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Chapter 2

Data Structure Index

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Chapter 4

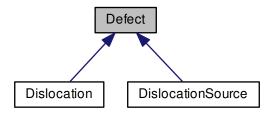
Data Structure Documentation

4.1 Defect Class Reference

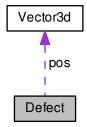
Class Defect representing a generic defect in a material.

#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 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.

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.

4.1.1 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 21 of file defect.h.

4.1.2 Constructor & Destructor Documentation

4.1.2.1 Defect::Defect ()

Default constructor.

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

Definition at line 17 of file defect.cpp.

```
{
  for (int i=0; i<3; i++)
    {
     this->pos.setValue(i, 0.0);
  }
}
```

4.1.2.2 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.

```
{
  this->pos.setValue (0, x);
  this->pos.setValue (1, y);
  this->pos.setValue (2, z);
```

4.1.2.3 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.

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

4.1.3 Member Function Documentation

4.1.3.1 double * Defect::getPosition()

Returns in an array the position.

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.

Definition at line 109 of file defect.cpp.

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

4.1.3.2 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 119 of file defect.cpp.

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

4.1.3.3 double Defect::getX()

Returns the X-coordinate of the defect.

Returns

X-coordinate of the defect.

Definition at line 128 of file defect.cpp.

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

4.1.3.4 double Defect::getY()

Returns the Y-coordinate of the defect.

Returns

Y-coordinate of the defect.

Definition at line 137 of file defect.cpp.

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

4.1.3.5 double Defect::getZ()

Returns the Z-coordinate of the defect.

Returns

Z-coordinate of the defect.

Definition at line 146 of file defect.cpp.

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

4.1 Defect Class Reference 11

4.1.3.6 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.

```
{
this->pos.setValue (a);
```

4.1.3.7 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.

```
this->pos.setValue (0, x);
this->pos.setValue (1, y);
this->pos.setValue (2, z);
```

4.1.3.8 void Defect::setX (double x)

Sets the X-coordinate of the defect.

Parameters

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

Definition at line 80 of file defect.cpp.

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

4.1.3.9 void Defect::setY (double y)

Sets the Y-coordinate of the defect.

Parameters

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

Definition at line 89 of file defect.cpp.

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

4.1.3.10 void Defect::setZ (double z)

Sets the Z-coordinate of the defect.

Parameters

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

Definition at line 98 of file defect.cpp.

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

4.1.3.11 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 122 of file defect.h.

```
{
  // This virtual function returns a zero matrix.
  // Inheriting classes will have functions implementing this in their own
  way
  // They will override this behaviour.
  Stress s;
  return (s);
```

4.1.4 Field Documentation

4.1.4.1 Vector3d Defect::pos [protected]

Position vector of the defect in 2D space.

Definition at line 27 of file defect.h.

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

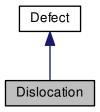
- · defect.h
- · defect.cpp

4.2 Dislocation Class Reference

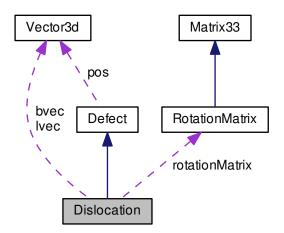
Dislocation class representing a dislocation in the simulation.

#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.

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 doe to the dislocation in the local co-ordinate system.

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 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.

• 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 lvec

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.

4.2.1 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.

4.2.2 Constructor & Destructor Documentation

4.2.2.1 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.

4.2.2.2 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.

```
this->bvec = burgers;
this->lvec = line;
this->pos = position;
this->mobile = m;
this->bmag = bm;
this->calculateRotationMatrix ();
```

4.2.3 Member Function Documentation

4.2.3.1 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 109 of file dislocation.cpp.

4.2.3.2 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.

```
{
  return ( this->bvec );
}
```

4.2.3.3 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.

```
{
  return ( this->lvec );
```

4.2.3.4 double * Defect::getPosition() [inherited]

Returns in an array the position.

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.

Definition at line 109 of file defect.cpp.

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

4.2.3.5 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 119 of file defect.cpp.

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

4.2.3.6 double Defect::getX() [inherited]

Returns the X-coordinate of the defect.

Returns

X-coordinate of the defect.

Definition at line 128 of file defect.cpp.

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

4.2.3.7 double Defect::getY() [inherited]

Returns the Y-coordinate of the defect.

Returns

Y-coordinate of the defect.

Definition at line 137 of file defect.cpp.

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

4.2.3.8 double Defect::getZ() [inherited]

Returns the Z-coordinate of the defect.

Returns

Z-coordinate of the defect.

Definition at line 146 of file defect.cpp.

```
{
   return (this->pos.getValue (2));
```

4.2.3.9 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.

```
this->bvec = burgers;
```

4.2.3.10 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.

```
{
  this->lvec = line;
```

4.2.3.11 void Dislocation::setMobile ()

Sets the dislocation as mobile.

Sets the flag mobile to true.

Definition at line 71 of file dislocation.cpp.

```
{
  this->mobile = true;
```

4.2.3.12 void Dislocation::setPinned()

Sets the dislocation as pinned.

Sets the flag mobile to false.

Definition at line 80 of file dislocation.cpp.

```
{
  this->mobile = false;
}
```

4.2.3.13 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.

```
{
  this->pos.setValue (a);
```

4.2.3.14 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.

```
{
  this->pos.setValue (0, x);
  this->pos.setValue (1, y);
  this->pos.setValue (2, z);
```

4.2.3.15 void Defect::setX (double x) [inherited]

Sets the X-coordinate of the defect.

