# DOS Extraction

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# Contents

# Chapter 1

# Index

## 1.1 Introduction

This program allows to extract the Density of States (DoS), assessed by means of capacitance-voltage measurements, in an organic semiconductor device. Simulated values are fitted to experimental data.

All source and header files are written in C++11 language.

The software is intended to be used on a Unix-like operating system.

## 1.2 Dependancies

The program requires the following software to be installed on your system:

- `CMake` (version 2.8 or above), a cross-platform configuration tool;
- `Make` (version 3.8.1 or above), a tool used to build executables;
- `GCC` (version 4.8 or above), the GNU Compiler Collection;
- `Eigen` (version 3.2 or above), to handle with matrices, vectors and linear algebra;
- `Gnuplot` (version 4.6.4 or above), a graphical utility to generate plots (the package **gnuplot-x11**, a terminal for X servers, is also required for the interactive interface);
- `Boost` (version 1.50 or above), a set of libraries used by gnuplot-iostream.

It also uses the following libraries, shipped in the *include/* folder:

- `GetPot` (version 1.1.18), to parse command-line and configuration files;
- `gnuplot-iostream` (version 2), a C++ interface for Gnuplot.

Parallel computing capabilities are provided through the `OpenMP` library, shipped together with GCC.

## 1.3 Compile

In order to generate the executable, first open the *CMakeLists.txt* file (in the top-level folder) and, if necessary, edit it to your needs.

Then create a build directory and move into it:

```
$ mkdir build
$ cd build
```

Now you're ready to configure your system:

```
$ cmake ..
```

**Note**

or, should you want the compiler to produce also debug symbols:

```
$ cmake -DCMAKE_BUILD_TYPE=Debug ..
```

and finally:

```
$ make
```

will build the *simulate_dos* executable and the *dosextraction* shared library under the *bin/* and *lib/* directories (or the ones specified in *CMakeLists.txt*) respectively.

If you wish to install:

- the executable, into */usr/bin/*;
- the shared library, into */usr/lib/*;
- the header files, into */usr/local/include/dosextraction/*;

just type:

```
# make install
```

while:

```
# make uninstall
```

will remove them.

If `Doxygen` (version 3.8.6 or above) and `GraphViz` are found, the following command will generate the present documentation under the *doc/* folder (or the one specified in *CMakeLists.txt*):

```
$ make doc
```

## 1.4 Set up the configurations

**Note**

The default configuration directory is *config/*.

Before you can run the executable, you have to set up the configuration file (default: *config.pot*). Within it you can find a list of parameters, each of which is commented out to explain what modifying it will entail.

Particularly, the variables *input_params* and *input_experim* can be set, i.e. the filenames where to find input fitting parameters and experimental data respectively. It's recommended (but not compulsory) to put these files in the same directory as the configuration file (otherwise you can specify a relative or absolute path to them).

**Warning**

The program never checks that the input values are numeric but will always cast them to floating point numbers, then please pay attention while setting up the variable *skipHeaders*.

You can create multiple configuration files, each with different parameter values: the one you aim to use can be specified in the command-line before running.

## 1.5 Run!

To run by using the default configuration filename (*config.pot*) simply move into the directory where the executable is located in and type:

```
$ ./simulate_dos
```

To specify a different configuration file previously saved in the configuration directory:

```
$ ./simulate_dos -f configuration_filename
```

or:

```
$ ./simulate_dos --file configuration_filename
```

The variable *configuration_filename* should **not** contain the path.

**Warning**

Furthermore, if you run the program from a different folder or if you chose a different configuration directory, you have also to manually specify the path to the configuration directory (either absolute or relative to the current directory) by using:

```
$ ./simulate_dos -d configuration_directory
```

or:

```
$ ./simulate_dos --directory configuration_directory
```

Once complete, the results of the simulation(s) will be saved in the output directory (relative to the current folder) specified in the configuration file (default: *output/*).

Gnuplot scripts are saved too for later re-use under the *gnuplot/* subdirectory; you can run them through:

```
$ gnuplot name_of_the_script
```

# Chapter 2

# Namespace Index

## 2.1 Namespace List

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

# Chapter 3

# Hierarchical Index

## 3.1 Class Hierarchy

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

# Chapter 4

# Class Index

## 4.1 Class List

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

# Chapter 5

# File Index

## 5.1 File List

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

# Chapter 6

# Namespace Documentation

## 6.1 constants Namespace Reference

Numerical constants.

### Variables

- const Real Q = 1.60217653000000e-19
  *Electron charge* $[C]$.
- const Real Q2 = Q $*$ Q
  *Electron charge squared* $\left[C^2\right]$.
- const Real K_B = 1.38065050000000e-23
  *Boltzmann's constant* $\left[J \cdot K^{-1}\right]$.
- const Real EPS0 = 8.854187817e-12
  *Vacuum electrical permittivity* $\left[C \cdot V^{-1} \cdot m^{-1}\right]$.
- const Real T = 300
  *Reference temperature* $[K]$.
- const Real V_TH = K_B $*$ T / Q
  *Treshold voltage* $[V]$.
- const Index PARAMS_NO = 26
  *Number of parameters required in input file.*
- const Real PI = M_PI
  $\pi$.
- const Real SQRT_PI = std::sqrt(PI)
  $\sqrt{\pi}$.
- const Real PI_M4 = 0.7511255444649425
  $\pi^{-\frac{1}{4}}$.
- const Real SQRT_2 = std::sqrt(2)
  $\sqrt{2}$.

### 6.1.1 Detailed Description

Numerical constants.

## 6.2 numerics Namespace Reference

Namespace for generic numeric algorithms.

## Functions

- template<typename ScalarType >
  VectorX< ScalarType > sort (const VectorX< ScalarType > &vector)

  *Function to sort Eigen vectors.*
- template<typename ScalarType >
  VectorXpair< ScalarType > sort_pair (const VectorX< ScalarType > &vector)

  *Function to sort Eigen vectors, keeping track of indexes.*
- Real trapz (const VectorXr &x, const VectorXr &y)

  *Function to compute approximate integral of y with spacing increment specified by x, using trapezoidal rule.*
- Real trapz (const VectorXr &y)

  *Compute the approximate integral of y with unit spacing, using trapezoidal rule.*
- VectorXr deriv (const VectorXr &, const VectorXr &)

  *Compute the numeric derivative:* $\frac{dy}{dx}$.
- Real interp1 (const VectorXr &, const VectorXr &, const Real &)

  *Linear 1D interpolation. Interpolate y, defined at points x, at the point xNew.*
- VectorXr interp1 (const VectorXr &, const VectorXr &, const VectorXr &)

  *Linear 1D interpolation. Interpolate y, defined at points x, at the points xNew.*
- Real error_L2 (const VectorXr &, const VectorXr &, const VectorXr &, const Real &)

  *Compute the* $L^2$*-norm error between simulated and interpolated values, using trapz.*

### 6.2.1 Detailed Description

Namespace for generic numeric algorithms.

### 6.2.2 Function Documentation

#### 6.2.2.1 VectorX< ScalarType > sort ( const VectorX< ScalarType > & *vector* )

Function to sort Eigen vectors.

**Template Parameters**

| | |
|---|---|
| *ScalarType* | : the scalar type. |

**Parameters**

| | | |
|---|---|---|
| in | *vector* | : the vector to be sorted. |

**Returns**

the sorted vector.

Definition at line 103 of file numerics.h.

#### 6.2.2.2 VectorXpair< ScalarType > sort_pair ( const VectorX< ScalarType > & *vector* )

Function to sort Eigen vectors, keeping track of indexes.

**Template Parameters**

| | |
|---|---|
| *ScalarType* | : the scalar type. |

**Parameters**

| | | |
|---|---|---|
| in | *vector* | : the vector to be sorted. |

**Returns**

an Eigen vector of pairs: (sorted value, corresponding index in the unsorted vector).

Definition at line 112 of file numerics.h.

#### 6.2.2.3 Real trapz ( const VectorXr & *x*, const VectorXr & *y* )

Function to compute approximate integral of *y* with spacing increment specified by *x*, using trapezoidal rule.

**Parameters**

| | | |
|---|---|---|
| in | *x* | : the vector of the discrete domain; |
| in | *y* | : the vector of values to integrate. |

**Returns**

the approximate integral value.

Definition at line 17 of file numerics.cc.

#### 6.2.2.4 Real trapz ( const VectorXr & *y* )

Compute the approximate integral of *y* with unit spacing, using trapezoidal rule.

**Parameters**

| | | |
|---|---|---|
| in | *y* | : the vector of values to integrate. |

**Returns**

the approximate integral value.

Definition at line 33 of file numerics.cc.

#### 6.2.2.5 VectorXr deriv ( const VectorXr & *y*, const VectorXr & *x* )

Compute the numeric derivative: $\frac{dy}{dx}$.

**Parameters**

| | | |
|---|---|---|
| in | *y* | : the vector of values to differentiate; |
| in | *x* | : the vector of the discrete domain. |

**Returns**

a vector of the same length as *y* containing the approximate derivative.

Definition at line 38 of file numerics.cc.

#### 6.2.2.6 Real interp1 ( const VectorXr & *x*, const VectorXr & *y*, const Real & *xNew* )

Linear 1D interpolation. Interpolate *y*, defined at points *x*, at the point *xNew*.

**Parameters**

| | | |
|---|---|---|
| in | *y* | : the vector of values to interpolate; |
| in | *x* | : the vector of the discrete domain; |
| in | *xNew* | : the point to interpolate at. |

**Returns**

a scalar containing the interpolated value.

Definition at line 58 of file numerics.cc.

#### 6.2.2.7 VectorXr interp1 ( const VectorXr & *x*, const VectorXr & *y*, const VectorXr & *xNew* )

Linear 1D interpolation. Interpolate *y*, defined at points *x*, at the points *xNew*.

**Parameters**

| | | |
|---|---|---|
| in | *y* | : the vector of values to interpolate; |
| in | *x* | : the vector of the discrete domain; |
| in | *xNew* | : the vector of points to interpolate at. |

**Returns**

a vector of the same length as *xNew* containing the interpolated values.

Definition at line 79 of file numerics.cc.

#### 6.2.2.8 Real error_L2 ( const VectorXr & *interp*, const VectorXr & *simulated*, const VectorXr & *V*, const Real & *V_shift* )

Compute the $L^2$-norm error between simulated and interpolated values, using *trapz*.

**Parameters**

| | | |
|---|---|---|
| in | *interp* | : the interpolated values; |
| in | *simulated* | : the simulated values; |
| in | *V* | : the vector of the electric potential; |
| in | *V_shift* | : shift to the electric potential. |

**Returns**

the value of the $L^2$-norm error.

Definition at line 94 of file numerics.cc.

## 6.3 utility Namespace Reference

Namespace for utilities and auxiliary functions.

### Functions

- std::string full_path (const std::string &, const std::string &)
  *Auxiliary function to return the full path to a file.*
- void print_block (const char *, std::ostream &=std::cout)
  *Auxiliary function to print a string inside a block.*
- void print_done (std::ostream &=std::cout)
  *Auxiliary function to print a "DONE!" string.*

### 6.3.1 Detailed Description

Namespace for utilities and auxiliary functions.

### 6.3.2 Function Documentation

#### 6.3.2.1 std::string full_path ( const std::string & *filename,* const std::string & *relative_directory* )

Auxiliary function to return the full path to a file.

**Parameters**

| | | |
|---|---|---|
| in | *filename* | : the filename; |
| in | *relative_directory* | : the directory for a relative path. |

**Returns**

the variable *filename*, if it contains an absolute path; otherwise returns the concatenation of *relative_directory* and *filename* (i.e. the relative path to *filename*).

Definition at line 17 of file typedefs.cc.

#### 6.3.2.2 void print_block ( const char * *string,* std::ostream & *os* = `std::cout` )

Auxiliary function to print a string inside a block.

**Parameters**

| | | |
|---|---|---|
| in | *string* | : the string to print; |
| out | *os* | : output stream. |

Definition at line 22 of file typedefs.cc.

#### 6.3.2.3 void print_done ( std::ostream & *os* = `std::cout` )

Auxiliary function to print a "DONE!" string.

**Parameters**

| | | |
|---|---|---|
| out | *os* | : output stream. |

Definition at line 47 of file typedefs.cc.

# Chapter 7

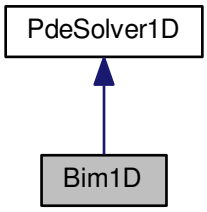
# Class Documentation

## 7.1 Bim1D Class Reference

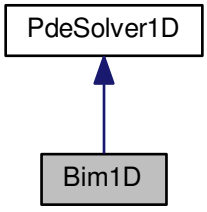
Class derived from PdeSolver1D, providing a finite volume Box Integration Method (BIM) solver.

`#include <solvers.h>`

Inheritance diagram for Bim1D:




Collaboration diagram for Bim1D:



### Public Member Functions

- Bim1D ()=delete

  *Default constructor (deleted since it is required to specify the mesh).*
- Bim1D (VectorXr &)

  *Constructor.*
- virtual ~Bim1D ()=default

  *Destructor (defaulted).*
- virtual void assembleAdvDiff (const VectorXr &, const VectorXr &, const VectorXr &, const VectorXr &) override

  *Assemble the matrix for an advection-diffusion term.*
- virtual void assembleStiff (const VectorXr &, const VectorXr &) override

  *Assemble the matrix for a diffusion term.*
- virtual void assembleMass (const VectorXr &, const VectorXr &) override

  *Assemble the matrix for a reaction term.*

### Static Public Member Functions

- static VectorXr log_mean (const VectorXr &, const VectorXr &)

  *Compute the element-wise logarithmic mean of two vectors.*
- static std::pair< VectorXr, VectorXr > bernoulli (const VectorXr &)

  *Compute the values of the Bernoulli function.*

### Additional Inherited Members

## 7.1.1 Detailed Description

Class derived from PdeSolver1D, providing a finite volume Box Integration Method (BIM) solver.

