# My Project

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## 1.1 Class List

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

# Chapter 2

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## 2.1 File List

Here is a list of all files with brief descriptions:

# Chapter 3

# Class Documentation

## 3.1 ConstantGridSolver Class Reference

`#include <ConstantGridSolver.h>`

### Public Member Functions

- arma::cx_mat calculateT (int j, double E) const

  *Calculates* $\mathbf{T}(x_j, E)$ *matrix.*
- arma::cx_mat calculateU (int j, double E)

  *Calculates* $\mathbf{U}(x_j, E)$ *matrix.*
- arma::cx_mat calculateEP (int j, double E)

  *Calculates* $\mathbf{E}^{+}(x_j, E)$ *matrix.*
- arma::cx_mat calculateEM (int j, double E)

  *Calculates* $\mathbf{E}^{-}(x_j, E)$ *matrix.*
- void modifyCCnj (arma::cx_mat &n1, arma::cx_mat &n0, arma::cx_mat &j1, arma::cx_mat &j0, double E)

  *Modifies closed channels elements.*
- arma::cx_mat fwdIteration (const arma::cx_mat &B, double E)

  *Iterates Numerov algorithm forward up to* $N-1$ *and returns* $\mathbf{R}_{N-1}$ *matrix for a given energy.*
- arma::cx_mat calculateS (const arma::cx_mat R_N, double E)

  *Calculates* $\mathbf{S}$ *matrix for given* $\mathbf{R}_{N-1}$*.*
- void saveS (const arma::cx_mat &S, const std::string S_type, const int E, const std::string directory)

  *Saves* $\mathbf{S}$ *matrix (Im and Re part separately).*
- void setParameters (const Parameters &parameters)
- ConstantGridSolver ()=default
- ∼ConstantGridSolver ()=default
- ConstantGridSolver (const Parameters &params)

  *Constructor.*
- void solveForEnergies (std::string directory)

  *Performs Numerov calculations for a given set of parameters for all energies.*

### 3.1.1 Constructor & Destructor Documentation

#### 3.1.1.1 ConstantGridSolver::ConstantGridSolver ( ) [default]

#### 3.1.1.2 ConstantGridSolver::∼ConstantGridSolver ( ) [default]

#### 3.1.1.3 ConstantGridSolver::ConstantGridSolver ( const Parameters & *params* ) [explicit]

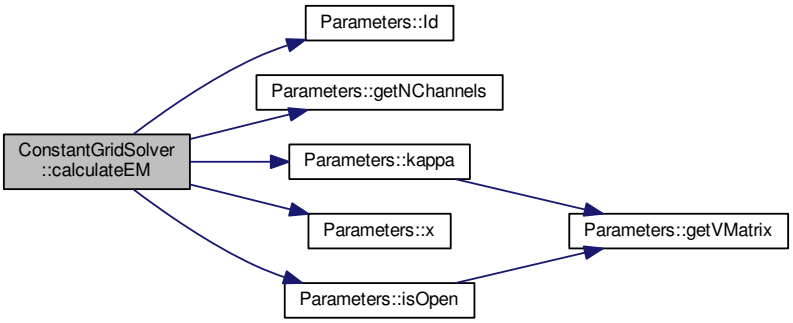
Constructor.

### 3.1.2 Member Function Documentation

#### 3.1.2.1 arma::cx_mat ConstantGridSolver::calculateEM ( int *j*, double *E* )

Calculates $\mathbf{E}^{-}(x_j, E)$ matrix.

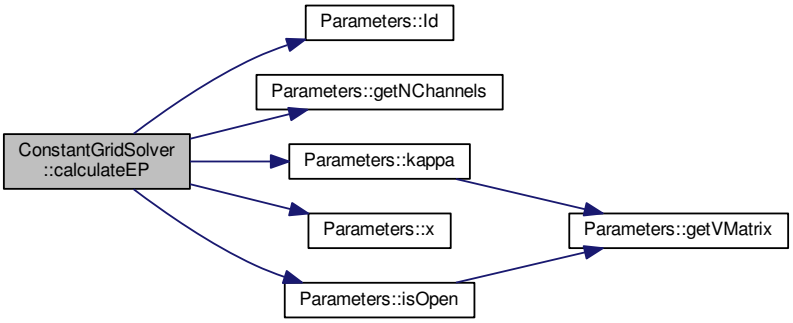
Here is the call graph for this function:




#### 3.1.2.2 arma::cx_mat ConstantGridSolver::calculateEP ( int *j*, double *E* )

Calculates $\mathbf{E}^{+}(x_j, E)$ matrix.

