationMatrix, 56
mobile	Strain, 81
Dislocation, 27	Stress, 91
DislocationSource, 39 moveDislocations	Vector3d, 100
SlipPlane, 69	PI
Slipi latie, 09	constants.h, 104
nlterations	populateMatrix
DislocationSource, 39	Strain, 82
normalVector	Stress, 92
SlipPlane, 73	pos
normalize	Defect, 15
Vector3d, 97	Dislocation, 27 DislocationSource, 40
operator*	position
Matrix33, 45, 46	SlipPlane, 73

principalStrains	Dislocation, 23
Strain, 83	setPosition
principalStresses	Defect, 13, 14
Stress, 94	Dislocation, 23, 24
, -	DislocationSource, 36, 37
resetIterationCounter	SlipPlane, 71
DislocationSource, 35	setTauCritical
rotate	DislocationSource, 37
Strain, 82	setValue
Stress, 93	Matrix33, 49
RotationMatrix, 50	RotationMatrix, 57
adjugate, 52	Strain, 83
getValue, 52	Stress, 93
operator*, 53, 54	Vector3d, 101
operator*=, 55	setVector
operator \sim , 57	Vector3d, 101
operator $^{\wedge}$, 57	setX
operator+, 55	Defect, 14
operator+=, 56	Dislocation, 24
operator-, <mark>56</mark>	DislocationSource, 38
operator-=, 56	setY
RotationMatrix, 51	Defect, 14
RotationMatrix, 51	Dislocation, 25
setValue, 57	DislocationSource, 38
x, 58	setZ
rotationMatrix	Defect, 14
Dislocation, 27	Dislocation, 25
DislocationSource, 40	DislocationSource, 38
SlipPlane, 73	shearStrains
rotationMatrix.cpp, 121	Strain, 83
rotationMatrix.h, 121	shearStresses
CORTO	Stress, 94
SQRT2	SlipPlane, 58
constants.h, 104	calculateDislocationForces, 61
SQRT3	calculateDislocationStresses, 62
constants.h, 104	calculateRotationMatrix, 62
SQRT5	calculateTimeIncrement, 63
constants.h, 104	calculate Velocities, 64
setBurgers	dislocationForces, 72
Dislocation, 23	dislocationSources, 72
DislocationSource, 35 setBurgersMagnitude	dislocationStresses, 72
DislocationSource, 36	dislocationVelocities, 72
setDislocationList	dislocations, 72
SlipPlane, 70	distanceFromExtremity, 65
setDislocationSourceList	dt, 72
SlipPlane, 70	extremities, 72
setExtremities	getAxis, 65
SlipPlane, 70	getDislocation, 66
setLineVector	getDislocationList, 66
Dislocation, 23	getDislocationSource, 67
Dislocation, 23 Dislocation Source, 36	getDislocationSourceList, 67
setMobile	getExtremities, 67
Dislocation, 23	getExtremity, 68
setNormal	getNormal, 68
SlipPlane, 71	getNormal, 00 getNumDislocationSources, 69
setNumIterations	getNumDislocations, 68
DislocationSource, 36	getPosition, 69
setPinned	getRotationMatrix, 69
33	gon totalloriviation, oo

moveDislocations, 69	x, 94
normalVector, 73	stress.cpp, 131
position, 73	stress.h, 133
rotationMatrix, 73	stressField
setDislocationList, 70	Defect, 15
setDislocationSourceList, 70	Dislocation, 25
	DislocationSource, 38
setExtremities, 70	
setNormal, 71	stressFieldLocal
setPosition, 71	Dislocation, 26
SlipPlane, 60, 61	sum
SlipPlane, 60, 61	Vector3d, 101
sortDislocations, 71	tauCritical
slipPlane.cpp, 123	
slipPlane.h, 124	DislocationSource, 40
slipPlaneDefaults.h, 125	Vector3d, 94
sortDislocations	
SlipPlane, 71	getValue, 96
Strain, 73	getVector, 97
adjugate, 76	magnitude, 97
getPrincipalStrains, 77	normalize, 97
getShearStrains, 77	operator*, 98
getValue, 77	operator*=, 98
operator*, 78, 79	operator^, 100
operator*=, 79, 80	operator [∧] =, 100
operator \sim , 82	operator+, 99
operator [^] , 81	operator+=, 99
•	operator-, 99
operator+, 80	operator-=, 100
operator+=, 80	setValue, 101
operator-, 81	setVector, 101
operator-=, 81	sum, 101
populateMatrix, 82	Vector3d, 95, 96
principalStrains, 83	x, 102
rotate, 82	vector3d.cpp, 135
setValue, 83	vector3d.h, 135
shearStrains, 83	
Strain, 75, 76	X
x, 84	Matrix33, 49
strain.cpp, 128	RotationMatrix, 58
strain.h, 130	Strain, 84
Stress, 84	Stress, 94
adjugate, 86	Vector3d, 102
getPrincipalStresses, 87	
getShearStresses, 87	
getValue, 87	
operator*, 88, 89	
operator*=, 90	
operator~, 92	
operator [^] , 92	
operator+, 90	
operator+=, 91	
operator-, 91	
•	
operator-=, 91	
populateMatrix, 92	
principalStresses, 94	
rotate, 93	
setValue, 93	
shearStresses, 94	
Stress, 86	