Matrices are held in a sparse format.

Definition at line 117 of file solvers.h.

## 7.1.2 Constructor & Destructor Documentation

### 7.1.2.1 Bim1D ( VectorXr & *mesh* )

Constructor.

**Parameters**

| | | |
|---|---|---|
| in | *mesh* | : the mesh coordinates. |

Definition at line 20 of file solvers.cc.

## 7.1.3 Member Function Documentation

### 7.1.3.1 VectorXr log_mean ( const VectorXr & *x1*, const VectorXr & *x2* ) [static]

Compute the element-wise logarithmic mean of two vectors.

$$M_{log}(x_1,x_2) = \frac{x_2 - x_1}{\log x_2 - \log x_1} = \frac{x_2 - x_1}{\log\left(\frac{x_2}{x_1}\right)} .$$

**Parameters**

| | | |
|---|---|---|
| in | *x1* | : the first vector; |
| in | *x2* | : the second vector. |

**Returns**

the vector of the logarithmic means.

Definition at line 23 of file solvers.cc.

#### 7.1.3.2 std::pair< VectorXr, VectorXr > bernoulli ( const VectorXr & *x* ) [static]

Compute the values of the Bernoulli function.

$$\mathfrak{B}(x) = \frac{x}{e^x - 1} .$$

**Parameters**

| | | |
|---|---|---|
| in | *x* | : the vector of the values to compute the Bernoulli function at. |

**Returns**

the pair $(\mathfrak{B}(x), \mathfrak{B}(-x))$.

Definition at line 54 of file solvers.cc.

#### 7.1.3.3 void assembleAdvDiff ( const VectorXr & *alpha,* const VectorXr & *gamma,* const VectorXr & *eta,* const VectorXr & *beta* ) [override], [virtual]

Assemble the matrix for an advection-diffusion term.

Build the Scharfetter-Gummel stabilized stiffness matrix for: $-\nabla \cdot (\alpha \cdot \gamma(\eta \nabla u - \beta u)) = f$.

**Parameters**

| | | |
|---|---|---|
| in | *alpha* | : $\alpha$, an element-wise constant function; |
| in | *gamma* | : $\gamma$, an element-wise linear function; |
| in | *eta* | : $\eta$, an element-wise linear function; |
| in | *beta* | : $\beta$, an element-wise constant function. |

Implements PdeSolver1D.

Definition at line 113 of file solvers.cc.

#### 7.1.3.4 void assembleStiff ( const VectorXr & *eps,* const VectorXr & *kappa* ) [override], [virtual]

Assemble the matrix for a diffusion term.

Build the standard finite element stiffness matrix for the diffusion problem: $-\nabla \cdot (\varepsilon \cdot \kappa \nabla u) = f$.

**Parameters**

| | | |
|---|---|---|
| in | *eps* | : $\varepsilon$, an element-wise constant function; |

| | | |
|---|---|---|
| in | *kappa* | : $\kappa$, an element-wise linear function. |

Implements PdeSolver1D.

Definition at line 173 of file solvers.cc.

#### 7.1.3.5 void assembleMass ( const VectorXr & *delta*, const VectorXr & *zeta* ) [override], [virtual]

Assemble the matrix for a reaction term.

Build the lumped finite element mass matrix for the reaction problem: $\delta \cdot \zeta u = f$.

**Parameters**

| | | |
|---|---|---|
| in | *delta* | : $\delta$, an element-wise constant function; |
| in | *zeta* | : $\zeta$, an element-wise linear function. |

Implements PdeSolver1D.

Definition at line 182 of file solvers.cc.

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

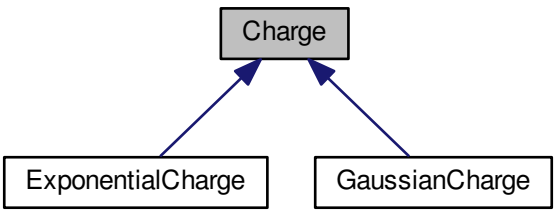
- DosExtraction/src/solvers.h
- DosExtraction/src/solvers.cc

## 7.2 Charge Class Reference

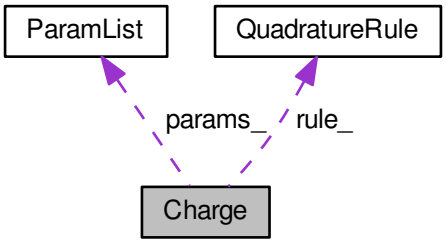
Abstract class providing methods to calculate total electric charge (the rhs in the Poisson equation).

`#include <charge.h>`

Inheritance diagram for Charge:



Collaboration diagram for Charge:




## Public Member Functions

- Charge ()=delete

  *Default constructor (deleted since it is required to specify a ParamList and a QuadratureRule).*
- Charge (const ParamList &, const QuadratureRule &)

  *Constructor.*
- virtual ~Charge ()=default

  *Destructor (defaulted).*
- virtual VectorXr charge (const VectorXr &phi)=0

  *Compute the total charge density.*
- virtual VectorXr dcharge (const VectorXr &phi)=0

  *Compute the derivative of the total charge density with respect to the electric potential.*

## Protected Attributes

- const ParamList & params_

  *Parameter list handler.*
- const QuadratureRule & rule_

  *Quadrature rule handler.*

### 7.2.1 Detailed Description

Abstract class providing methods to calculate total electric charge (the rhs in the Poisson equation).

Definition at line 30 of file charge.h.

### 7.2.2 Constructor & Destructor Documentation

#### 7.2.2.1 Charge ( const ParamList & *params*, const QuadratureRule & *rule* )

Constructor.

**Parameters**

| | | |
|---|---|---|
| in | *params* | : a list of simulation parameters; |
| in | *rule* | : a quadrature rule. |

Definition at line 19 of file charge.cc.

### 7.2.3 Member Function Documentation

#### 7.2.3.1 virtual VectorXr charge ( const VectorXr & *phi* ) [pure virtual]

Compute the total charge density.

**Parameters**

| | | |
|---|---|---|
| in | *phi* | : the electric potential $\varphi$. |

**Returns**

the total charge density $q(\varphi)$ $\left[C \cdot m^{-3}\right]$.

Implemented in ExponentialCharge, and GaussianCharge.

#### 7.2.3.2 virtual VectorXr dcharge ( const VectorXr & *phi* ) [pure virtual]

Compute the derivative of the total charge density with respect to the electric potential.

**Parameters**

| | | |
|---|---|---|
| in | *phi* | : the electric potential $\varphi$. |

**Returns**

the derivative: $\frac{\mathrm{d}q(\varphi)}{\mathrm{d}\varphi}$ $\left[C \cdot m^{-3} \cdot V^{-1}\right]$.

Implemented in ExponentialCharge, and GaussianCharge.

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

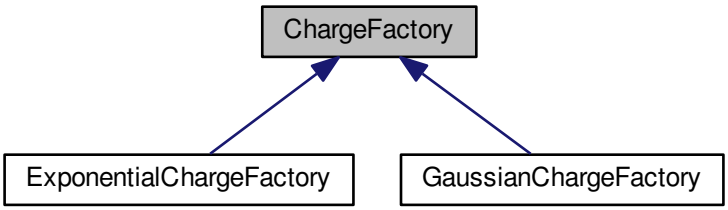
- DosExtraction/src/charge.h
- DosExtraction/src/charge.cc

## 7.3 ChargeFactory Class Reference

Abstract factory to handle the constitutive relation for the Density of States.

`#include <factory.h>`

Inheritance diagram for ChargeFactory:




## Public Member Functions

- ChargeFactory ()=default

  *Default constructor (defaulted).*
- virtual ~ChargeFactory ()=default

  *Destructor (defaulted).*
- virtual Charge * BuildCharge (const ParamList &params, const QuadratureRule &rule)=0

  *Factory method to build an abstract Charge object.*

### 7.3.1 Detailed Description

Abstract factory to handle the constitutive relation for the Density of States.

Definition at line 30 of file factory.h.

### 7.3.2 Member Function Documentation

#### 7.3.2.1 virtual Charge* BuildCharge ( const ParamList & *params*, const QuadratureRule & *rule* ) [pure virtual]

Factory method to build an abstract Charge object.

**Parameters**

| | | |
|---|---|---|
| in | *params* | : a list of simulation parameters; |
| in | *rule* | : a quadrature rule. |

**Returns**

a pointer to Charge.

Implemented in ExponentialChargeFactory, and GaussianChargeFactory.

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

- DosExtraction/src/factory.h

## 7.4 CsvParser Class Reference

Class providing methods to read **numeric** content from a .csv file and to store it in Eigen matrices or vectors.

`#include <csvParser.h>`

### Public Member Functions

- CsvParser ()=delete

  *Default constructor (deleted since it is required to specify at least a filename).*
- CsvParser (const std::string &, const bool &=true)

  *Constructor: load the input file and check its compatibility with the code.*
- virtual ~CsvParser ()

  *Destructor: close the input file.*
- RowVectorXr importRow (const Index &)

  *Method to import a row from the input file.*
- MatrixXr importRows (const std::initializer_list< Index > &)

  *Method to import multiple rows from the input file.*
- MatrixXr importFirstRows (const Index &)

  *Method to import the first nRows rows from the input file.*
- VectorXr importCol (const Index &)

  *Method to import a column from the input file.*
- MatrixXr importCols (const std::initializer_list< Index > &)

  *Method to import multiple columns from the input file.*
- MatrixXr importFirstCols (const Index &)

  *Method to import the first nCols columns from the input file.*
- Real importCell (const Index &, const Index &)

  *Method to import a single cell from the input file.*
- MatrixXr importAll ()

  *Method to import the whole input file.*

#### Getter methods

- const Index & **nRows** () const
- const Index & **nCols** () const

### Private Member Functions

- void reset ()

  *Reset all the flags for input_ and go back to the beginning of file (possibly by ignoring headers).*

### Private Attributes

- bool hasHeaders_

  *bool to determine if first row contains headers or not.*
- Index nRows_

  *Number of rows in the input file.*
- Index nCols_

  *Number of columns in the input file.*
- std::ifstream input_

  *Input stream to input_filename.*

- std::string line_
  *Auxiliary variable to store currently processed line.*
- char separator_
  *The separator character detected.*

### 7.4.1 Detailed Description

Class providing methods to read **numeric** content from a .csv file and to store it in Eigen matrices or vectors.

Definition at line 34 of file csvParser.h.

### 7.4.2 Constructor & Destructor Documentation

#### 7.4.2.1 CsvParser ( const std::string & *input_filename*, const bool & *hasHeaders* = `true` )

Constructor: load the input file and check its compatibility with the code.

**Parameters**

| | | |
|---|---|---|
| in | *input_filename* | : the name of the input file; |
| in | *hasHeaders* | : bool to specify if first row contains headers or not; if **true**, first row is always ignored. |

Definition at line 24 of file csvParser.cc.

### 7.4.3 Member Function Documentation

#### 7.4.3.1 RowVectorXr importRow ( const Index & *index* )

Method to import a row from the input file.

**Parameters**

| | | |
|---|---|---|
| in | *index* | : the row index. |

**Returns**

a row vector containing the content read.

Definition at line 96 of file csvParser.cc.

#### 7.4.3.2 MatrixXr importRows ( const std::initializer_list< Index > & *indexes* )

Method to import multiple rows from the input file.

**Parameters**

| | | |
|---|---|---|
| in | *indexes* | : initializer list containing the row indexes (e.g. something like {1, 3, 4}). |

**Returns**

a matrix containing the content read (row by row).

Definition at line 129 of file csvParser.cc.

#### 7.4.3.3 MatrixXr importFirstRows ( const Index & *nRows* )

Method to import the first *nRows* rows from the input file.

**Parameters**

| | | |
|---|---|---|
| in | *nRows* | : the number of rows to import. |

**Returns**

a matrix containing the content read (row by row).

Definition at line 146 of file csvParser.cc.

#### 7.4.3.4 VectorXr importCol ( const Index & *index* )

Method to import a column from the input file.

**Parameters**

| | | |
|---|---|---|
| in | *index* | : the column index. |

**Returns**

a column vector containing the content read.

Definition at line 160 of file csvParser.cc.

#### 7.4.3.5 MatrixXr importCols ( const std::initializer_list< Index > & *indexes* )

Method to import multiple columns from the input file.

**Parameters**

| | | |
|---|---|---|
| in | *indexes* | : initializer list containing the column indexes (e.g. something like {1, 3, 4}). |

**Returns**

a matrix containing the content read (column by column).

Definition at line 189 of file csvParser.cc.

#### 7.4.3.6 MatrixXr importFirstCols ( const Index & *nCols* )

Method to import the first *nCols* columns from the input file.

**Parameters**

| | | |
|---|---|---|
| in | *nCols* | : the number of columns to import. |

**Returns**

a matrix containing the content read (column by column).

Definition at line 206 of file csvParser.cc.

#### 7.4.3.7 Real importCell ( const Index & *rowIndex,* const Index & *colIndex* )

Method to import a single cell from the input file.

**Parameters**

| | | |
|---|---|---|
| in | *rowIndex* | : the cell row index. |
| in | *colIndex* | : the cell column index. |

**Returns**

a scalar containing the value read.

Definition at line 220 of file csvParser.cc.

#### 7.4.3.8 MatrixXr importAll ( )

Method to import the whole input file.

**Returns**

a matrix containing the content read (cell by cell).