Parameters

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

Definition at line 80 of file defect.cpp.

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

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

Sets the Y-coordinate of the defect.

Parameters

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

Definition at line 89 of file defect.cpp.

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

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

Sets the Z-coordinate of the defect.

Parameters

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

Definition at line 98 of file defect.cpp.

```
(
this->pos.setValue (2, z);
```

4.2.3.18 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 137 of file dislocation.cpp.

```
double principalStresses[3];
double shearStresses[3];
Vector3d r; // Vector joining the present dislocation to the point p

r = p - this->pos; // Still in global coordinate system
Vector3d rLocal = this->rotationMatrix * r; //
Rotated to local co-ordinate system

// Calculate the stress field in the local co-ordinate system
Stress sLocal = this->stressFieldLocal (rLocal, mu, nu)
;

// Calculate the stress field in the global co-ordinate system
Stress sGlobal = (this->rotationMatrix) * sLocal * (^(
```

```
this->rotationMatrix));
return (sGlobal);
```

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

Calculates the stress field doe 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 163 of file dislocation.cpp.

```
double D = ( mu * this->bm ) / ( 2.0 * PI * ( 1.0 - nu ) ); // Constant for
    all components of the stress tensor

double x, y, denominator; // Terms that appear repeatedly in the stress
    tensor

x = p.getValue (0);
y = p.getValue (1);
denominator = pow ( ((x*x) + (y*y)), 2);

principalStresses[0] = -1.0 * D * y * ( (3.0*x*x) + (y*y) ) / denominator;
principalStresses[1] = D * y * ( (x*x) - (y*y) ) / denominator;
principalStresses[2] = nu * ( principalStresses[0] + principalStresses[1] );

shearStresses[0] = D * x * ( (x*x) - (y*y) ) / denominator;
shearStresses[1] = 0.0;
shearStresses[2] = 0.0;
```

4.2.4 Field Documentation

4.2.4.1 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.

4.2.4.2 Vector3d Dislocation::bvec [protected]

Burgers vector of the dislocation.

Definition at line 27 of file dislocation.h.

4.2.4.3 Vector3d Dislocation::lvec [protected]

Line vector if the dislocation.

Definition at line 32 of file dislocation.h.

4.2.4.4 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.

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

Position vector of the defect in 2D space.

Definition at line 27 of file defect.h.

4.2.4.6 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:

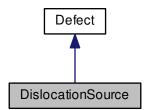
- · dislocation.h
- · dislocation.cpp

4.3 DislocationSource Class Reference

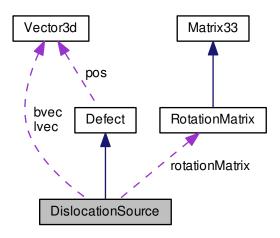
DislocationSource class representing a source of dislocations in the simulation.

#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 setPosition (double *a)

Sets the position of the defect.

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

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.

• 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.

Vector3d pos

Position vector of the defect in 2D space.

4.3.1 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. The properties of this class and the member functions will be declared here.

Definition at line 21 of file dislocationSource.h.

4.3.2 Constructor & Destructor Documentation

4.3.2.1 DislocationSource::DislocationSource ()

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. Tau critical: Default value set in the defaults file. Interations: Default value set in the defaults file.

Definition at line 22 of file dislocationSource.cpp.

4.3.2.2 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.
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 42 of file dislocationSource.cpp.

```
{
  this->bvec = burgers;
  this->lvec = line;
  this->pos = position;
  this->bmag = bm;
  this->tauCritical = tau;
  this->nIterations = nIter;
```

4.3.3 Member Function Documentation

4.3.3.1 double * Defect::getPosition() [inherited]

Returns in an array the position.

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.

Definition at line 109 of file defect.cpp.

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

4.3.3.2 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 119 of file defect.cpp.

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

4.3.3.3 double Defect::getX() [inherited]

Returns the X-coordinate of the defect.

Returns

X-coordinate of the defect.

Definition at line 128 of file defect.cpp.

```
{
  return (this->getValue (0));
```

4.3.3.4 double Defect::getY() [inherited]

Returns the Y-coordinate of the defect.

Returns

Y-coordinate of the defect.

Definition at line 137 of file defect.cpp.

```
(
  return (this->pos.getValue (1));
}
```

4.3.3.5 double Defect::getZ() [inherited]

Returns the Z-coordinate of the defect.

Returns

Z-coordinate of the defect.

Definition at line 146 of file defect.cpp.

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

4.3.3.6 void DislocationSource::setBurgers (Vector3d burgers)

Sets the Burgers vector of the dislocation.

Parameters

```
burgers | Bergers vector of the dislocation.
```

Definition at line 56 of file dislocationSource.cpp.

```
this->bvec = burgers;
```

4.3.3.7 void DislocationSource::setLineVector (Vector3d line)

Sets the line vector of the dislocation.

Parameters

line Line vector of the dislocation.	
--------------------------------------	--

Definition at line 65 of file dislocationSource.cpp.

```
{
  this->lvec = line;
}
```

4.3.3.8 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

а	Pointer to the array containing the coordinates of the defect.
---	--

Definition at line 56 of file defect.cpp.

```
{
  this->pos.setValue (a);
}
```

4.3.3.9 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.

```
this->pos.setValue (0, x);
this->pos.setValue (1, y);
this->pos.setValue (2, z);
}
```

4.3.3.10 void Defect::setX (double x) [inherited]

Sets the X-coordinate of the defect.