Here is the call graph for this function:




#### 3.1.2.3 arma::cx_mat ConstantGridSolver::calculateS ( const arma::cx_mat *R_N*, double *E* )

Calculates $\mathbf{S}$ matrix for given $\mathbf{R}_{N-1}$.

This method calculates the scattering matrix $\mathbf{S}(E)$. Its value is given by

$$\mathbf{S} = (\mathbf{R}_{N-1}\mathbf{e}_{N-1}^{+} - \mathbf{e}_{N}^{+}) - 1(\mathbf{R}_{N-1}\mathbf{e}_{N-1}^{-} - \mathbf{e}_{N}^{-}) \tag{3.1}$$

where $\mathbf{e}_i^{\pm} = (\mathbf{I} - \mathbf{T}_i)\mathbf{E}_i^{\pm}$.

**Parameters**

| | |
|---|---|
| *R_N* | - $\mathbf{R}_{N-1}$ |
| *E* | - energy |

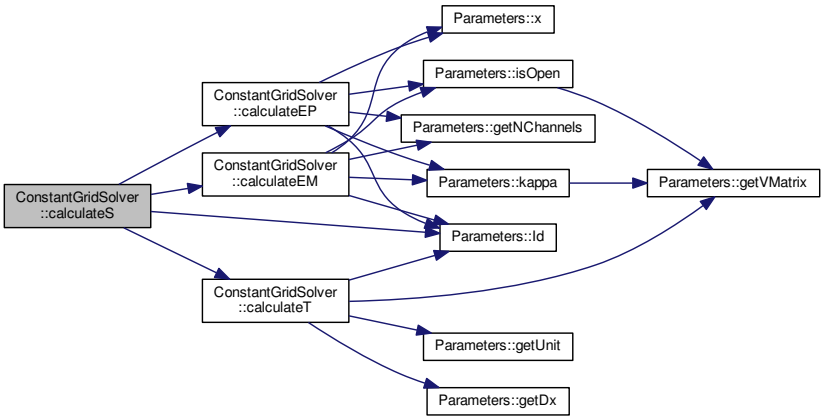
**Returns**

$\mathbf{S}$

**Exceptions**

| | |
|---|---|
| *std::runtime_error* | if there is a problem with calculating |

Here is the call graph for this function:




#### 3.1.2.4 arma::cx_mat ConstantGridSolver::calculateT ( int *j*, double *E* ) const

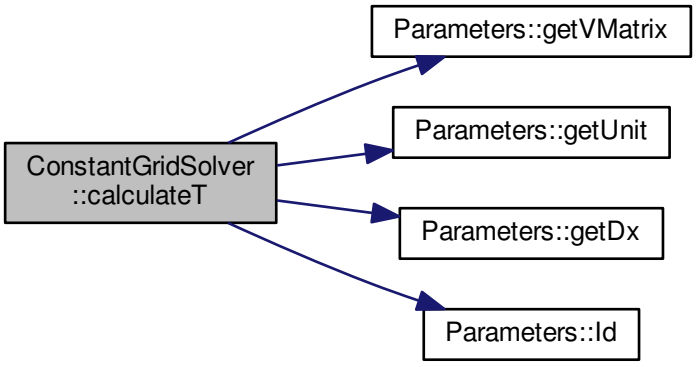
Calculates $\mathbf{T}(x_j, E)$ matrix.

This method calculates T matrix for given index j and set of parameters [in] j - index of x value for which T is calculated [in] params - Parameters object for which T is calculated

**Returns**

T matrix

Here is the call graph for this function:




#### 3.1.2.5 arma::cx_mat ConstantGridSolver::calculateU ( int *j*, double *E* )

Calculates $\mathbf{U}(x_j, E)$ matrix.