Definition at line 228 of file csvParser.cc.

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

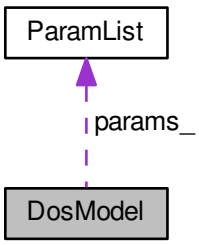
- DosExtraction/src/csvParser.h
- DosExtraction/src/csvParser.cc

## 7.5 DosModel Class Reference

Class providing methods to process a simulation to extract the Density of States starting from a parameter list.

`#include <dosModel.h>`

Collaboration diagram for DosModel:




### Public Member Functions

- DosModel ()

  *Default constructor.*
- DosModel (const ParamList &)

  *Explicit conversion constructor.*

- virtual ~DosModel ()=default

  *Destructor (defaulted).*
- const ParamList & params () const

  *Getter method.*
- void simulate (const GetPot &, const std::string &, const std::string &, const std::string &, const std::string &)

  *Perform the simulation.*
- void post_process (const GetPot &, const std::string &, std::ostream &, std::ostream &, const Real &, const Real &, const VectorXr &, const VectorXr &, const VectorXr &, const VectorXr &)

  *Perform post-processing.*
- void gnuplot_commands (const std::string &, std::ostream &) const

  *Defines commands to generate Gnuplot output files.*
- void save_plot (const std::string &, const std::string &, const std::string &, const std::string &) const

  *Save the Gnuplot output files.*

### Private Attributes

- bool initialized_

  *bool to determine if DosModel param_ has been properly initialized.*
- ParamList params_

  *The parameter list.*
- Real V_shift_

  *Peak shift between experimental data and simulated values* $[V]$.

## 7.5.1 Detailed Description

Class providing methods to process a simulation to extract the Density of States starting from a parameter list.

Definition at line 42 of file dosModel.h.

## 7.5.2 Constructor & Destructor Documentation

### 7.5.2.1 DosModel ( const ParamList & *params* ) [explicit]

Explicit conversion constructor.

**Parameters**

| | | |
|---|---|---|
| in | *params* | : a parameter list. |

Definition at line 24 of file dosModel.cc.

## 7.5.3 Member Function Documentation

### 7.5.3.1 void simulate ( const GetPot & *config*, const std::string & *input_experim*, const std::string & *output_directory*, const std::string & *output_plot_subdir*, const std::string & *output_filename* )

Perform the simulation.

**Parameters**

| | | |
|---|---|---|
| in | *config* | : the GetPot configuration object; |
| in | *input_experim* | : the file containing experimental data; |
| in | *output_directory* | : directory where to store output files; |
| in | *output_plot_subdir* | : sub-directory where to store Gnuplot files; |
| in | *output_filename* | : prefix for the output filename. |

Definition at line 27 of file dosModel.cc.

#### 7.5.3.2 void post_process ( const GetPot & *config*, const std::string & *input_experim*, std::ostream & *output_fitting*, std::ostream & *output_CV*, const Real & *A_semic*, const Real & *C_sb*, const VectorXr & *x_semic*, const VectorXr & *dens*, const VectorXr & *V_simulated*, const VectorXr & *C_simulated* )

Perform post-processing.

**Parameters**

| | | |
|---|---|---|
| in | *config* | : the GetPot configuration object; |
| in | *input_experim* | : the file containing experimental data; |
| out | *output_fitting* | : output file containing infos about fitting experimental data; |
| out | *output_CV* | : output file containing infos about capacitance-voltage data; |
| in | *A_semic* | : area of the semiconductor; |
| in | *C_sb* | : stray border capacitance (see ParamList); |
| in | *x_semic* | : the mesh corresponding to the semiconductor domain; |
| in | *dens* | : charge density $[C \cdot m^{-3}]$; |
| in | *V_simulated* | : simulated voltage values; |
| in | *C_simulated* | : simulated capacitance values. |

Definition at line 273 of file dosModel.cc.

#### 7.5.3.3 void gnuplot_commands ( const std::string & *output_CV_filename*, std::ostream & *os* ) const

Defines commands to generate Gnuplot output files.

**Parameters**

| | | |
|---|---|---|
| in | *output_CV_filename* | : output CV filename; |
| out | *os* | : output stream. |

Definition at line 364 of file dosModel.cc.

#### 7.5.3.4 void save_plot ( const std::string & *output_directory*, const std::string & *output_plot_subdir*, const std::string & *output_CV_filename*, const std::string & *output_filename* ) const

Save the Gnuplot output files.

**Parameters**

| | | |
|---|---|---|
| in | *output_directory* | : directory where to store output files; |
| in | *output_plot_subdir* | : sub-directory where to store Gnuplot files; |
| in | *output_CV_filename* | : output CV filename; |

| | | |
|---|---|---|
| in | *output_filename* | : prefix for the output filename. |

Definition at line 398 of file dosModel.cc.

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

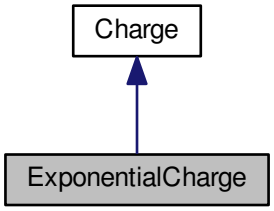
- DosExtraction/src/dosModel.h
- DosExtraction/src/dosModel.cc

## 7.6 ExponentialCharge Class Reference

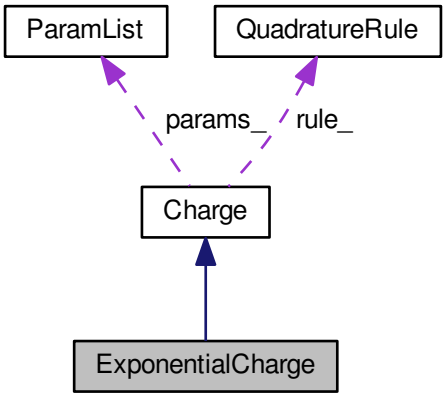
Class derived from Charge, under the hypothesis that Density of States is a single exponential.

`#include <charge.h>`

Inheritance diagram for ExponentialCharge:




Collaboration diagram for ExponentialCharge:




### Public Member Functions

- ExponentialCharge ()=delete

*Default constructor (deleted since it is required to specify a ParamList and a QuadratureRule).*

- ExponentialCharge (const ParamList &, const QuadratureRule &)

  *Constructor.*
- virtual ~ExponentialCharge ()=default

  *Destructor (defaulted).*
- virtual VectorXr charge (const VectorXr &) override

  *Compute the total charge density.*
- virtual VectorXr dcharge (const VectorXr &) override

  *Compute the derivative of the total charge density with respect to the electric potential.*

### Private Member Functions

- Real n_approx (const Real &, const Real &, const Real &) const

  *Compute electrons density (per unit volume).*
- Real dn_approx (const Real &, const Real &, const Real &) const

  *Compute the approximate derivative of electrons density (per unit volume) with respect to the electric potential.*

### Private Attributes

- Real N0_

  *Parameter of the exponential density.*

### Additional Inherited Members

## 7.6.1 Detailed Description

Class derived from Charge, under the hypothesis that Density of States is a single exponential.

Provide methods to compute total electric charge and its derivative under the hypothesis that Density of States is a single exponential, whose parameter is got by the constructor, of the form:

$$\frac{N_0}{\lambda}\exp\left(-\frac{(\cdot)}{\lambda}\right) .$$

Definition at line 127 of file charge.h.

## 7.6.2 Constructor & Destructor Documentation

### 7.6.2.1 ExponentialCharge ( const ParamList & *params*, const QuadratureRule & *rule* )

Constructor.

**Parameters**

| | | |
|---|---|---|
| in | *params* | : a list of simulation parameters; |
| in | *rule* | : a quadrature rule. |

Definition at line 112 of file charge.cc.

## 7.6.3 Member Function Documentation

### 7.6.3.1 VectorXr charge ( const VectorXr & *phi* ) [override], [virtual]

Compute the total charge density.

**Parameters**

| | | |
|---|---|---|
| in | *phi* | : the electric potential $\varphi$. |

**Returns**

the total charge density $q(\varphi)\ \left[C \cdot m^{-3}\right]$.

Implements Charge.

Definition at line 143 of file charge.cc.

#### 7.6.3.2 VectorXr dcharge ( const VectorXr & *phi* ) [override], [virtual]

Compute the derivative of the total charge density with respect to the electric potential.

**Parameters**

| | | |
|---|---|---|
| in | *phi* | : the electric potential $\varphi$. |

**Returns**

the derivative: $\frac{\mathrm{d}q(\varphi)}{\mathrm{d}\varphi}\ \left[C \cdot m^{-3} \cdot V^{-1}\right]$.

Implements Charge.

Definition at line 155 of file charge.cc.

#### 7.6.3.3 Real n_approx ( const Real & *phi,* const Real & *N0,* const Real & *lambda* ) const [private]

Compute electrons density (per unit volume).

**Parameters**

| | | |
|---|---|---|
| in | *phi* | : the electric potential $\varphi$; |
| in | *N0* | : the exponential $N_0$; |
| in | *lambda* | : the exponential $\lambda$. |

**Returns**

the electrons density $n(\varphi)\ \left[m^{-3}\right]$.

Definition at line 115 of file charge.cc.

#### 7.6.3.4 Real dn_approx ( const Real & *phi,* const Real & *N0,* const Real & *lambda* ) const [private]

Compute the approximate derivative of electrons density (per unit volume) with respect to the electric potential.

**Parameters**

| | | |
|---|---|---|
| in | *phi* | : the electric potential $\varphi$; |
| in | *N0* | : the exponential $N_0$; |
| in | *lambda* | : the exponential $\lambda$. |

**Returns**

the derivative: $\frac{\mathrm{d}n(\varphi)}{\mathrm{d}\varphi}\ \left[m^{-3} \cdot V^{-1}\right]$.

Definition at line 129 of file charge.cc.

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

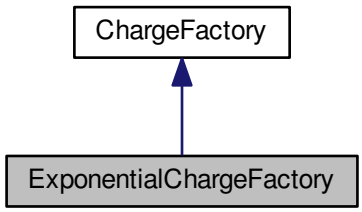
- DosExtraction/src/charge.h
- DosExtraction/src/charge.cc

## 7.7 ExponentialChargeFactory Class Reference

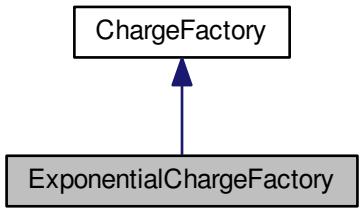
Concrete factory to handle a single exponential DOS constitutive relation.

`#include <factory.h>`

Inheritance diagram for ExponentialChargeFactory:




Collaboration diagram for ExponentialChargeFactory:




### Public Member Functions

- ExponentialChargeFactory ()=default

  *Default constructor (defaulted).*
- virtual ~ExponentialChargeFactory ()=default

  *Destructor (defaulted).*
- virtual Charge * BuildCharge (const ParamList &, const QuadratureRule &) override

  *Factory method to build a concrete Charge object.*

### 7.7.1 Detailed Description

Concrete factory to handle a single exponential DOS constitutive relation.

Definition at line 84 of file factory.h.

### 7.7.2 Member Function Documentation

#### 7.7.2.1 Charge * BuildCharge ( const ParamList & *params*, const QuadratureRule & *rule* ) [override], [virtual]

Factory method to build a concrete Charge object.

**Parameters**

| | | |
|---|---|---|
| in | *params* | : a list of simulation parameters; |
| in | *rule* | : a quadrature rule. |

**Returns**

a pointer to ExponentialCharge.

Implements ChargeFactory.

Definition at line 22 of file factory.cc.

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

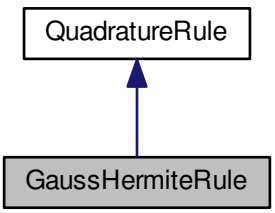
- DosExtraction/src/factory.h
- DosExtraction/src/factory.cc

## 7.8 GaussHermiteRule Class Reference

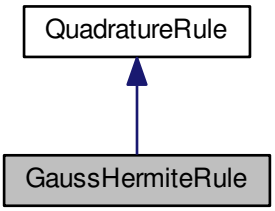
Class derived from QuadratureRule providing the Gauss-Hermite quadrature rule.

`#include <quadratureRule.h>`

Inheritance diagram for GaussHermiteRule:



Collaboration diagram for GaussHermiteRule:




## Public Member Functions

- GaussHermiteRule ()=delete

  *Default constructor (deleted since it is required to specify the number of nodes).*
- GaussHermiteRule (const Index &)

  *Constructor.*
- virtual ~GaussHermiteRule ()=default

  *Destructor (defaulted).*
- virtual void apply () override

  *Apply the quadrature rule in order to compute the nodes and weights.*
- virtual void apply (const GetPot &) override

  *Apply the quadrature rule reading parameters from a configuration file.*
- void apply_iterative_algorithm (const Index &=1000, const Real &=1.0e-14)

  *Compute nodes and weights using an adapted version of the algorithm presented in:*
  *William H. Press, Saul A. Teukolsky, William T. Vetterling, and Brian P. Flannery. 2007.*
  *Numerical Recipes: The Art of Scientific Computing (3rd edition).*
  *Cambridge University Press, New York, NY, USA.*
- void apply_using_eigendecomposition ()

  *Compute nodes and weights using an eigendecomposition-based algorithm.*

## Additional Inherited Members

### 7.8.1 Detailed Description

Class derived from QuadratureRule providing the Gauss-Hermite quadrature rule.

Compute nodes and weights for the *nNodes_*-points approximation of:

$$\int_{-\infty}^{+\infty} w(x) f(x)\ \mathrm{d}x$$

where $w(x) = e^{-x^2}$.

Definition at line 94 of file quadratureRule.h.

### 7.8.2 Constructor & Destructor Documentation

#### 7.8.2.1 GaussHermiteRule ( const Index & *nNodes* )

Constructor.