Parameters

X	X-coordinate of the defect.

Definition at line 80 of file defect.cpp.

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

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

Sets the Y-coordinate of the defect.

Parameters

У	Y-coordinate of the defect.

Definition at line 89 of file defect.cpp.

```
{
  this->pos.setValue (1, y);
```

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

Sets the Z-coordinate of the defect.

Parameters

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

Definition at line 98 of file defect.cpp.

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

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

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 122 of file defect.h.

```
{
  // This virtual function returns a zero matrix.
  // Inheriting classes will have functions implementing this in their own
  way
  // They will override this behaviour.
  Stress s;
  return (s);
```

4.3.4 Field Documentation

4.3.4.1 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 44 of file dislocationSource.h.

4.3.4.2 Vector3d DislocationSource::bvec [protected]

Burgers vector of the dislocation.

Definition at line 27 of file dislocationSource.h.

4.3.4.3 Vector3d DislocationSource::lvec [protected]

Line vector if the dislocation.

Definition at line 32 of file dislocationSource.h.

4.3.4.4 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 38 of file dislocationSource.h.

4.3.4.5 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 62 of file dislocationSource.h.

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

Position vector of the defect in 2D space.

Definition at line 27 of file defect.h.

4.3.4.7 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 50 of file dislocationSource.h.

4.3.4.8 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 56 of file dislocationSource.h.

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

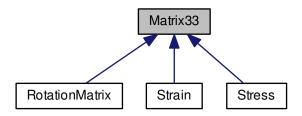
- · dislocationSource.h
- · dislocationSource.cpp

4.4 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.

Determinant.

• Matrix33 operator! () const

Inverse.

Protected Attributes

double x [3][3]

Array containing the elements of the matrix.

4.4.1 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.

4.4.2 Constructor & Destructor Documentation

4.4.2.1 Matrix33::Matrix33 ()

Default constructor.

Initializes the matrix with all elements equal to 0.0.

Definition at line 17 of file matrix33.cpp.

4.4.2.2 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.

```
{
  int i, j;
  for (i=0; i<3; i++)
    {
     for (j=0; j<3; j++)
        {
          this->x[i][j] = a[i][j];
        }
}
```

4.4.2.3 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.

4.4.2.4 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.

```
{
  int i, j;
  for (i=0; i<3; i++)
    {
     for (j=0; j<3; j++)
        {
        this->x[i][j] = a.x[i] * b.x[j];
     }
}
```

4.4.3 Member Function Documentation

4.4.3.1 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.

4.4.3.2 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.

4.4.3.3 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.

4.4.3.4 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.

4.4.3.5 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.

4.4.3.6 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.

```
{
    Vector3d r(0.0, 0.0, 0.0);
    int i, j;

    for (i=0; i<3; i++)
        {
        for (j=0; j<3; j++)
             {
                  r[i] += this->x[i][j] * v.x[j];
             }
        return (r);
}
```

4.4.3.7 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.

4.4.3.8 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.

```
{
   Matrix33* r = new Matrix33;
   *r = (*this) * p;
   *this = *r;
   delete(r);
   r = NULL;
}
```

4.4.3.9 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.

4.4.3.10 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.

4.4.3.11 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.

4.4.3.12 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.

4.4.3.13 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.

4.4.3.14 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.

4.4.3.15 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

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

Definition at line 93 of file matrix33.cpp.

```
{
   if (row>=0 && row<3)
     {
      if (column>=0 && column<3)
          {
          this->x[row][column] = value;
      }
}
```

4.4.4 Field Documentation

4.4.4.1 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:

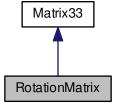
- matrix33.h
- matrix33.cpp

4.5 RotationMatrix Class Reference

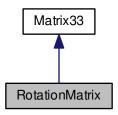
RotationMatrix class to represent a rotation matrix.

```
#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.

• double operator \sim () const

Determinant.

· Matrix33 operator! () const

Inverse.

Protected Attributes

double x [3][3]

Array containing the elements of the matrix.

4.5.1 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.

4.5.2 Constructor & Destructor Documentation

4.5.2.1 RotationMatrix::RotationMatrix ()

Default constructor.

Initializes the rotation matrix with a unit matrix.

Definition at line 14 of file rotationMatrix.cpp.

```
{
  int i, j;
  for ( i=0; i<3; i++ ) {
    for ( j=0; i<3; j++ ) {
      if ( i==j ) {
         this->setValue ( i, j, 1.0 );
      }
    else {
        this->setValue ( i, j, 0.0 );
    }
}
```

4.5.2.2 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.

```
{
   int i, j;
   for ( i=0; i<3; i++ ) {
      for ( j=0; j<3; j++ ) {
            this->setValue ( i, j, primed[i]*unPrimed[j] );
      }
}
```

4.5.3 Member Function Documentation

4.5.3.1 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.

```
{
    Matrix33 adj;
    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]);
    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]);
    adj.x[2][0] = (this->x[0][1]*this->x[1][2]) - (this->x[0][2]*this->x[1][1]);
    adj.x[2][2] = (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]);
    return (adj);
}
```

4.5.3.2 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.

4.5.3.3 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.

4.5.3.4 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.

4.5.3.5 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.

4.5.3.6 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.