This method calculates $\mathbf{U}$ matrix for given index j using the set of parameters provided to the ConstantGridSolver object.

**Parameters**

| | | |
|---|---|---|
| in | *j* | - index on the grid of x value |
| in | *E* | - energy value |

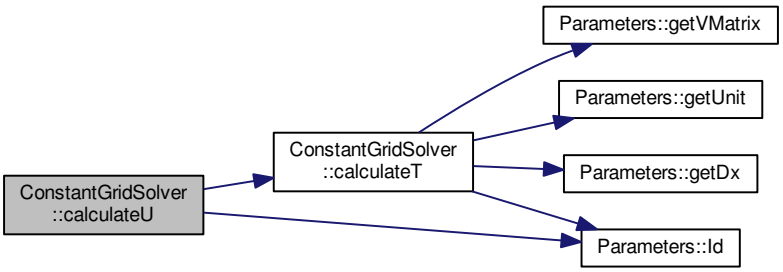
**Returns**

$\mathbf{U}(x_j, E)$

**Exceptions**

| | |
|---|---|
| *std::invalid_argument* | if $x_j$ does not exist |

Here is the call graph for this function:




#### 3.1.2.6 arma::cx_mat ConstantGridSolver::fwdIteration ( const arma::cx_mat & *B*, double *E* )

Iterates Numerov algorithm forward up to $N-1$ and returns $\mathbf{R}_{N-1}$ matrix for a given energy.

This method performs the Numerov iteration for a given energy for a case of some particular symmetry.

The initial value $\mathbf{R}_0^{-1}$:

- $\mathbf{R}_0^{-1} = \mathbf{0}$ if no symmetries
- $\mathbf{R}_0^{-1} = \mathbf{U}_0^{-1}(\mathbf{I}+\mathbf{B})$ if the symmetry is described by $\mathbf{B}$

Every value depends on the previous one: $\mathbf{R}_j = \mathbf{U}_j - \mathbf{R}_{j-1}^{-1}$.

**Parameters**

| | | |
|---|---|---|
| in | *B* | - $\mathbf{B}$ matrix to calculate the initial value |
| in | *E* | - energy |

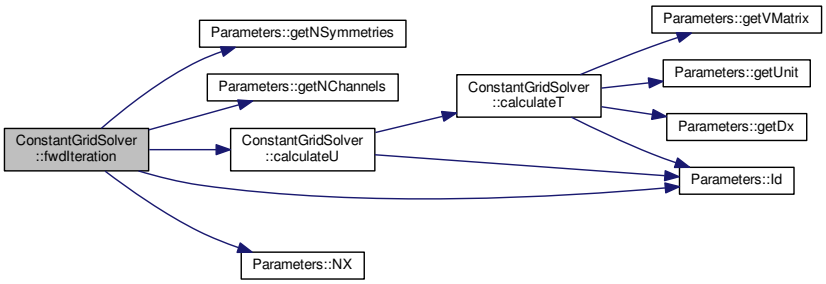
**Returns**

$\mathbf{R}_{N-1}$

**Exceptions**

| | |
|---|---|
| *std::invalid_argument* | if $\mathbf{U}_i$ cannot be calculated for given iteration $i$ |
| *std::runtime_error* | |

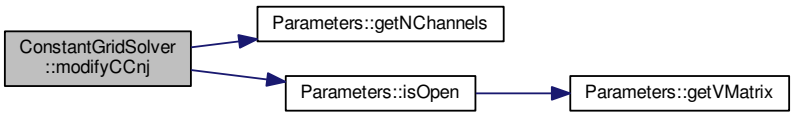
Here is the call graph for this function:




#### 3.1.2.7 void ConstantGridSolver::modifyCCnj ( arma::cx_mat & *n1*, arma::cx_mat & *n0*, arma::cx_mat & *j1*, arma::cx_mat & *j0*, double *E* )

Modifies closed channels elements.