**Parameters**

| | | |
|---|---|---|
| in | *nNodes* | : the number of nodes to be used for the quadrature rule. |

Definition at line 28 of file quadratureRule.cc.

### 7.8.3 Member Function Documentation

#### 7.8.3.1 void apply ( const GetPot & *config* ) [override], [virtual]

Apply the quadrature rule reading parameters from a configuration file.

**Parameters**

| | | |
|---|---|---|
| in | *config* | : the GetPot configuration object. |

Implements QuadratureRule.

Definition at line 36 of file quadratureRule.cc.

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

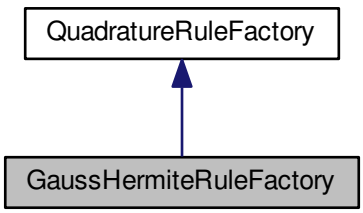
- DosExtraction/src/quadratureRule.h
- DosExtraction/src/quadratureRule.cc

## 7.9 GaussHermiteRuleFactory Class Reference

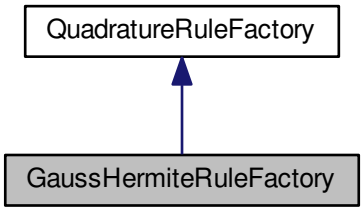
Concrete factory to handle a Gauss-Hermite quadrature rule.

`#include <factory.h>`

Inheritance diagram for GaussHermiteRuleFactory:



Collaboration diagram for GaussHermiteRuleFactory:




## Public Member Functions

- GaussHermiteRuleFactory ()=default

  *Default constructor (defaulted).*
- virtual ~GaussHermiteRuleFactory ()=default

  *Destructor (defaulted).*
- virtual QuadratureRule * BuildRule (const Index &) override

  *Factory method to build a concrete QuadratureRule object.*

### 7.9.1 Detailed Description

Concrete factory to handle a Gauss-Hermite quadrature rule.

Definition at line 137 of file factory.h.

### 7.9.2 Member Function Documentation

#### 7.9.2.1 QuadratureRule * BuildRule ( const Index & *nNodes* ) [override], [virtual]

Factory method to build a concrete QuadratureRule object.

**Parameters**

| | | |
|---|---|---|
| in | *nNodes* | : the number of nodes to be used for the quadrature rule. |

**Returns**

a pointer to GaussHermiteRule.

Implements QuadratureRuleFactory.

Definition at line 27 of file factory.cc.

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

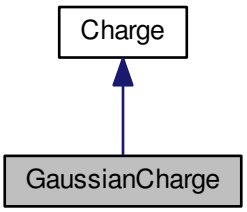
- DosExtraction/src/factory.h
- DosExtraction/src/factory.cc

## 7.10 GaussianCharge Class Reference

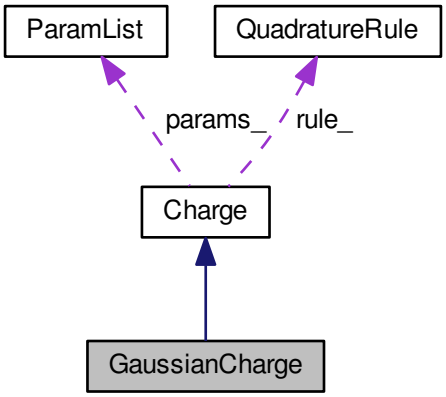
Class derived from Charge, under the hypothesis that Density of States is a combination of gaussians.

`#include <charge.h>`

Inheritance diagram for GaussianCharge:




Collaboration diagram for GaussianCharge:




### Public Member Functions

- GaussianCharge ()=delete

  *Default constructor (deleted since it is required to specify a ParamList and a QuadratureRule).*
- GaussianCharge (const ParamList &, const QuadratureRule &)

  *Constructor.*
- virtual ~GaussianCharge ()=default

  *Destructor (defaulted).*
- virtual VectorXr charge (const VectorXr &) override

  *Compute the total charge density.*
- virtual VectorXr dcharge (const VectorXr &) override

*Compute the derivative of the total charge density with respect to the electric potential.*

### Private Member Functions

- Real n_approx (const Real &, const Real &, const Real &) const

  *Compute electrons density (per unit volume).*
- Real dn_approx (const Real &, const Real &, const Real &) const

  *Compute the approximate derivative of electrons density (per unit volume) with respect to the electric potential.*

### Additional Inherited Members

## 7.10.1 Detailed Description

Class derived from Charge, under the hypothesis that Density of States is a combination of gaussians.

Provide methods to compute total electric charge and its derivative under the hypothesis that Density of States is a linear combination of multiple gaussians, whose parameters are read from a ParamList object, of the form:

$$\frac{N_0}{\sqrt{2\pi\sigma^2}}\exp\left(-\frac{(\cdot)^2}{2\sigma^2}\right).$$

Definition at line 76 of file charge.h.

## 7.10.2 Constructor & Destructor Documentation

### 7.10.2.1 GaussianCharge ( const ParamList & *params*, const QuadratureRule & *rule* )

Constructor.

**Parameters**

| | | |
|---|---|---|
| in | *params* | : a list of simulation parameters; |
| in | *rule* | : a quadrature rule. |

Definition at line 22 of file charge.cc.

## 7.10.3 Member Function Documentation

### 7.10.3.1 VectorXr charge ( const VectorXr & *phi* ) [override], [virtual]

Compute the total charge density.

**Parameters**

| | | |
|---|---|---|
| in | *phi* | : the electric potential $\varphi$. |

**Returns**

the total charge density $q(\varphi)\left[C\cdot m^{-3}\right]$.

Implements Charge.

Definition at line 53 of file charge.cc.

### 7.10.3.2 VectorXr dcharge ( const VectorXr & *phi* ) [override], [virtual]

Compute the derivative of the total charge density with respect to the electric potential.

**Parameters**

| | | |
|---|---|---|
| in | *phi* | : the electric potential $\varphi$. |

**Returns**

the derivative: $\frac{\mathrm{d}q(\varphi)}{\mathrm{d}\varphi}\left[C\cdot m^{-3}\cdot V^{-1}\right]$.

Implements Charge.

Definition at line 80 of file charge.cc.

#### 7.10.3.3 Real n_approx ( const Real & *phi,* const Real & *N0,* const Real & *sigma* ) const [private]

Compute electrons density (per unit volume).

**Parameters**

| | | |
|---|---|---|
| in | *phi* | : the electric potential $\varphi$; |
| in | *N0* | : the gaussian mean $N_0$; |
| in | *sigma* | : the gaussian standard deviation $\sigma$. |

**Returns**

the electrons density $n(\varphi)\left[m^{-3}\right]$.

Definition at line 25 of file charge.cc.

#### 7.10.3.4 Real dn_approx ( const Real & *phi,* const Real & *N0,* const Real & *sigma* ) const [private]

Compute the approximate derivative of electrons density (per unit volume) with respect to the electric potential.

**Parameters**

| | | |
|---|---|---|
| in | *phi* | : the electric potential $\varphi$; |
| in | *N0* | : the gaussian mean $N_0$; |
| in | *sigma* | : the gaussian standard deviation $\sigma$. |

**Returns**

the derivative: $\frac{\mathrm{d}n(\varphi)}{\mathrm{d}\varphi}\left[m^{-3}\cdot V^{-1}\right]$.

Definition at line 39 of file charge.cc.

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

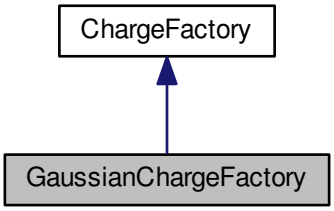
- DosExtraction/src/charge.h
- DosExtraction/src/charge.cc

## 7.11 GaussianChargeFactory Class Reference

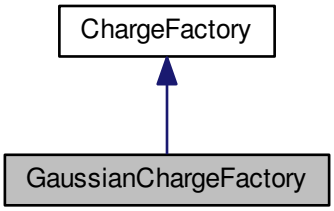
Concrete factory to handle a multiple gaussians DOS constitutive relation.

`#include <factory.h>`

Inheritance diagram for GaussianChargeFactory:




Collaboration diagram for GaussianChargeFactory:




### Public Member Functions

- GaussianChargeFactory ()=default

  *Default constructor (defaulted).*
- virtual ~GaussianChargeFactory ()=default

  *Destructor (defaulted).*
- virtual Charge * BuildCharge (const ParamList &, const QuadratureRule &) override

  *Factory method to build a concrete Charge object.*

## 7.11.1 Detailed Description

Concrete factory to handle a multiple gaussians DOS constitutive relation.

Definition at line 57 of file factory.h.

## 7.11.2 Member Function Documentation

### 7.11.2.1 Charge * BuildCharge ( const ParamList & *params*, const QuadratureRule & *rule* ) [override], [virtual]

Factory method to build a concrete Charge object.

**Parameters**

| | | |
|---|---|---|
| in | *params* | : a list of simulation parameters; |
| in | *rule* | : a quadrature rule. |

**Returns**

a pointer to GaussianCharge.

Implements ChargeFactory.

Definition at line 17 of file factory.cc.

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

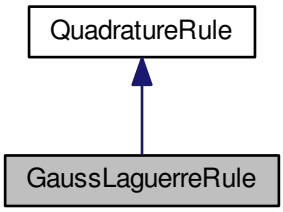
- DosExtraction/src/factory.h
- DosExtraction/src/factory.cc

## 7.12 GaussLaguerreRule Class Reference

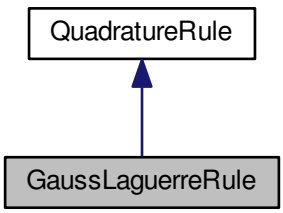
Class derived from QuadratureRule providing the Gauss-Laguerre quadrature rule.

`#include <quadratureRule.h>`

Inheritance diagram for GaussLaguerreRule:




Collaboration diagram for GaussLaguerreRule:



### Public Member Functions

- GaussLaguerreRule ()=delete

  *Default constructor (deleted since it is required to specify the number of nodes).*
- GaussLaguerreRule (const Index &)

  *Constructor.*
- virtual ~GaussLaguerreRule ()=default

  *Destructor (defaulted).*
- virtual void apply () override

  *Apply the quadrature rule in order to compute the nodes and weights.*
- virtual void apply (const GetPot &) override

  *Apply the quadrature rule reading parameters from a configuration file.*
- void apply_iterative_algorithm (const Index &=1000, const Real &=1.0e-14)

  *Compute nodes and weights using an adapted version of the algorithm presented in:*
  *William H. Press, Saul A. Teukolsky, William T. Vetterling, and Brian P. Flannery. 2007.*
  *Numerical Recipes: The Art of Scientific Computing (3rd edition).*
  *Cambridge University Press, New York, NY, USA.*
- void apply_using_eigendecomposition ()

  *Compute nodes and weights using an eigendecomposition-based algorithm.*

### Static Public Member Functions

- static Real log_gamma (const Real &)

  *Auxiliary function to compute* $\log\Gamma(x)$.

### Additional Inherited Members

## 7.12.1 Detailed Description

Class derived from QuadratureRule providing the Gauss-Laguerre quadrature rule.

Compute nodes and weights for the *nNodes_*-points approximation of:

$$\int_0^{+\infty} w(x) f(x)\, \mathrm{d}x$$

where $w(x) = e^{-x}$.

Definition at line 137 of file quadratureRule.h.

## 7.12.2 Constructor & Destructor Documentation

### 7.12.2.1 GaussLaguerreRule ( const Index & *nNodes* )

Constructor.

**Parameters**

| | | |
|---|---|---|
| in | *nNodes* | : the number of nodes to be used for the quadrature rule. |

Definition at line 148 of file quadratureRule.cc.

## 7.12.3 Member Function Documentation

### 7.12.3.1 Real log_gamma ( const Real & *x* ) [static]

Auxiliary function to compute $\log\Gamma(x)$.

**Parameters**

| | | |
|---|---|---|
| in | *x* | : the point to compute the function at. |

**Returns**

the natural logarithm of the gamma function evaluated at *x*.

Definition at line 151 of file quadratureRule.cc.

#### 7.12.3.2 void apply ( const GetPot & *config* ) [override], [virtual]

Apply the quadrature rule reading parameters from a configuration file.

**Parameters**

| | | |
|---|---|---|
| in | *config* | : the GetPot configuration object. |

Implements QuadratureRule.

Definition at line 184 of file quadratureRule.cc.

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

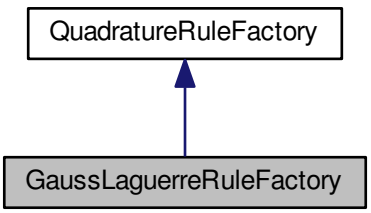
- DosExtraction/src/quadratureRule.h
- DosExtraction/src/quadratureRule.cc

## 7.13 GaussLaguerreRuleFactory Class Reference

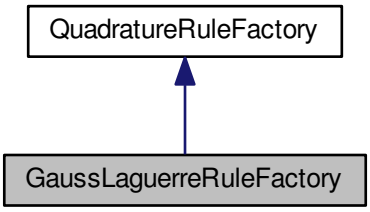
Concrete factory to handle a Gauss-Laguerre quadrature rule.

`#include <factory.h>`

Inheritance diagram for GaussLaguerreRuleFactory:



Collaboration diagram for GaussLaguerreRuleFactory:




## Public Member Functions

- GaussLaguerreRuleFactory ()=default

  *Default constructor (defaulted).*
- virtual ~GaussLaguerreRuleFactory ()=default

  *Destructor (defaulted).*
- virtual QuadratureRule * BuildRule (const Index &) override

  *Factory method to build a concrete QuadratureRule object.*

### 7.13.1 Detailed Description

Concrete factory to handle a Gauss-Laguerre quadrature rule.