```
{
    Vector3d r(0.0, 0.0, 0.0);
    int i, j;

    for (i=0; i<3; i++)
        {
        for (j=0; j<3; j++)
             {
                  r[i] += this->x[i][j] * v.x[j];
             }
        return (r);
}
```

4.5.3.7 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.

4.5.3.8 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.

```
{
   Matrix33* r = new Matrix33;
   *r = (*this) * p;
   *this = *r;
   delete(r);
   r = NULL;
```

4.5.3.9 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.

4.5.3.10 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.

4.5.3.11 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.

4.5.3.12 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.

4.5.3.13 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.

4.5.3.14 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.

4.5.3.15 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.

```
{
   if (row>=0 && row<3)
    {
      if (column>=0 && column<3)
        {
            this->x[row][column] = value;
        }
    }
}
```

4.5.4 Field Documentation

4.5.4.1 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:

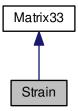
- · rotationMatrix.h
- rotationMatrix.cpp

4.6 Strain Class Reference

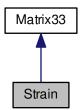
Strain class to represent the strain tensor.

#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.

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

Array containing the elements of the matrix.

4.6.1 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.

4.6.2 Constructor & Destructor Documentation

4.6.2.1 Strain::Strain()

Default constructor.

Initializes the strain tensor with zeros.

Definition at line 16 of file strain.cpp.

```
{
  int i, j;
  for (i=0; i<3; i++)
    {
     principalStrains [i] = 0.0;
     shearStrains [i] = 0.0;
  }
  this->populateMatrix ();
}
```

4.6.2.2 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.

```
{
  int i;
  for (i=0; i<3; i++)
    {
     this->principalStrains [i] = principal [i];
     this->shearStrains [i] = shear [i];
}
  this->populateMatrix ();
}
```

4.6.3 Member Function Documentation

4.6.3.1 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.

4.6 Strain Class Reference 51

```
return (adj);
```

4.6.3.2 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.

4.6.3.3 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.

```
{
  double s[3];
  int i;
  for (i=0; i<3; i++)
      {
       s[i] = this->shearStrains[i];
    }
  return (s);
```

4.6.3.4 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.

4.6.3.5 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.

4.6.3.6 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.

4.6 Strain Class Reference 53

4.6.3.7 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.

4.6.3.8 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.

```
{
    Vector3d r(0.0, 0.0, 0.0);
    int i, j;

    for (i=0; i<3; i++)
        {
        for (j=0; j<3; j++)
             {
                  r[i] += this->x[i][j] * v.x[j];
             }
        return (r);
}
```

4.6.3.9 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.

```
{
  int i, j;
  for (i=0; i<3; i++)
    {
      for (j=0; j<3; j++)
        {
            this->x[i][j] *= p;
      }
}
```

4.6.3.10 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.

```
{
   Matrix33* r = new Matrix33;
   *r = (*this) * p;
   *this = *r;
   delete(r);
   r = NULL;
}
```

4.6.3.11 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.

4.6 Strain Class Reference 55

4.6.3.12 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.

4.6.3.13 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.

4.6.3.14 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.

4.6.3.15 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.

```
{
   Matrix33 r;
   int i, j;

   for (i=0; i<3; i++)
        {
        for (j=0; j<3; j++)
             {
                  r.x[i][j] = this->x[j][i];
             }
        }
   return (r);
}
```

4.6.3.16 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.

4.6.3.17 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.

```
{
  this->x[0][0] = this->principalStrains [0];
  this->x[1][1] = this->principalStrains [1];
  this->x[2][2] = this->principalStrains [2];

  this->x[0][1] = this->x[1][0] = this->shearStrains [0];
  this->x[0][2] = this->x[2][0] = this->shearStrains [1];
  this->x[1][2] = this->x[2][1] = this->shearStrains [2];
```

4.6 Strain Class Reference 57

4.6.3.18 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.

```
{
  Matrix33 alphaT = ^alpha; // Transpose
  Strain sNew;

sNew = alpha * (*this) * alphaT; // Rotate the strain matrix
  return (sNew);
}
```

4.6.3.19 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.

4.6.4 Field Documentation

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

The three principal strains: s11, s22, s33.

Definition at line 27 of file strain.h.

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

The three shear strains: s12, s13, s23,

Definition at line 31 of file strain.h.

4.6.4.3 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:

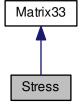
- strain.h
- strain.cpp

4.7 Stress Class Reference

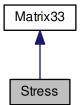
Stress class to represent the stress tensor.

#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.

4.7.1 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.

4.7.2 Constructor & Destructor Documentation

4.7.2.1 Stress::Stress()

Default constructor.

Initializes the stress tensor with zeros.

Definition at line 16 of file stress.cpp.

```
{
  int i, j;
  for (i=0; i<3; i++)
    {
     principalStresses [i] = 0.0;
     shearStresses [i] = 0.0;
  }
  this->populateMatrix ();
}
```

4.7.2.2 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

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

Definition at line 35 of file stress.cpp.

```
{
  int i;
  for (i=0; i<3; i++)
    {
      this->principalStresses [i] = principal [i];
      this->shearStresses [i] = shear [i];
    }
  this->populateMatrix ();
```

4.7.3 Member Function Documentation

4.7.3.1 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.

4.7.3.2 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.

```
{
    double p[3];
    int i;

    for (i=0; i<3; i++)
        {
            p[i] = this->principalStresses[i];
        }

    return (p);
}
```

4.7.3.3 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.

4.7.3.4 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.

4.7.3.5 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.

4.7 Stress Class Reference 63

4.7.3.6 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.

4.7.3.7 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.

4.7.3.8 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.