Here is the call graph for this function:




#### 3.1.2.8 void ConstantGridSolver::saveS ( const arma::cx_mat & *S*, const std::string *S_type*, const int *E*, const std::string *directory* )

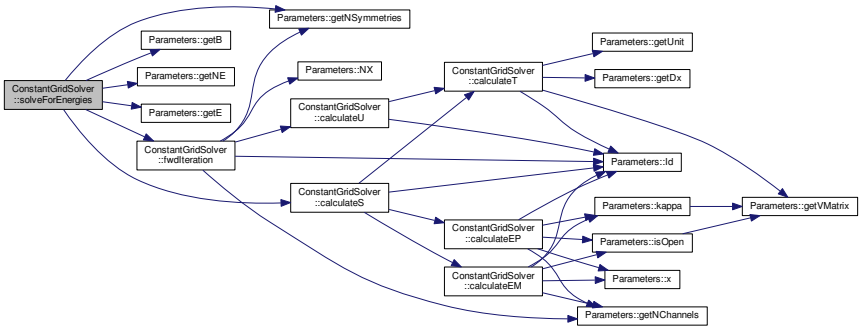
Saves $\mathbf{S}$ matrix (Im and Re part separately).

#### 3.1.2.9 void ConstantGridSolver::setParameters ( const Parameters & *parameters* ) [inline]

#### 3.1.2.10 void ConstantGridSolver::solveForEnergies ( std::string *directory* )

Performs Numerov calculations for a given set of parameters for all energies.

Here is the call graph for this function:




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

- ConstantGridSolver.h
- ConstantGridSolver.cpp

## 3.2 Parameters Class Reference

`#include <Parameters.h>`

### Public Member Functions

- void loadParams (std::string="Params.txt")

  *Reading the values of parameters from the file generated in Mathematica.*
- void setXValues ()

  *Setting xValues.*
- FRIEND_TEST (ParametersInputTest, setXValues_failsIfXMaxLessOrEqualXMin)
- FRIEND_TEST (ParametersInputTest, setXValues_failsIfInvalidDX)
- FRIEND_TEST (ParametersInputTest, setXValues_failsIfInvalidCombinationOfXMinXMaxDx)
- FRIEND_TEST (ParametersInputTest, setXValues_worksGoodForCorrectValues)
- void loadE (std::string filename="E.dat")

  *Reading the values of energies from the file generated in Mathematica.*
- void loadV (std::string filename="V.dat")

  *Reading the values of V from the file generated in Mathematica.*
- FRIEND_TEST (Parameters_loadV_Test, failsForIncorrectNumberOfRows)
- FRIEND_TEST (Parameters_loadV_Test, worksGoodForGoodFileOneChannel)
- FRIEND_TEST (Parameters_loadV_Test, worksGoodForGoodFileTwoChannels)
- void loadB (std::string filename="B")

  *Reading the values of B from the file generated in Mathematica.*
- FRIEND_TEST (ParametersInputTest, loadB_failsIfAnyFileDoesNotExistAndPositiveNSymmetries)
- FRIEND_TEST (ParametersInputTest, loadB_worksGoodForGoodFilesOneChannel)
- FRIEND_TEST (ParametersInputTest, loadB_failsIfAnyFileIsIncorrect)
- bool checkNumberOfRowsInFile (std::string filename, const int required_number_of_columns)
- Parameters ()=default
- ~Parameters ()=default
- Parameters (std::vector< std::string > filenames)

  *From a given directory takes all the needed values and creates Parameters object.*

- arma::cx_mat getVMatrix (int) const

  *V matrix for a given x_i.*
- double getE (int) const
- int NX () const
- double getXMin () const
- double getXMax () const
- double getDx () const
- double x (int i) const
- FRIEND_TEST (ParametersOutputTest, x_worksCorrectForNegativeIndices)
- double getUnit () const
- int getNChannels () const
- int getNE () const
- arma::cx_mat getB (int i) const
- int getNSymmetries () const
- int getGrid_points_per_lambda () const
- arma::cx_mat Id () const
- bool isOpen (int nChannel, double energy) const

  *Check if the channel is open.*
- double kappa (int n1, int n2, int i, double E) const
- double kappa (int n1, int n2, double x, double E) const
- arma::cx_mat getV (double x) const

  *Linear interpolation of V (works also for V given on non-constant grid if needed)*
- double lambda (double x, double E) const

  *de Broglie length for a given potential and x*
- double requiredDx (double x, double E) const