Definition at line 163 of file factory.h.

### 7.13.2 Member Function Documentation

#### 7.13.2.1 QuadratureRule * BuildRule ( const Index & *nNodes* ) [override], [virtual]

Factory method to build a concrete QuadratureRule object.

**Parameters**

| | | |
|---|---|---|
| in | *nNodes* | : the number of nodes to be used for the quadrature rule. |

**Returns**

a pointer to GaussLaguerreRule.

Implements QuadratureRuleFactory.

Definition at line 32 of file factory.cc.

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

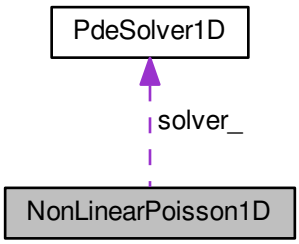
- DosExtraction/src/factory.h
- DosExtraction/src/factory.cc

## 7.14 NonLinearPoisson1D Class Reference

Provide a solver for a non-linear Poisson equation.

`#include <solvers.h>`

Collaboration diagram for NonLinearPoisson1D:




### Public Member Functions

- NonLinearPoisson1D ()=delete

  *Default constructor (deleted since it is required to specify the solver to be used).*
- NonLinearPoisson1D (const PdeSolver1D &, const Index &=100, const Real &=1.0e-6)

  *Constructor.*
- virtual ~NonLinearPoisson1D ()=default

  *Destructor (defaulted).*
- void apply (const VectorXr &, const VectorXr &, Charge &)

  *Apply a Newton method to the equation and then discretize it using the solver specified.*

#### Getter methods

- const VectorXr & **phi** () const
- const VectorXr & **norm** () const
- const Real & **qTot** () const
- const Real & **cTot** () const

### Private Member Functions

- SparseXr computeJac (const VectorXr &) const

  *Compute the Jacobi matrix.*

### Private Attributes

- const PdeSolver1D & solver_

  *Solver handler.*
- Index maxIterationsNo_

  *Maximum number of iterations.*
- Real tolerance_

*Tolerance.*

- VectorXr phi_

  *The electric potential.*

- VectorXr norm_

  *Vector holding $L^\infty$-norm errors for each iteration.*

- Real qTot_

  *Total charge.*

- Real cTot_

  *Total capacitance.*

### 7.14.1 Detailed Description

Provide a solver for a non-linear Poisson equation.

A Newton method is applied in order to solve:

$$-\frac{\mathrm{d}}{\mathrm{d}z}\left(\varepsilon(z)\cdot\frac{\mathrm{d}\varphi}{\mathrm{d}z}(z)\right)=-q\cdot\frac{N_0}{\sqrt{\pi}}\int_{-\infty}^{+\infty}\exp\left(-\alpha^2\right)\left(1+\exp\left(\frac{\sqrt{2}\sigma\alpha-q\varphi(z)}{K_B\cdot T}\right)\right)^{-1}\mathrm{d}\alpha\ .$$

Definition at line 194 of file solvers.h.

### 7.14.2 Constructor & Destructor Documentation

#### 7.14.2.1 NonLinearPoisson1D ( const PdeSolver1D & *solver*, const Index & *maxIterationsNo* = `100`, const Real & *tolerance* = `1.0e-6` )

Constructor.

**Parameters**

| | | |
|---|---|---|
| in | *solver* | : the solver to be used; |
| in | *maxIterationsNo* | : maximum number of iterations desired; |
| in | *tolerance* | : tolerance desired. |

Definition at line 204 of file solvers.cc.

### 7.14.3 Member Function Documentation

#### 7.14.3.1 void apply ( const VectorXr & *mesh*, const VectorXr & *init_guess*, Charge & *charge_fun* )

Apply a Newton method to the equation and then discretize it using the solver specified.

**Parameters**

| | | |
|---|---|---|
| in | *mesh* | : the mesh; |
| in | *init_guess* | : initial guess for the Newton algorithm; |
| in | *charge_fun* | : an object of class Charge specifying how to compute total electric charge. |

Definition at line 211 of file solvers.cc.

#### 7.14.3.2 SparseXr computeJac ( const VectorXr & *x* ) const [private]

Compute the Jacobi matrix.

**Parameters**

| | | |
|---|---|---|
| in | *x* | : the vector where to start from. |

**Returns**

the Jacobi matrix in a sparse format.

Definition at line 332 of file solvers.cc.

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

- DosExtraction/src/solvers.h
- DosExtraction/src/solvers.cc

## 7.15 ParamList Class Reference

Class providing methods to handle a list of parameters.

`#include <paramList.h>`

### Public Member Functions

- ParamList ()=default

  *Default constructor (defaulted).*
- ParamList (const RowVectorXr &)

  *Explicit conversion constructor.*
- virtual ~ParamList ()=default

  *Destructor (defaulted).*

#### Getter methods

- const Index & **simulationNo** () const
- const Real & **t_semic** () const
- const Real & **t_ins** () const
- const Real & **eps_semic** () const
- const Real & **eps_ins** () const
- const Real & **Wf** () const
- const Real & **Ea** () const
- const Real & **N0** () const
- const Real & **sigma** () const
- const Real & **N0_2** () const
- const Real & **sigma_2** () const
- const Real & **shift_2** () const
- const Real & **N0_3** () const
- const Real & **sigma_3** () const
- const Real & **shift_3** () const
- const Real & **N0_4** () const
- const Real & **sigma_4** () const
- const Real & **shift_4** () const
- const Real & **N0_exp** () const
- const Real & **lambda_exp** () const
- const Real & **A_semic** () const
- const Real & **C_sb** () const
- const Index & **nNodes** () const
- const Index & **nSteps** () const
- const Real & **V_min** () const
- const Real & **V_max** () const

## Private Attributes

- Index simulationNo_
  *Simulation number index.*
- Real t_semic_
  *Thickness of the semiconductor layer* $[m]$.
- Real t_ins_
  *Thickness of the insulator layer* $[m]$.
- Real eps_semic_
  *Relative electrical permittivity of the semiconductor layer* [ ].
- Real eps_ins_
  *Relative electrical permittivity of the insulator layer* [ ].
- Real Wf_
  *Work-function (normalized by* $Q$*)* $[V]$.
- Real Ea_
  *Electron affinity (normalized by* $Q$*)* $[V]$.
- Real N0_
  *1st gaussian* $N_0$ $\left[m^{-3}\right]$.
- Real sigma_
  *1st gaussian standard deviation* $\sigma$ *(normalized by* $K_B \cdot T$*)* [ ].
- Real N0_2_
  *2nd gaussian* $N_0$ $\left[m^{-3}\right]$.
- Real sigma_2_
  *2nd gaussian standard deviation* $\sigma$ *(normalized by* $K_B \cdot T$*)* [ ].
- Real shift_2_
  *2nd gaussian shift with respect to the 1st gaussian electric potential (normalized by* $-Q$*)* $[V]$.
- Real N0_3_
  *3rd gaussian* $N_0$ $\left[m^{-3}\right]$.
- Real sigma_3_
  *3rd gaussian standard deviation* $\sigma$ *(normalized by* $K_B \cdot T$*)* [ ].
- Real shift_3_
  *3rd gaussian shift with respect to the 1st gaussian electric potential (normalized by* $-Q$*)* $[V]$.
- Real N0_4_
  *4th gaussian* $N_0$ $\left[m^{-3}\right]$.
- Real sigma_4_
  *4th gaussian standard deviation* $\sigma$ *(normalized by* $K_B \cdot T$*)* [ ].
- Real shift_4_
  *4th gaussian shift with respect to the 1st gaussian electric potential (normalized by* $-Q$*)* $[V]$.
- Real N0_exp_
  *Exponential* $N_0$ $\left[m^{-3}\right]$.
- Real lambda_exp_
  *Exponential* $\lambda$ *(normalized by* $K_B \cdot T$*)* [ ].
- Real A_semic_
  *Area of the semiconductor* $\left[m^2\right]$.
- Real C_sb_
  *Equivalent capacitance of the series semiconductor-insulator (stray-border capacitance)* $[F]$.
- Index nNodes_
  *Number of nodes that form the mesh.*
- Index nSteps_
  *Number of steps to simulate.*
- Real V_min_
  *Minimum voltage* $[V]$.
- Real V_max_
  *Maximum voltage* $[V]$.

### Friends

- class **GaussianCharge**
- class **ExponentialCharge**
- class **DosModel**

### 7.15.1 Detailed Description

Class providing methods to handle a list of parameters.

It can include up to 4 gaussians (later combined to compute total charge) and an exponential.

Definition at line 30 of file paramList.h.

### 7.15.2 Constructor & Destructor Documentation

#### 7.15.2.1 ParamList ( const RowVectorXr & *list* ) [explicit]

Explicit conversion constructor.

**Parameters**

| | | |
|---|---|---|
| in | *list* | : a row vector containing a list of parameters (for example got by a CsvParser object). Parameters should be sorted in the same order as specified above. |

Definition at line 19 of file paramList.cc.

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

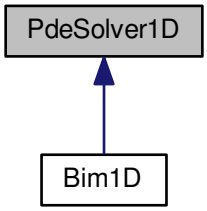
- DosExtraction/src/paramList.h
- DosExtraction/src/paramList.cc

## 7.16 PdeSolver1D Class Reference

Abstract class providing methods to assemble matrices to solve one-dimensional PDEs.

`#include <solvers.h>`

Inheritance diagram for PdeSolver1D:




### Public Member Functions

- PdeSolver1D ()=delete

*Default constructor (deleted since it is required to specify the mesh).*

- PdeSolver1D (VectorXr &)

  *Constructor.*

- virtual ~PdeSolver1D ()=default

  *Destructor (defaulted).*

- virtual void assembleAdvDiff (const VectorXr &alpha, const VectorXr &gamma, const VectorXr &eta, const VectorXr &beta)=0

  *Assemble the matrix for an advection-diffusion term.*

- virtual void assembleStiff (const VectorXr &eps, const VectorXr &kappa)=0

  *Assemble the matrix for a diffusion term.*

- virtual void assembleMass (const VectorXr &delta, const VectorXr &zeta)=0

  *Assemble the matrix for a reaction term.*

**Getter methods**

- const SparseXr & **AdvDiff** () const
- const SparseXr & **Stiff** () const
- const SparseXr & **Mass** () const

## Protected Attributes

- VectorXr mesh_

  *The mesh.*

- Index nNodes_

  *Number of nodes that form the mesh.*

- SparseXr AdvDiff_

  *Matrix for an advection-diffusion term.*

- SparseXr Stiff_

  *Stiffness matrix.*

- SparseXr Mass_

  *Mass matrix.*

## Friends

- class **NonLinearPoisson1D**

### 7.16.1 Detailed Description

Abstract class providing methods to assemble matrices to solve one-dimensional PDEs.

Matrices are held in a sparse format.

Definition at line 36 of file solvers.h.

### 7.16.2 Constructor & Destructor Documentation

#### 7.16.2.1 PdeSolver1D ( VectorXr & *mesh* )

Constructor.

**Parameters**

| | | |
|---|---|---|
| in | *mesh* | : the mesh. |

Definition at line 17 of file solvers.cc.

### 7.16.3 Member Function Documentation

#### 7.16.3.1 virtual void assembleAdvDiff ( const VectorXr & *alpha,* const VectorXr & *gamma,* const VectorXr & *eta,* const VectorXr & *beta* ) [pure virtual]

Assemble the matrix for an advection-diffusion term.

Build the matrix for the advection-diffusion problem: $-\nabla \cdot (\alpha \cdot \gamma(\eta \nabla u - \beta u)) = f$.

**Parameters**

| | | |
|---|---|---|
| in | *alpha* | : $\alpha$, an element-wise constant function; |
| in | *gamma* | : $\gamma$, an element-wise linear function; |
| in | *eta* | : $\eta$, an element-wise linear function; |
| in | *beta* | : $\beta$, an element-wise constant function. |

Implemented in Bim1D.

#### 7.16.3.2 virtual void assembleStiff ( const VectorXr & *eps,* const VectorXr & *kappa* ) [pure virtual]

Assemble the matrix for a diffusion term.

Build the matrix for the diffusion problem: $-\nabla \cdot (\varepsilon \cdot \kappa \nabla u) = f$.

**Parameters**

| | | |
|---|---|---|
| in | *eps* | : $\varepsilon$, an element-wise constant function; |
| in | *kappa* | : $\kappa$, an element-wise linear function. |

Implemented in Bim1D.

#### 7.16.3.3 virtual void assembleMass ( const VectorXr & *delta,* const VectorXr & *zeta* ) [pure virtual]

Assemble the matrix for a reaction term.

Build the mass matrix for the reaction problem: $\delta \cdot \zeta u = f$.

**Parameters**

| | | |
|---|---|---|
| in | *delta* | : $\delta$, an element-wise constant function; |
| in | *zeta* | : $\zeta$, an element-wise linear function. |

Implemented in Bim1D.

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

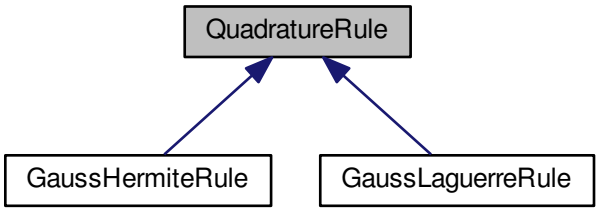
- DosExtraction/src/solvers.h
- DosExtraction/src/solvers.cc

## 7.17 QuadratureRule Class Reference

Abstract class providing a quadrature rule.