```
{
    Vector3d r(0.0, 0.0, 0.0);
    int i, j;

    for (i=0; i<3; i++)
        {
        for (j=0; j<3; j++)
             {
                  r[i] += this->x[i][j] * v.x[j];
             }
    }
    return (r);
}
```

4.7.3.9 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.

4.7.3.10 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.

```
{
   Matrix33* r = new Matrix33;
   *r = (*this) * p;
   *this = *r;
   delete(r);
   r = NULL;
```

4.7.3.11 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.

4.7 Stress Class Reference 65

Returns

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

Definition at line 155 of file matrix33.cpp.

4.7.3.12 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.

4.7.3.13 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.

4.7.3.14 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.

4.7.3.15 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.

4.7.3.16 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.

4.7 Stress Class Reference 67

4.7.3.17 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.

```
this->x[0][0] = this->principalStresses [0];
this->x[1][1] = this->principalStresses [1];
this->x[2][2] = this->principalStresses [2];
this->x[0][1] = this->x[1][0] = this->shearStresses [0];
this->x[0][2] = this->x[2][0] = this->shearStresses [1];
this->x[1][2] = this->x[2][1] = this->shearStresses [2];
```

4.7.3.18 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.

```
{
  Matrix33 alphaT = ^alpha; // Transpose
  Stress sNew;

sNew = alpha * (*this) * alphaT; // Rotate the stress matrix
  return (sNew);
}
```

4.7.3.19 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.

```
this->x[row][column] = value;
}
```

4.7.4 Field Documentation

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

The three principal stresses: s11, s22, s33.

Definition at line 27 of file stress.h.

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

The three shear stresses: s12, s13, s23,

Definition at line 31 of file stress.h.

4.7.4.3 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:

- · stress.h
- · stress.cpp

4.8 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.

4.8.1 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.

4.8.2 Constructor & Destructor Documentation

4.8.2.1 Vector3d::Vector3d()

Default constructor.

Initializes the vector with all elements equal to 0.0.

Definition at line 16 of file vector3d.cpp.

```
{
  this->x[0] = 0.0;
  this->x[1] = 0.0;
  this->x[2] = 0.0;
}
```

4.8.2.2 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.

```
{
    this->x[0] = a[0];
    this->x[1] = a[1];
    this->x[2] = a[2];
```

4.8.2.3 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.

```
{
  this->x[0] = a1;
  this->x[1] = a2;
  this->x[2] = a3;
```

4.8.3 Member Function Documentation

4.8.3.1 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.

```
if (index>=0 && index<3)
    {
       return (this->x[index]);
    }
else
```

```
return (0);
}
```

4.8.3.2 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.

```
{
  double* a = new double[3];
  a[0] = this->x[0];
  a[1] = this->x[1];
  a[2] = this->x[2];
  return (a);
```

4.8.3.3 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.

```
{
  double s = 0.0;
  int i;

  for (i=0; i<3; i++)
   {
     s += this->x[i] * this->x[i];
  }

  return ( sqrt (s) );
}
```

4.8.3.4 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.

```
{
  double m = this->magnitude ();
  if (m==0.0)
  {
    return (Vector3d ());
  }
  else
  {
    return ((*this) * (1.0/m));
  }
}
```

4.8.3.5 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.

```
{
    Vector3d r(0.0, 0.0, 0.0);
    int i;
    for (i=0; i<3; i++)
        {
        r.x[i] = this->x[i] * p;
    }
    return (r);
```

4.8.3.6 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.

4.8.3.7 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.

```
{
  int i;
  for (i=0; i<3; i++)
      {
      this->x[i] *= p;
    }
}
```

4.8.3.8 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.

```
{
  Vector3d r (0.0, 0.0, 0.0);
  int i;

  for (i=0; i<3; i++)
      {
      r.x[i] = this->x[i] + p.x[i];
    }

  return (r);
}
```

4.8.3.9 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.

```
{
  int i;
  for (i=0; i<3; i++)
      {
      this->x[i] += p.x[i];
      }
}
```

4.8.3.10 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.

```
{
    Vector3d r(0.0, 0.0, 0.0);
    int i;

    for (i=0; i<3; i++)
        {
        r.x[i] = this->x[i] - p.x[i];
    }

    return (r);
}
```

4.8.3.11 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.

```
{
  int i;
  for (i=0; i<3; i++)
      {
      this->x[i] -= p.x[i];
      }
}
```

4.8.3.12 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.

```
{
    Vector3d r(0.0, 0.0, 0.0);

    r.x[0] = (this->x[1] * p.x[2]) - (this->x[2] * p.x[1]);
    r.x[1] = (this->x[2] * p.x[0]) - (this->x[0] * p.x[2]);
    r.x[2] = (this->x[0] * p.x[1]) - (this->x[1] * p.x[0]);
    return (r);
}
```

4.8.3.13 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.

```
{
    Vector3d* r = Vector3d(0.0, 0.0, 0.0);

    r->x[0] = (this->x[1] * p.x[2]) - (this->x[2] * p.x[1]);
    r->x[1] = (this->x[2] * p.x[0]) - (this->x[0] * p.x[2]);
    r->x[2] = (this->x[0] * p.x[1]) - (this->x[1] * p.x[0]);

    *this = *r;

    delete (r);
    r = NULL;
}
```

4.8.3.14 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.