### Friends

- class Parameters_loadV_Test
- class Parameters_isOpen_Test
- class Parameters_kappaInt_Test
- class Parameters_kappaDouble_Test
- class Parameters_getV_Test
- class Parameters_lambda_Test
- class Parameters_requiredDX_Test

## 3.2.1 Constructor & Destructor Documentation

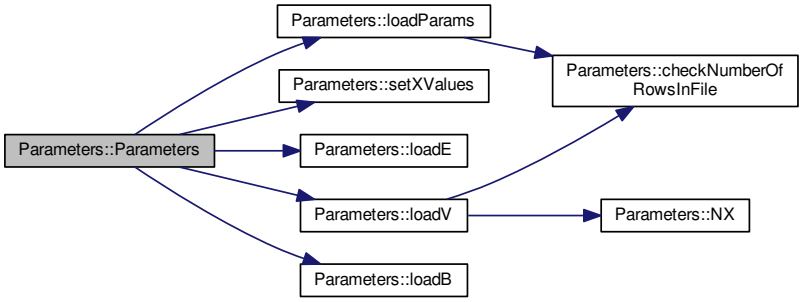
#### 3.2.1.1 Parameters::Parameters ( ) [default]

#### 3.2.1.2 Parameters::~Parameters ( ) [default]

#### 3.2.1.3 Parameters::Parameters ( std::vector< std::string > *filenames* ) [explicit]

From a given directory takes all the needed values and creates Parameters object.

Here is the call graph for this function:




### 3.2.2 Member Function Documentation

#### 3.2.2.1 bool Parameters::checkNumberOfRowsInFile ( std::string *filename,* const int *required_number_of_columns* )

#### 3.2.2.2 Parameters::FRIEND_TEST ( ParametersInputTest , setXValues_failsIfXMaxLessOrEqualXMin )

#### 3.2.2.3 Parameters::FRIEND_TEST ( ParametersInputTest , setXValues_failsIfInvalidDX )

#### 3.2.2.4 Parameters::FRIEND_TEST ( ParametersInputTest , setXValues_failsIfInvalidCombinationOfXMinXMaxDx )

#### 3.2.2.5 Parameters::FRIEND_TEST ( ParametersInputTest , setXValues_worksGoodForCorrectValues )

#### 3.2.2.6 Parameters::FRIEND_TEST ( Parameters_loadV_Test , failsForIncorrectNumberOfRows )

#### 3.2.2.7 Parameters::FRIEND_TEST ( Parameters_loadV_Test , worksGoodForGoodFileOneChannel )

#### 3.2.2.8 Parameters::FRIEND_TEST ( Parameters_loadV_Test , worksGoodForGoodFileTwoChannels )

#### 3.2.2.9 Parameters::FRIEND_TEST ( ParametersInputTest , loadB_failsIfAnyFileDoesNotExistAndPositiveNSymmetries )

#### 3.2.2.10 Parameters::FRIEND_TEST ( ParametersInputTest , loadB_worksGoodForGoodFilesOneChannel )

#### 3.2.2.11 Parameters::FRIEND_TEST ( ParametersInputTest , loadB_failsIfAnyFileIsIncorrect )

#### 3.2.2.12 Parameters::FRIEND_TEST ( ParametersOutputTest , x_worksCorrectForNegativeIndices )

#### 3.2.2.13 arma::cx_mat Parameters::getB ( int *i* ) const [inline]

#### 3.2.2.14 double Parameters::getDx ( ) const [inline]

#### 3.2.2.15 double Parameters::getE ( int *i* ) const

#### 3.2.2.16 int Parameters::getGrid_points_per_lambda ( ) const [inline]

#### 3.2.2.17 int Parameters::getNChannels ( ) const [inline]

#### 3.2.2.18 int Parameters::getNE ( ) const [inline]

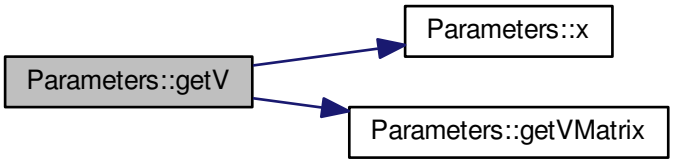
#### 3.2.2.19 int Parameters::getNSymmetries ( ) const [inline]

#### 3.2.2.20 double Parameters::getUnit ( ) const [inline]

#### 3.2.2.21 arma::cx_mat Parameters::getV ( double *x* ) const

Linear interpolation of V (works also for V given on non-constant grid if needed)

Here is the call graph for this function:




#### 3.2.2.22 arma::cx_mat Parameters::getVMatrix ( int *i* ) const

V matrix for a given x_i.