`#include <quadratureRule.h>`

Inheritance diagram for QuadratureRule:




## Public Member Functions

- QuadratureRule ()=delete

  *Default constructor (deleted since it is required to specify the number of nodes).*
- QuadratureRule (const Index &)

  *Constructor.*
- virtual ~QuadratureRule ()=default

  *Destructor (defaulted).*
- virtual void apply ()=0

  *Apply the quadrature rule in order to compute the nodes and weights.*
- virtual void apply (const GetPot &config)=0

  *Apply the quadrature rule reading parameters from a configuration file.*

### Getter methods

- const Index & **nNodes** () const
- const VectorXr & **nodes** () const
- const VectorXr & **weights** () const

## Protected Attributes

- Index nNodes_

  *Number of nodes of quadrature.*
- VectorXr nodes_

  *Vector containing the computed nodes coordinates.*
- VectorXr weights_

  *Vector containing the computed weights.*

## Friends

- class **GaussianCharge**
- class **ExponentialCharge**

### 7.17.1 Detailed Description

Abstract class providing a quadrature rule.

Approximate the integral:

$$\int_a^b f(x)\,\mathrm{d}x$$

with the finite sum:

$$\sum_{i=1}^{nNodes\_} w_i \cdot f(x_i)$$

where $\{x_i\}_{i=1}^{nNodes\_}$ and $\{w_i\}_{i=1}^{nNodes\_}$ are called respectively nodes and weights.

Definition at line 34 of file quadratureRule.h.

### 7.17.2 Constructor & Destructor Documentation

#### 7.17.2.1 QuadratureRule ( const Index & *nNodes* )

Constructor.

**Parameters**

| | | |
|---|---|---|
| in | *nNodes* | : the number of nodes to be used for the quadrature rule. |

Definition at line 19 of file quadratureRule.cc.

### 7.17.3 Member Function Documentation

#### 7.17.3.1 virtual void apply ( const GetPot & *config* ) [pure virtual]

Apply the quadrature rule reading parameters from a configuration file.

**Parameters**

| | | |
|---|---|---|
| in | *config* | : the GetPot configuration object. |

Implemented in GaussLaguerreRule, and GaussHermiteRule.

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

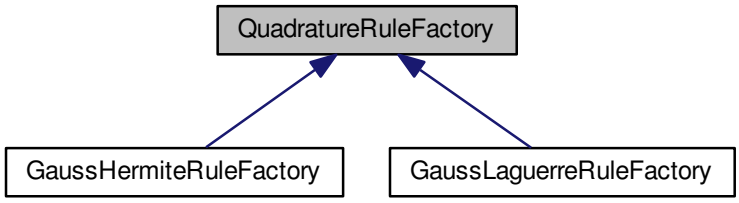
- DosExtraction/src/quadratureRule.h
- DosExtraction/src/quadratureRule.cc

## 7.18 QuadratureRuleFactory Class Reference

Abstract factory to handle a quadrature rule.

`#include <factory.h>`

Inheritance diagram for QuadratureRuleFactory:




## Public Member Functions

- QuadratureRuleFactory ()=default

  *Default constructor (defaulted).*
- virtual ~QuadratureRuleFactory ()=default

  *Destructor (defaulted).*
- virtual QuadratureRule * BuildRule (const Index &nNodes)=0

  *Factory method to build an abstract QuadratureRule object.*

### 7.18.1 Detailed Description

Abstract factory to handle a quadrature rule.

Definition at line 111 of file factory.h.

### 7.18.2 Member Function Documentation

#### 7.18.2.1 virtual QuadratureRule* BuildRule ( const Index & *nNodes* ) [pure virtual]

Factory method to build an abstract QuadratureRule object.

**Parameters**

| | | |
|---|---|---|
| in | *nNodes* | : the number of nodes to be used for the quadrature rule. |

**Returns**

a pointer to QuadratureRule.

Implemented in GaussLaguerreRuleFactory, and GaussHermiteRuleFactory.

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

- DosExtraction/src/factory.h

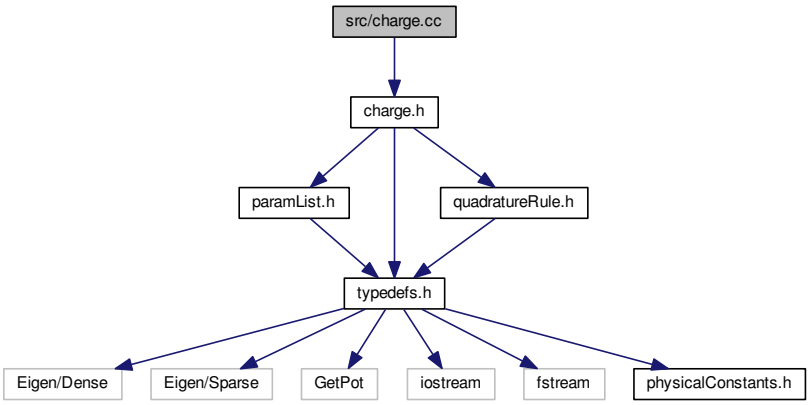
# Chapter 8

# File Documentation

## 8.1 DosExtraction/src/charge.cc File Reference

```
#include "charge.h"
```

Include dependency graph for charge.cc:




### 8.1.1 Detailed Description

**Author**

Pasquale Claudio Africa pasquale.africa@gmail.com

**Date**

2014

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**Copyright**



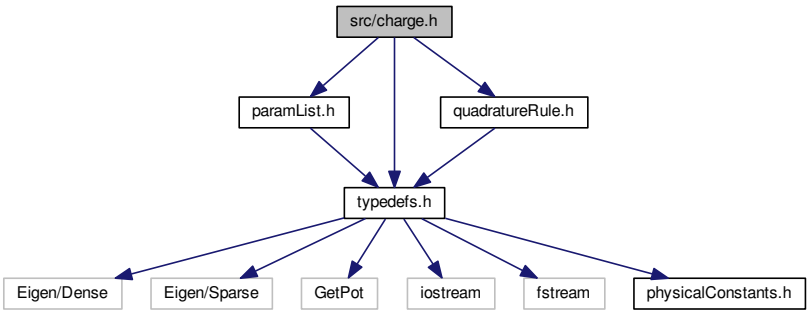
Definition in file charge.cc.

## 8.2 DosExtraction/src/charge.h File Reference

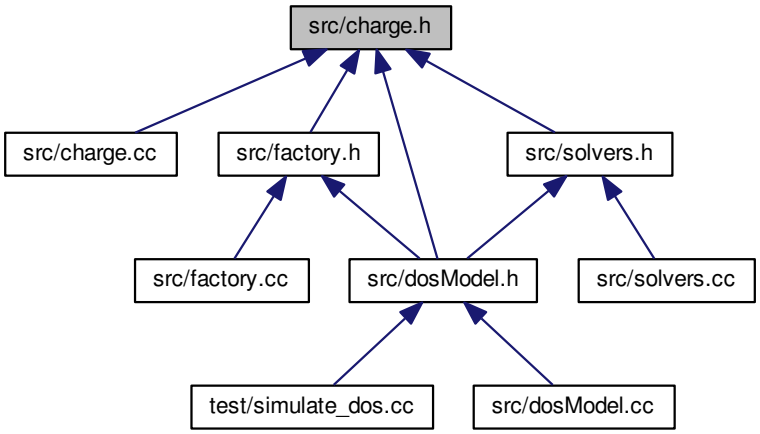
Classes for computing total electric charge.

```
#include "paramList.h"
#include "quadratureRule.h"
#include "typedefs.h"
```

Include dependency graph for charge.h:




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




### Classes

- class Charge

  *Abstract class providing methods to calculate total electric charge (the rhs in the Poisson equation).*
- class GaussianCharge

  *Class derived from Charge, under the hypothesis that Density of States is a combination of gaussians.*
- class ExponentialCharge

  *Class derived from Charge, under the hypothesis that Density of States is a single exponential.*

### 8.2.1 Detailed Description

Classes for computing total electric charge.

**Author**

Pasquale Claudio Africa pasquale.africa@gmail.com

**Date**

2014

This file is part of the "DosExtraction" project.

**Copyright**

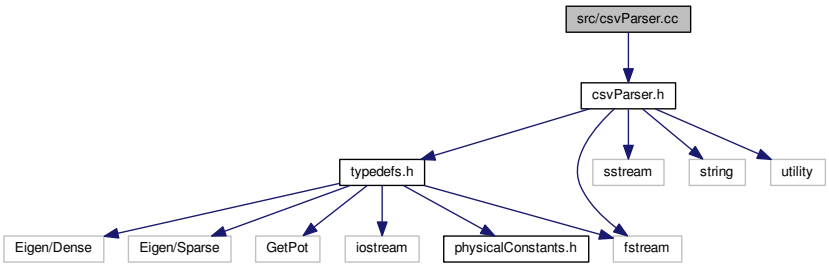


Definition in file charge.h.

## 8.3 DosExtraction/src/csvParser.cc File Reference

```
#include "csvParser.h"
```

Include dependency graph for csvParser.cc:




### 8.3.1 Detailed Description

**Author**

Pasquale Claudio Africa pasquale.africa@gmail.com

**Date**

2014

This file is part of the "DosExtraction" project.

**Copyright**



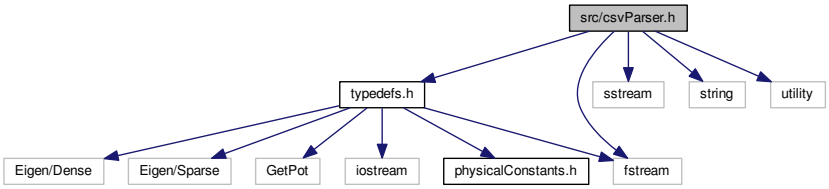
Definition in file csvParser.cc.

## 8.4 DosExtraction/src/csvParser.h File Reference

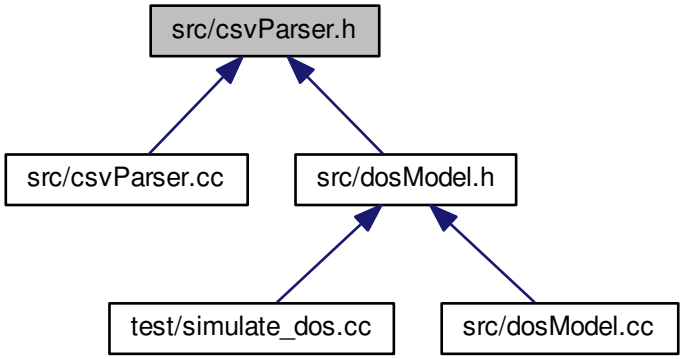
Tools to store content from a .csv file in matrices or vectors.

```
#include "typedefs.h"
#include <fstream>
#include <sstream>
#include <string>
#include <utility>
```

Include dependency graph for csvParser.h:




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




### Classes

- class CsvParser

  *Class providing methods to read **numeric** content from a .csv file and to store it in Eigen matrices or vectors.*

### 8.4.1 Detailed Description

Tools to store content from a .csv file in matrices or vectors.

**Author**

Pasquale Claudio Africa pasquale.africa@gmail.com

**Date**

2014

This file is part of the "DosExtraction" project.

**Copyright**

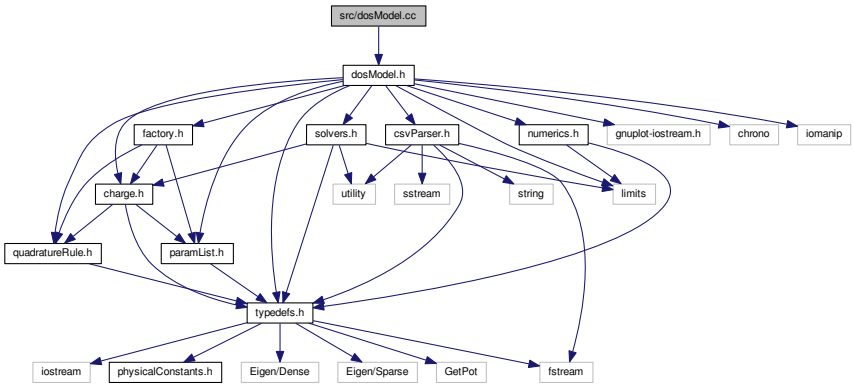


Definition in file csvParser.h.

## 8.5 DosExtraction/src/dosModel.cc File Reference

```
#include "dosModel.h"
```

Include dependency graph for dosModel.cc:




### 8.5.1 Detailed Description

**Author**

Pasquale Claudio Africa pasquale.africa@gmail.com

**Date**

2014

This file is part of the "DosExtraction" project.

**Copyright**



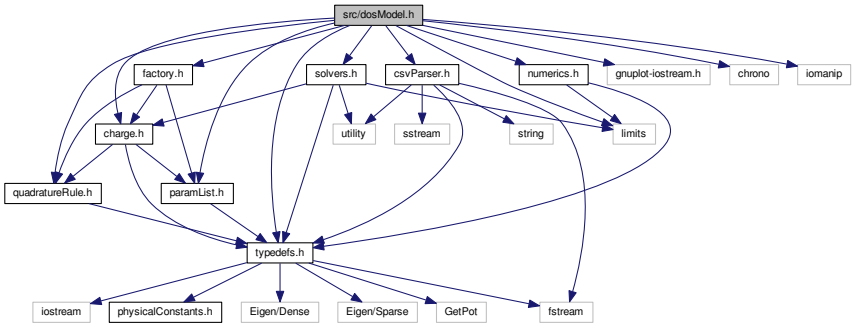
Definition in file dosModel.cc.