```
{
   if (index>=0 && index <3)
     {
      this->x[index] = value;
   }
}
```

4.8.3.15 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.

```
{
	this->x[0] = a[0];
	this->x[1] = a[1];
	this->x[2] = a[2];
```

4.8.3.16 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.

4.8.4 Field Documentation

4.8.4.1 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

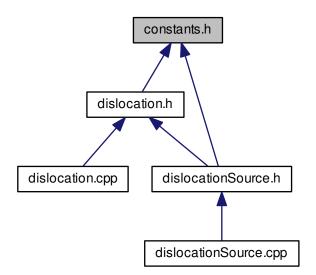
Chapter 5

File Documentation

5.1 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.

5.1.1 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.

5.1.2 Macro Definition Documentation

5.1.2.1 #define PI 3.141592654

The irrational number pi.

Definition at line 16 of file constants.h.

5.1.2.2 #define SQRT2 1.414213562

The square root of 2.

Definition at line 21 of file constants.h.

5.1.2.3 #define SQRT3 1.732050808

The square root of 3.

Definition at line 26 of file constants.h.

5.1.2.4 #define SQRT5 2.236067978

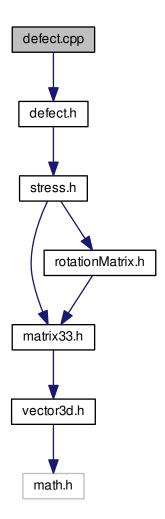
The square root of 5.

Definition at line 31 of file constants.h.

5.2 defect.cpp File Reference

Definition of member functions of the Defect class.

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



5.2.1 Detailed Description

Definition of member functions of the Defect class.

Author

Adhish Majumdar

Version

0.0

Date

22/04/2013

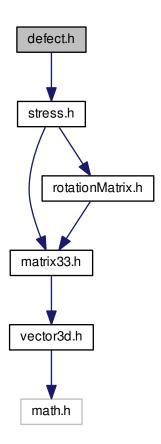
This file defines the member functions of the Defect class representing a single defect in the simulation. Definition in file defect.cpp.

5.3 defect.h File Reference

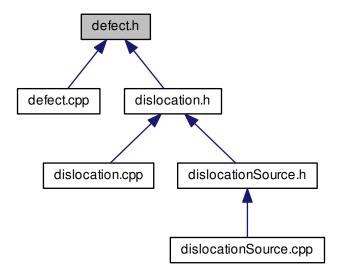
Definition of the **Defect** class.

#include "stress.h"

Include dependency graph for defect.h:



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



Data Structures

· class Defect

Class Defect representing a generic defect in a material.

5.3.1 Detailed Description

Definition of the **Defect** class.

Author

Adhish Majumdar

Version

0.0

Date

22/04/2013

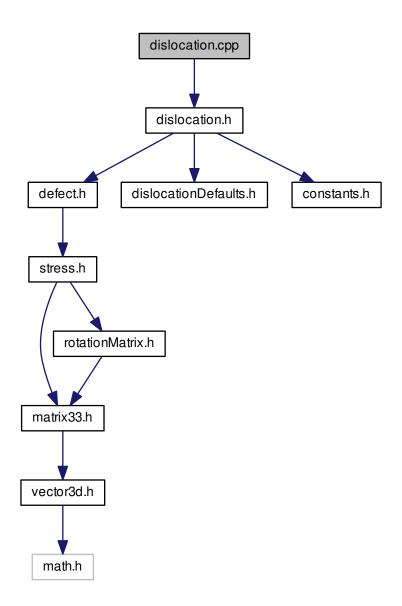
This file defines the Defect class representing an defect in the simulation. This is simply a generic description class with virtual functions. Later classes like dislocations, precipitates, boundaries etc will inherit from this class.

Definition in file defect.h.

5.4 dislocation.cpp File Reference

Definition of constructors and member functions of the Dislocation class.

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



5.4.1 Detailed Description

Definition of constructors and member functions of the Dislocation class.

Author

Adhish Majumdar

Version

0.0

Date

29/04/2013

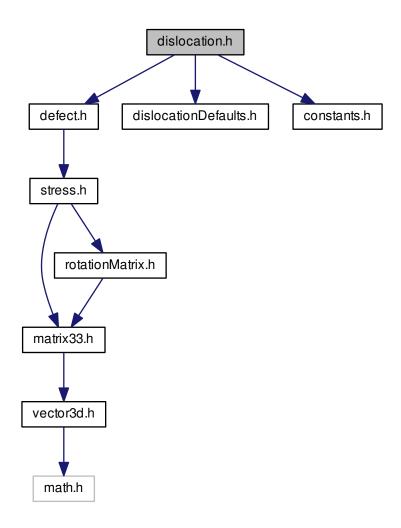
This file defines the constructors and member functions of the Dislocation class. This class inherits from the Defect class.

Definition in file dislocation.cpp.

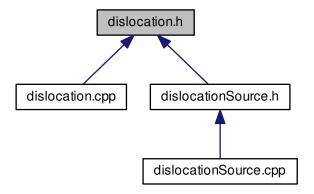
5.5 dislocation.h File Reference

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.

5.5.1 Detailed Description

Definition of the Dislocation class.

Author

Adhish Majumdar

Version

0.0

Date

29/04/2013

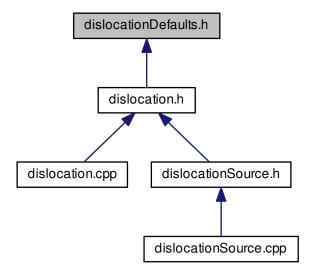
This file defines the Dislocation class representing a dislocation in the simulation. This class inherits from the Defect class.

Definition in file dislocation.h.

5.6 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_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.

5.6.1 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.

5.6.2 Macro Definition Documentation

5.6.2.1 #define DEFAULT_BURGERS_0 1.0

Default value of the Burgers vector x-coordinate.

Definition at line 21 of file dislocationDefaults.h.

5.6.2.2 #define DEFAULT_BURGERS_1 1.0

Default value of the Burgers vector y-coordinate.

Definition at line 25 of file dislocationDefaults.h.

5.6.2.3 #define DEFAULT_BURGERS_2 0.0

Default value of the Burgers vector z-coordinate.

Definition at line 29 of file dislocationDefaults.h.

5.6.2.4 #define DEFAULT_BURGERS_MAGNITUDE 5.0e-09

Default value of the magnitude of the Burgers vector.

Definition at line 16 of file dislocationDefaults.h.

5.6.2.5 #define DEFAULT_LINEVECTOR_0 1.0

Default value of the line vector x-coordinate.

Definition at line 34 of file dislocationDefaults.h.

5.6.2.6 #define DEFAULT_LINEVECTOR_1 -1.0

Default value of the line vector y-coordinate.

Definition at line 38 of file dislocationDefaults.h.

5.6.2.7 #define DEFAULT_LINEVECTOR_2 -2.0

Default value of the line vector z-coordinate.

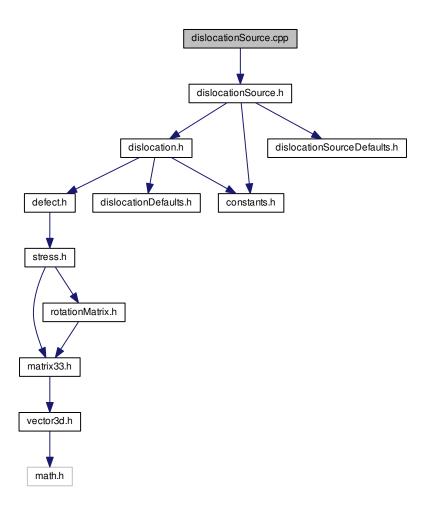
Definition at line 42 of file dislocationDefaults.h.

5.7 dislocationSource.cpp File Reference

Definition of the member functions of the DislocationSource class.

#include "dislocationSource.h"

Include dependency graph for dislocationSource.cpp:



5.7.1 Detailed Description

Definition of the member functions of the DislocationSource class.

Author

Adhish Majumdar

Version

0.0

Date

02/05/2013

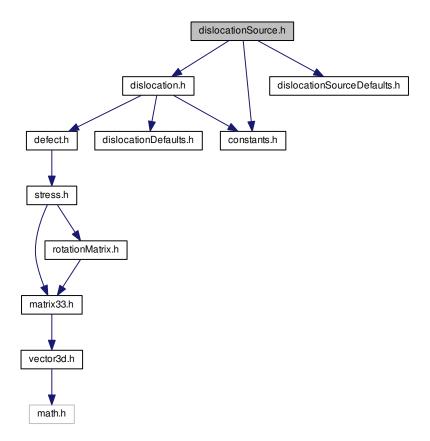
This file defines the member functions of the DislocationSource class representing a source of dislocations in the simulation. This class inherits from the Defect class. This object is basically the representation of a Frank-Read source emitting dislocation dipoles.

Definition in file dislocationSource.cpp.

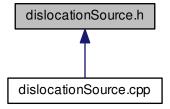
5.8 dislocationSource.h File Reference

Definition of the DislocationSource class.