#### 3.2.2.23 double Parameters::getXMax ( ) const [inline]

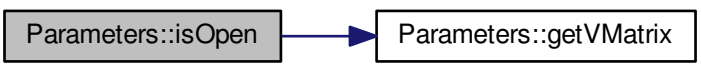
#### 3.2.2.24 double Parameters::getXMin ( ) const [inline]

#### 3.2.2.25 arma::cx_mat Parameters::Id ( ) const [inline]

#### 3.2.2.26 bool Parameters::isOpen ( int *nChannel*, double *energy* ) const

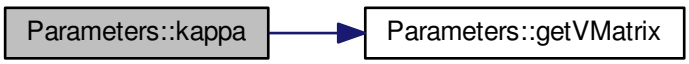
Check if the channel is open.

Here is the call graph for this function:



#### 3.2.2.27 double Parameters::kappa ( int *n1*, int *n2*, int *i*, double *E* ) const

Here is the call graph for this function:



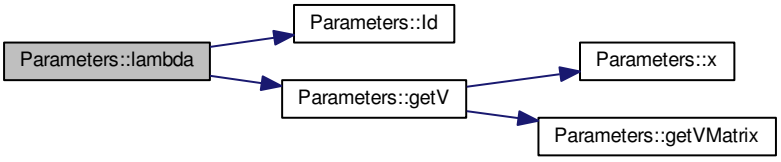

#### 3.2.2.28 double Parameters::kappa ( int *n1*, int *n2*, double *x*, double *E* ) const

Here is the call graph for this function:


#### 3.2.2.29 double Parameters::lambda ( double *x*, double *E* ) const

de Broglie length for a given potential and x

Here is the call graph for this function:




#### 3.2.2.30 void Parameters::loadB ( std::string *filename* = "B" )

Reading the values of B from the file generated in Mathematica.

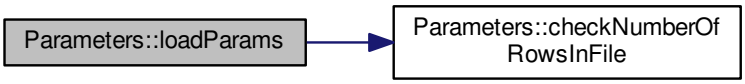
#### 3.2.2.31 void Parameters::loadE ( std::string *filename* = "E.dat" )

Reading the values of energies from the file generated in Mathematica.

#### 3.2.2.32 void Parameters::loadParams ( std::string *filename* = "Params.txt" )

Reading the values of parameters from the file generated in Mathematica.

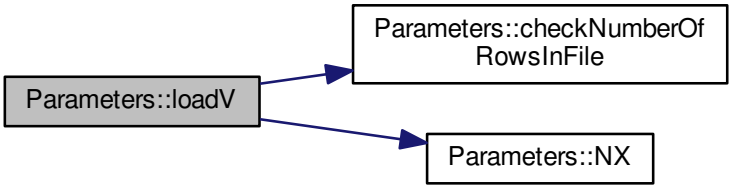
Here is the call graph for this function:




#### 3.2.2.33 void Parameters::loadV ( std::string *filename* = "V.dat" )

Reading the values of V from the file generated in Mathematica.

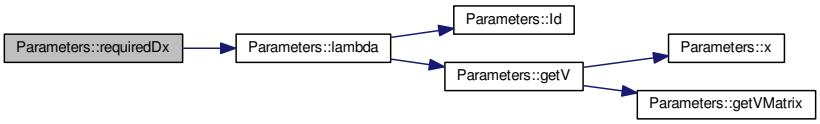
Here is the call graph for this function:




#### 3.2.2.34 int Parameters::NX ( ) const

#### 3.2.2.35 double Parameters::requiredDx ( double *x*, double *E* ) const

Here is the call graph for this function:




#### 3.2.2.36 void Parameters::setXValues ( )

Setting xValues.