## 8.6 DosExtraction/src/dosModel.h File Reference

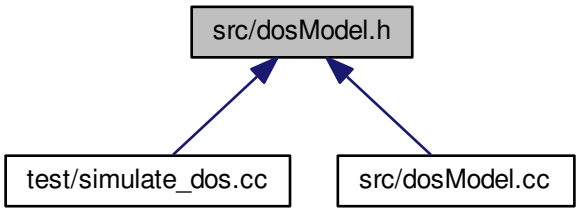
Mathematical model for Density of States extraction.

```
#include "charge.h"
#include "csvParser.h"
#include "factory.h"
#include "numerics.h"
#include "paramList.h"
#include "quadratureRule.h"
#include "solvers.h"
#include "typedefs.h"
#include "gnuplot-iostream.h"
#include <chrono>
#include <iomanip>
#include <limits>
```

Include dependency graph for dosModel.h:




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




### Classes

- class DosModel

  *Class providing methods to process a simulation to extract the Density of States starting from a parameter list.*

### 8.6.1 Detailed Description

Mathematical model for Density of States extraction.

**Author**

Pasquale Claudio Africa pasquale.africa@gmail.com

**Date**

2014

This file is part of the "DosExtraction" project.

**Copyright**

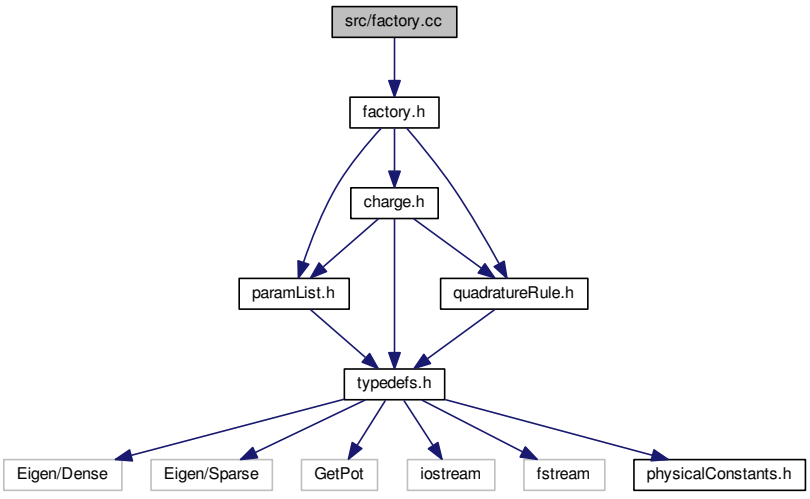


Definition in file dosModel.h.

## 8.7 DosExtraction/src/factory.cc File Reference

```
#include "factory.h"
```

Include dependency graph for factory.cc:




### 8.7.1 Detailed Description

**Author**

Pasquale Claudio Africa pasquale.africa@gmail.com

**Date**

2014

This file is part of the "DosExtraction" project.

**Copyright**



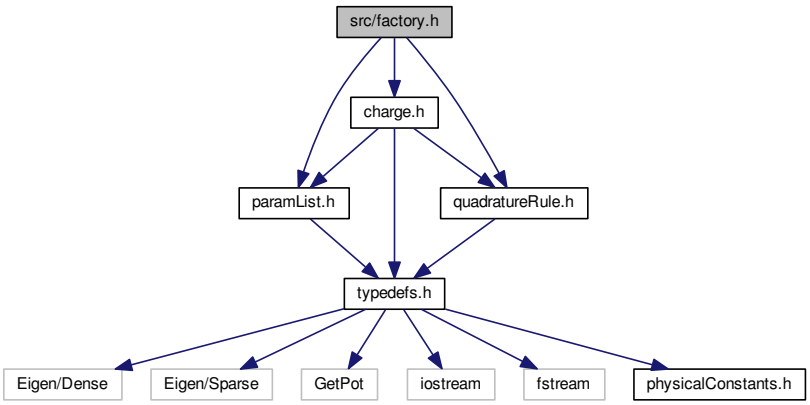
Definition in file factory.cc.

## 8.8 DosExtraction/src/factory.h File Reference

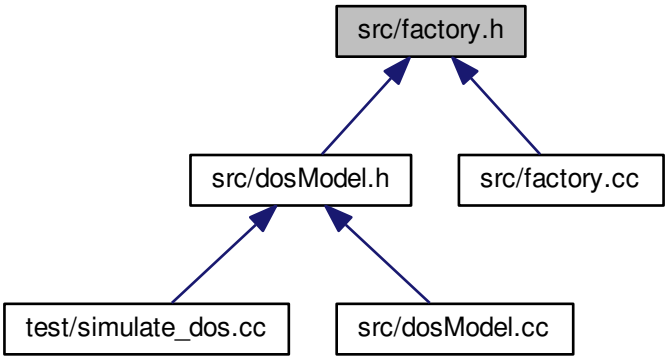
Abstract factory design patterns.

```
#include "charge.h"
#include "paramList.h"
#include "quadratureRule.h"
```

Include dependency graph for factory.h:



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




## Classes

- class ChargeFactory

  *Abstract factory to handle the constitutive relation for the Density of States.*
- class GaussianChargeFactory

  *Concrete factory to handle a multiple gaussians DOS constitutive relation.*
- class ExponentialChargeFactory

  *Concrete factory to handle a single exponential DOS constitutive relation.*
- class QuadratureRuleFactory

  *Abstract factory to handle a quadrature rule.*
- class GaussHermiteRuleFactory

  *Concrete factory to handle a Gauss-Hermite quadrature rule.*
- class GaussLaguerreRuleFactory

  *Concrete factory to handle a Gauss-Laguerre quadrature rule.*

### 8.8.1 Detailed Description

Abstract factory design patterns.

**Author**

Pasquale Claudio Africa pasquale.africa@gmail.com

**Date**

2014

This file is part of the "DosExtraction" project.

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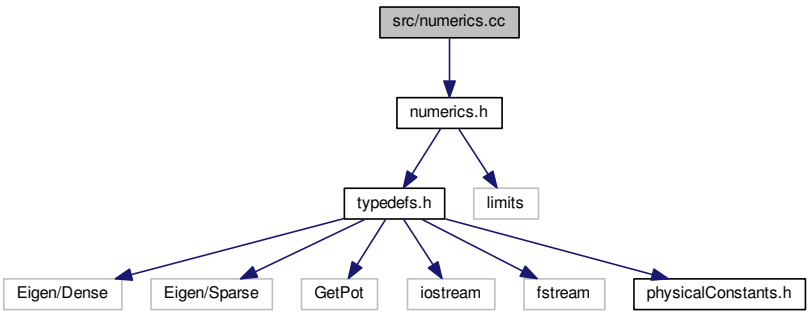
Definition in file factory.h.

## 8.9 DosExtraction/src/numerics.cc File Reference

```
#include "numerics.h"
```

Include dependency graph for numerics.cc:




### 8.9.1 Detailed Description

**Author**

Pasquale Claudio Africa pasquale.africa@gmail.com

**Date**

2014

This file is part of the "DosExtraction" project.

**Copyright**



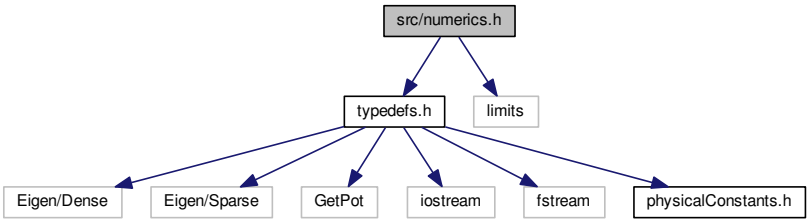
Definition in file numerics.cc.

## 8.10 DosExtraction/src/numerics.h File Reference

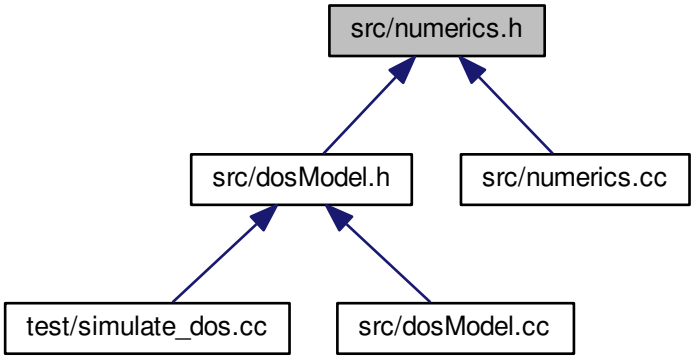
Generic numeric algorithms.

```
#include "typedefs.h"
#include <limits>
```

Include dependency graph for numerics.h:




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




## Namespaces

- numerics

  *Namespace for generic numeric algorithms.*

## Functions

- template<typename ScalarType >
  VectorX< ScalarType > sort (const VectorX< ScalarType > &vector)

  *Function to sort Eigen vectors.*
- template<typename ScalarType >
  VectorXpair< ScalarType > sort_pair (const VectorX< ScalarType > &vector)

  *Function to sort Eigen vectors, keeping track of indexes.*
- Real trapz (const VectorXr &x, const VectorXr &y)

  *Function to compute approximate integral of y with spacing increment specified by x, using trapezoidal rule.*
- Real trapz (const VectorXr &y)

  *Compute the approximate integral of y with unit spacing, using trapezoidal rule.*
- VectorXr deriv (const VectorXr &, const VectorXr &)

*Compute the numeric derivative:* $\frac{dy}{dx}$.

- Real interp1 (const VectorXr &, const VectorXr &, const Real &)

  *Linear 1D interpolation. Interpolate y, defined at points x, at the point xNew.*
- VectorXr interp1 (const VectorXr &, const VectorXr &, const VectorXr &)

  *Linear 1D interpolation. Interpolate y, defined at points x, at the points xNew.*
- Real error_L2 (const VectorXr &, const VectorXr &, const VectorXr &, const Real &)

  *Compute the* $L^2$*-norm error between simulated and interpolated values, using trapz.*

### 8.10.1 Detailed Description

Generic numeric algorithms.

**Author**

Pasquale Claudio Africa pasquale.africa@gmail.com

**Date**

2014

This file is part of the "DosExtraction" project.

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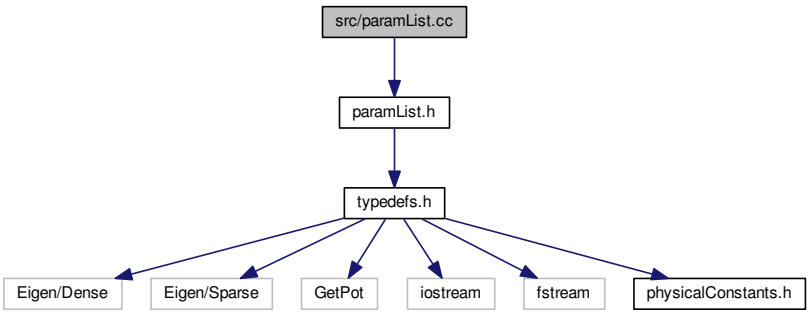
Definition in file numerics.h.

## 8.11 DosExtraction/src/paramList.cc File Reference

```
#include "paramList.h"
```

Include dependency graph for paramList.cc:




### 8.11.1 Detailed Description

**Author**

Pasquale Claudio Africa pasquale.africa@gmail.com

**Date**

2014

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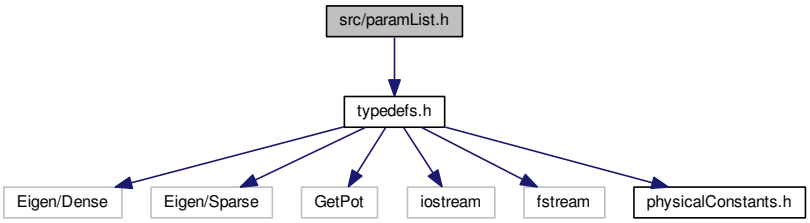
Definition in file paramList.cc.

## 8.12 DosExtraction/src/paramList.h File Reference

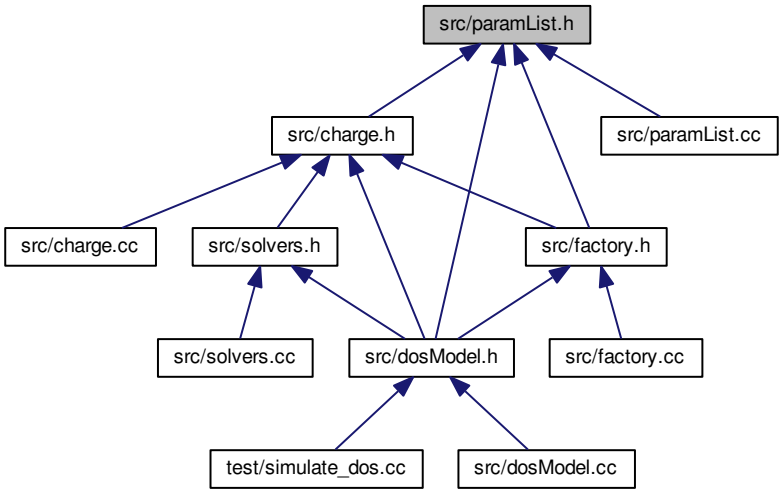
Interface to process a list of simulation parameters.

```
#include "typedefs.h"
```

Include dependency graph for paramList.h:



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




### Classes

- class ParamList

  *Class providing methods to handle a list of parameters.*

### 8.12.1 Detailed Description

Interface to process a list of simulation parameters.