```
#include "dislocation.h"
#include "constants.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.

5.8.1 Detailed Description

Definition of the DislocationSource class.

Author

Adhish Majumdar

Version

0.0

Date

02/05/2013

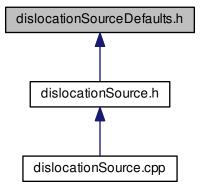
This file defines the DislocationSource class representing a source of dislocations in the simulation. This class inherits from the Defect class. This object is basically the representation of a Frank-Read source emitting dislocation dipoles.

Definition in file dislocationSource.h.

5.9 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.

5.9.1 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.

5.9.2 Macro Definition Documentation

5.9.2.1 #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.

5.9.2.2 #define DEFAULT_TAU_CRITICAL 1.0e09

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

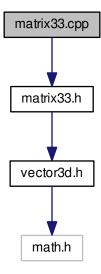
Default value of the critical shear stress for a dislocation source to emit a dipole. The number is expressed in Pa.

Definition at line 17 of file dislocationSourceDefaults.h.

5.10 matrix33.cpp File Reference

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

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



5.10.1 Detailed Description

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

Author

Adhish Majumdar

Version

0.0

Date

22/04/2013

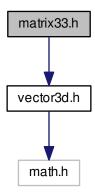
This file defines the member functions and operators of the Matrix33 class representing a 3x3 matrix in the simulation.

Definition in file matrix33.cpp.