#### 3.2.2.37 double Parameters::x ( int *i* ) const [inline]

### 3.2.3 Friends And Related Function Documentation

#### 3.2.3.1 friend class Parameters_getV_Test [friend]

#### 3.2.3.2 friend class Parameters_isOpen_Test [friend]

#### 3.2.3.3 friend class Parameters_kappaDouble_Test [friend]

#### 3.2.3.4 friend class Parameters_kappaInt_Test [friend]

#### 3.2.3.5 friend class Parameters_lambda_Test [friend]

#### 3.2.3.6 friend class Parameters_loadV_Test [friend]

#### 3.2.3.7 friend class Parameters_requiredDX_Test [friend]

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

- Parameters.h
- Parameters.cpp

# Chapter 4

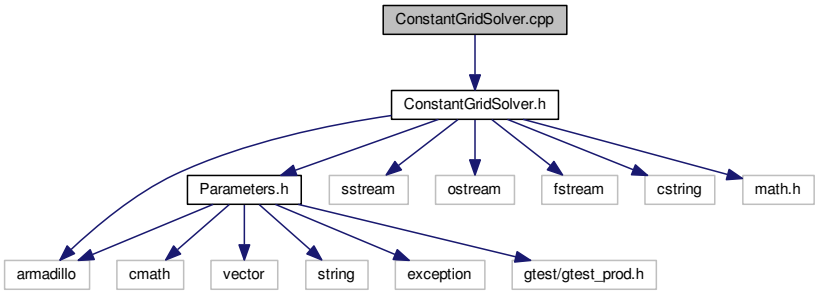
# File Documentation

## 4.1 ConstantGridSolver.cpp File Reference

Definitions of ConstantGridSolver class methods.

```
#include "ConstantGridSolver.h"
```

Include dependency graph for ConstantGridSolver.cpp:




### 4.1.1 Detailed Description

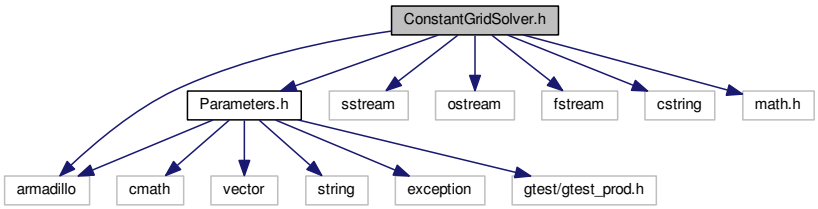
Definitions of ConstantGridSolver class methods.

## 4.2 ConstantGridSolver.h File Reference

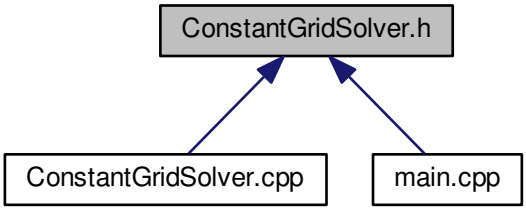
Definition of ConstantGridSolver class.

```
#include "armadillo"
#include "Parameters.h"
#include <sstream>
#include <ostream>
#include <fstream>
#include <cstring>
#include <math.h>
```

Include dependency graph for ConstantGridSolver.h:




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




### Classes

- class ConstantGridSolver

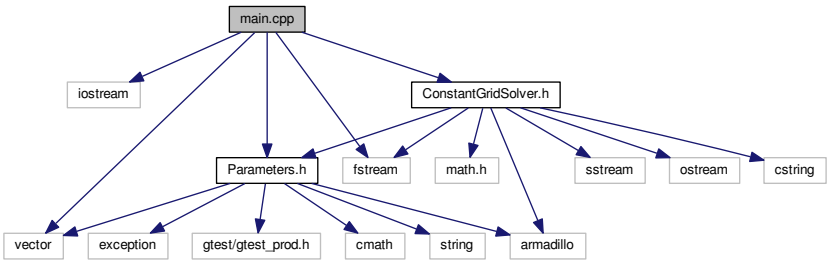
#### 4.2.1 Detailed Description

Definition of ConstantGridSolver class. This file contains a definition of ConstantGridSolver class, performing the calculations for a given set of parameters (Parameters object).

## 4.3 main.cpp File Reference

```
#include <iostream>
#include <vector>
#include <fstream>
#include "Parameters.h"
#include "ConstantGridSolver.h"
```

Include dependency graph for main.cpp:



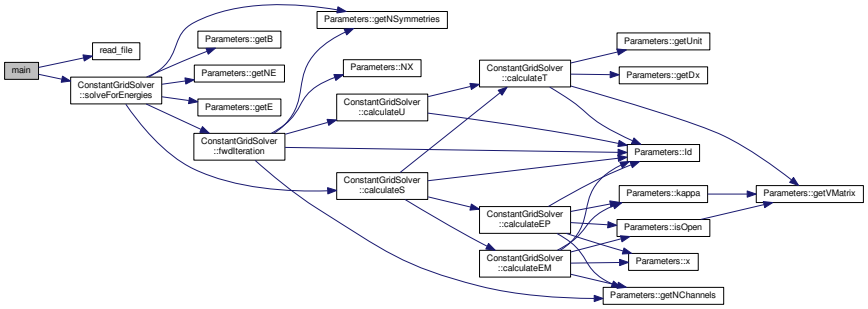

## Functions

- std::vector< std::string > read_file (std::string filename)
- int main ()

### 4.3.1 Function Documentation

#### 4.3.1.1 int main ( )

Here is the call graph for this function:



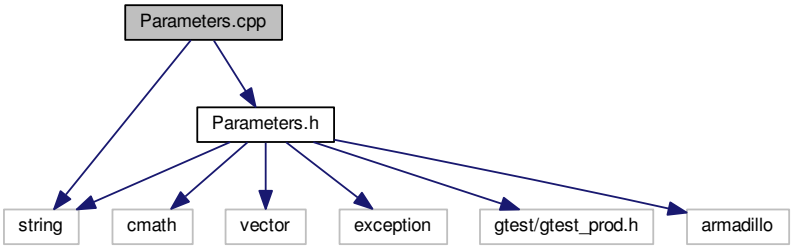

#### 4.3.1.2 std::vector<std::string> read_file ( std::string *filename* )

## 4.4 Parameters.cpp File Reference

Definitions of Parameters class methods.

```
#include <string>
#include "Parameters.h"
```

Include dependency graph for Parameters.cpp:




### 4.4.1 Detailed Description

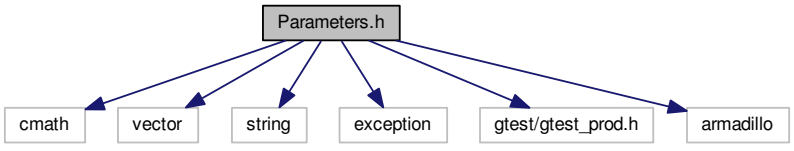
Definitions of Parameters class methods.

## 4.5 Parameters.h File Reference

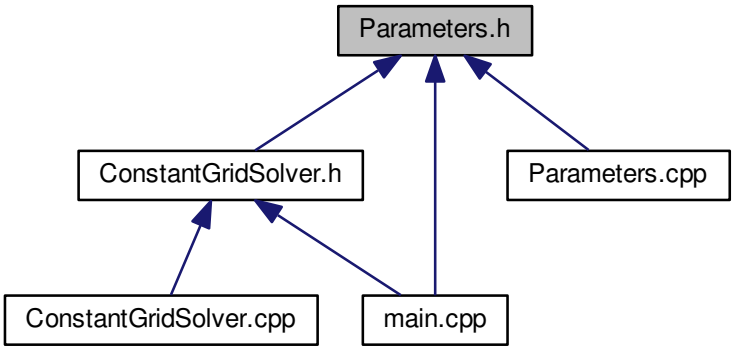
Definition of Parameters class.

```
#include <cmath>
#include <vector>
#include <string>
#include <exception>
#include <gtest/gtest_prod.h>
#include "armadillo"
```

Include dependency graph for Parameters.h:



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




## Classes

- class Parameters

### 4.5.1 Detailed Description

Definition of Parameters class. This file contains the definition of Parameters class.

# Index