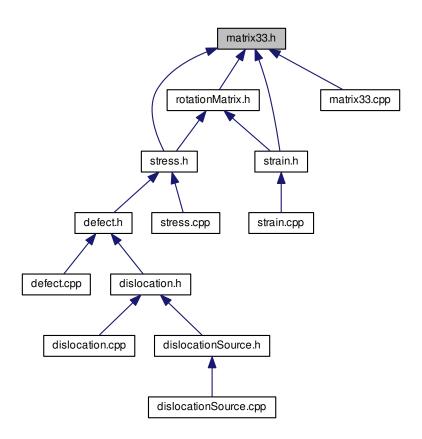
5.11 matrix33.h File Reference

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.

5.11.1 Detailed Description

Definition of the Matrix33 class.

Author

Adhish Majumdar

Version

0.0

Date

22/04/2013

This file defines the Matrix33 class representing a 3x3 matrix in the simulation.

Definition in file matrix33.h.

5.12 rotationMatrix.cpp File Reference

Definition of the RotationMatrix class member functions.

5.12.1 Detailed Description

Definition of the RotationMatrix class member functions.

Author

Adhish Majumdar

Version

0.0

Date

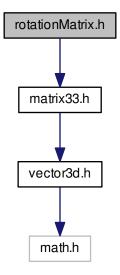
25/04/2013

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

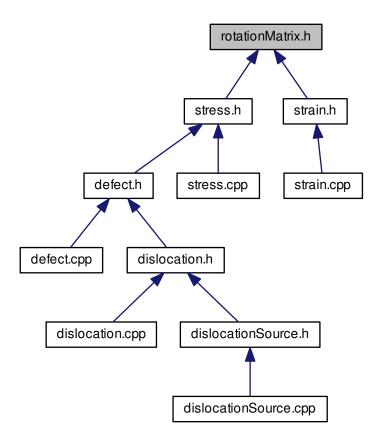
5.13 rotationMatrix.h File Reference

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.

5.13.1 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.

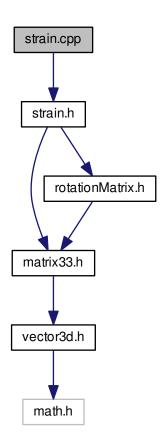
Definition in file rotationMatrix.h.

5.14 strain.cpp File Reference

Definition of the member functions if the Strain class.

#include "strain.h"

Include dependency graph for strain.cpp:



5.14.1 Detailed Description

Definition of the member functions if the Strain class.

Author

Adhish Majumdar

5.15 strain.h File Reference 97

Version

0.0

Date

22/04/2013

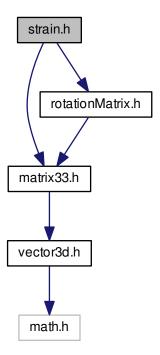
This file defines the member functions of the Strain class for the strain tensor.

Definition in file strain.cpp.

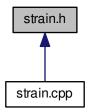
5.15 strain.h File Reference

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.

5.15.1 Detailed Description

Definition of the Strain class.

Author

Adhish Majumdar

Version

0.0

Date

25/04/2013

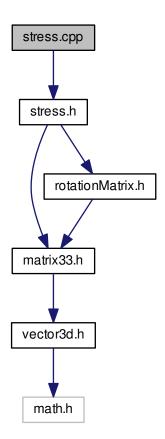
This file defines the Strain class for the strain tensor.

Definition in file strain.h.

5.16 stress.cpp File Reference

Definition of the member functions if the Stress class.

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



5.16.1 Detailed Description

Definition of the member functions if the Stress class.

Author

Adhish Majumdar

Version

0.0

Date

22/04/2013

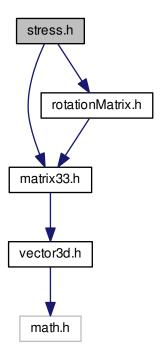
This file defines the member functions of the Stress class for the stress tensor.

Definition in file stress.cpp.

5.17 stress.h File Reference

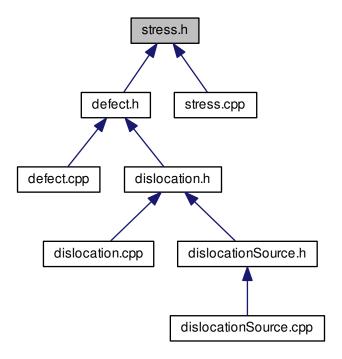
Definition of the Stress class.

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



5.17 stress.h File Reference

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



Data Structures

class Stress

Stress class to represent the stress tensor.

5.17.1 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.

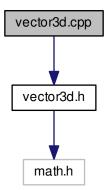
Definition in file stress.h.

5.18 vector3d.cpp File Reference

Definition of member functions and operators of the Vector3d class.

#include "vector3d.h"

Include dependency graph for vector3d.cpp:



5.18.1 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.

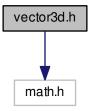
Definition in file vector3d.cpp.

5.19 vector3d.h File Reference

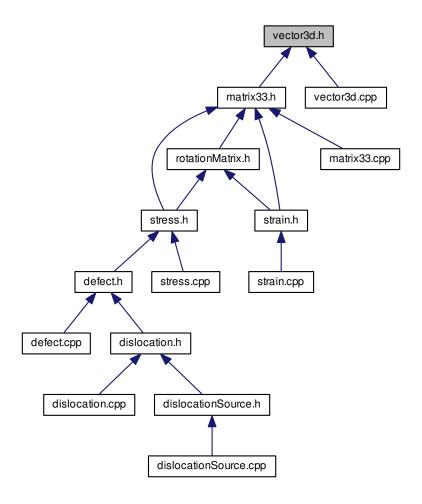
Definition of the Vector3d class.

#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.

5.19.1 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.

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