**Author**

Pasquale Claudio Africa pasquale.africa@gmail.com

**Date**

2014

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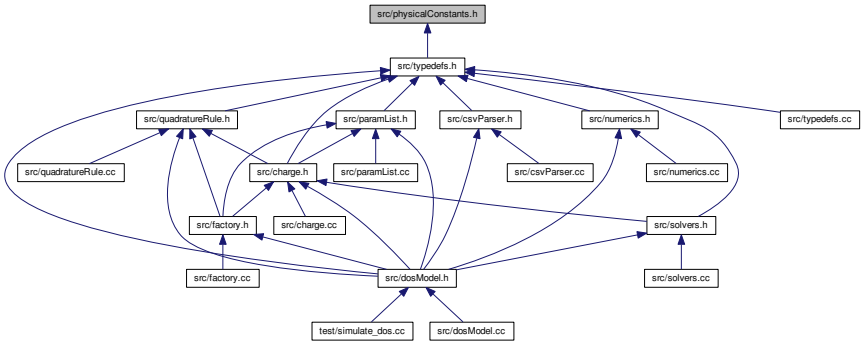
Definition in file paramList.h.

## 8.13 DosExtraction/src/physicalConstants.h File Reference

Physical constants.

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




## Namespaces

- constants

  *Numerical constants.*

## Variables

- const Real Q = 1.60217653000000e-19

  *Electron charge* $[C]$.
- const Real Q2 = Q ∗ Q

  *Electron charge squared* $\left[C^2\right]$.
- const Real K_B = 1.38065050000000e-23

  *Boltzmann's constant* $\left[J \cdot K^{-1}\right]$.
- const Real EPS0 = 8.854187817e-12

  *Vacuum electrical permittivity* $\left[C \cdot V^{-1} \cdot m^{-1}\right]$.
- const Real T = 300

  *Reference temperature* $[K]$.
- const Real V_TH = K_B ∗ T / Q

  *Treshold voltage* $[V]$.

### 8.13.1 Detailed Description

Physical constants.

**Author**

Pasquale Claudio Africa pasquale.africa@gmail.com

**Date**

2014

This file is part of the "DosExtraction" project.

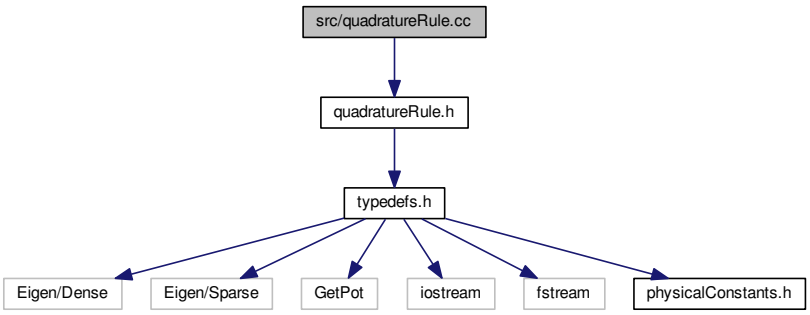
**Copyright**



Definition in file physicalConstants.h.

## 8.14 DosExtraction/src/quadratureRule.cc File Reference

```
#include "quadratureRule.h"
```
Include dependency graph for quadratureRule.cc:




### 8.14.1 Detailed Description

**Author**

Pasquale Claudio Africa pasquale.africa@gmail.com

**Date**

2014

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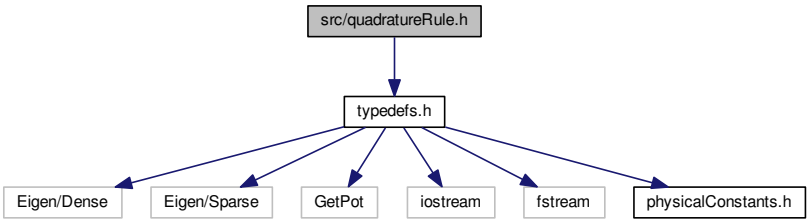
Definition in file quadratureRule.cc.

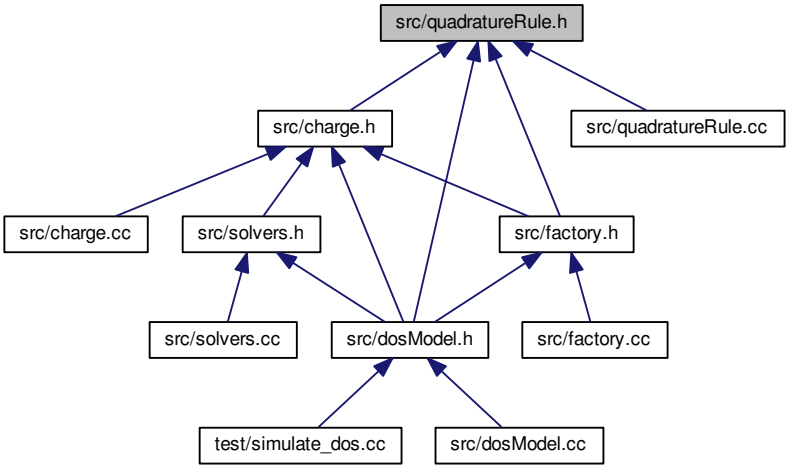
## 8.15 DosExtraction/src/quadratureRule.h File Reference

Quadrature rules.

```
#include "typedefs.h"
```
Include dependency graph for quadratureRule.h:



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




## Classes

- class QuadratureRule

  *Abstract class providing a quadrature rule.*
- class GaussHermiteRule

  *Class derived from QuadratureRule providing the Gauss-Hermite quadrature rule.*
- class GaussLaguerreRule

  *Class derived from QuadratureRule providing the Gauss-Laguerre quadrature rule.*

### 8.15.1 Detailed Description

Quadrature rules.

**Author**

Pasquale Claudio Africa pasquale.africa@gmail.com

**Date**

2014

This file is part of the "DosExtraction" project.

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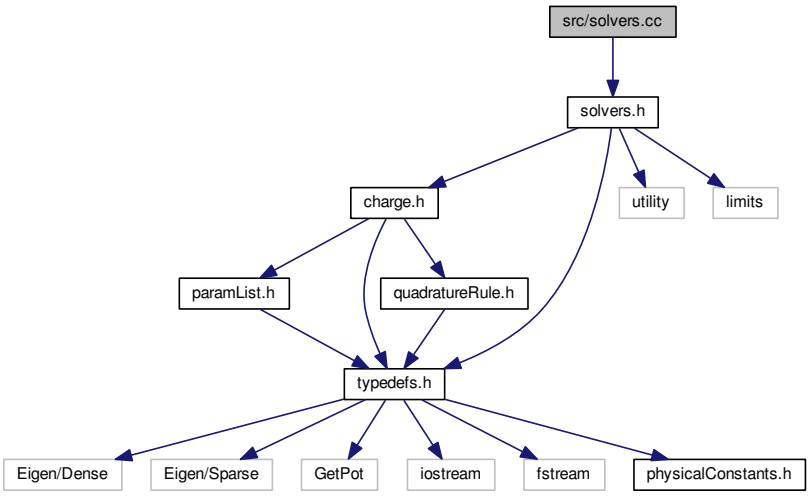
Definition in file quadratureRule.h.

## 8.16 DosExtraction/src/solvers.cc File Reference

```
#include "solvers.h"
```

Include dependency graph for solvers.cc:




### 8.16.1 Detailed Description

**Author**

Pasquale Claudio Africa pasquale.africa@gmail.com

**Date**

2014

This file is part of the "DosExtraction" project.

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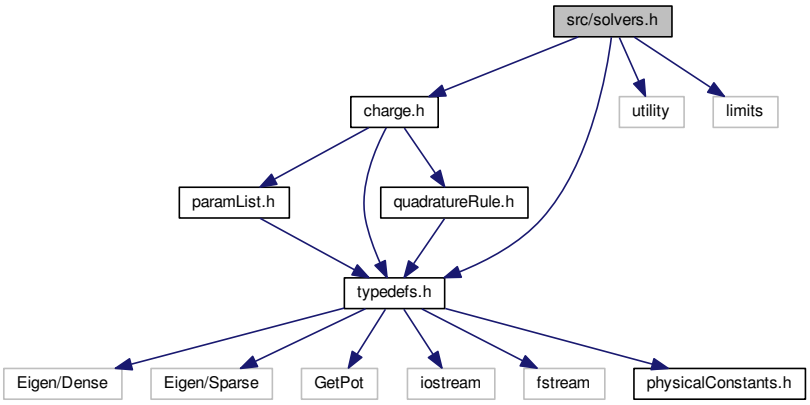
Definition in file solvers.cc.

## 8.17 DosExtraction/src/solvers.h File Reference

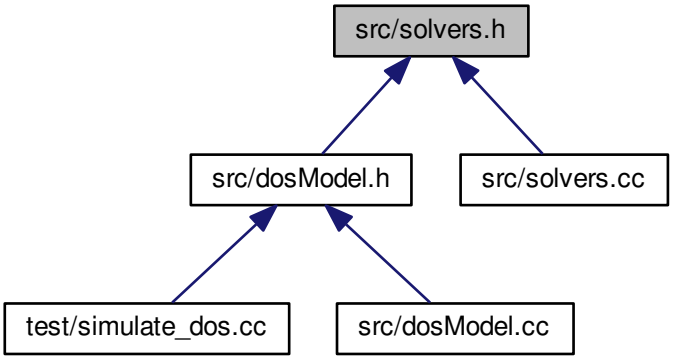
Generic solvers for PDEs.

```
#include "charge.h"
#include "typedefs.h"
#include <utility>
#include <limits>
```

Include dependency graph for solvers.h:




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




## Classes

- class PdeSolver1D

  *Abstract class providing methods to assemble matrices to solve one-dimensional PDEs.*
- class Bim1D

  *Class derived from PdeSolver1D, providing a finite volume Box Integration Method (BIM) solver.*
- class NonLinearPoisson1D

  *Provide a solver for a non-linear Poisson equation.*

### 8.17.1 Detailed Description

Generic solvers for PDEs.

**Author**

Pasquale Claudio Africa pasquale.africa@gmail.com

**Date**

2014

This file is part of the "DosExtraction" project.

**Copyright**

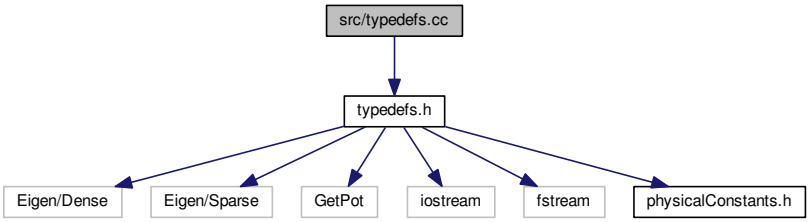


Definition in file solvers.h.

## 8.18 DosExtraction/src/typedefs.cc File Reference

```
#include "typedefs.h"
```

Include dependency graph for typedefs.cc:




### 8.18.1 Detailed Description

**Author**

Pasquale Claudio Africa pasquale.africa@gmail.com

**Date**

2014

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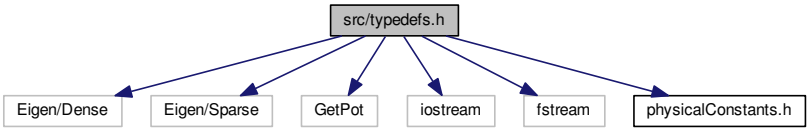
Definition in file typedefs.cc.

## 8.19 DosExtraction/src/typedefs.h File Reference

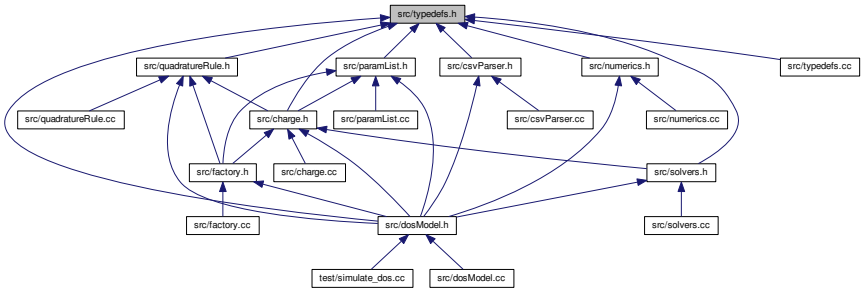
Typedefs and utility functions.

```
#include <Eigen/Dense>
#include <Eigen/Sparse>
#include "GetPot"
#include <iostream>
#include <fstream>
#include "physicalConstants.h"
```

Include dependency graph for typedefs.h:




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




### Namespaces

- constants

  *Numerical constants.*
- utility

  *Namespace for utilities and auxiliary functions.*

### Macros

- #define Real double

  *Pre-processor macro for real numbers.*
- #define Index ptrdiff_t

  *Pre-processor macro for indexing variables.*

### Typedefs

- typedef Matrix< Real, Dynamic, Dynamic > MatrixXr

*Typedef for dense real-valued dynamic-sized matrices.*

- typedef Matrix< Real, Dynamic, 1 > VectorXr

  *Typedef for dense real-valued dynamic-sized column vectors.*
- typedef Matrix< Real, 1, Dynamic > RowVectorXr

  *Typedef for dense real-valued dynamic-sized row vectors.*
- typedef SparseMatrix< Real > SparseXr

  *Typedef for sparse real-valued dynamic-sized matrices.*
- template<typename ScalarType >
  using VectorX = Matrix< ScalarType, Dynamic, 1 >

  *Template alias for Eigen vectors.*
- template<typename T >
  using VectorXpair = VectorX< std::pair< T, Index > >

  *Template alias for an Eigen vector of pairs: (ScalarType, Index).*

## Functions

- std::string full_path (const std::string &, const std::string &)

  *Auxiliary function to return the full path to a file.*
- void print_block (const char *, std::ostream &=std::cout)

  *Auxiliary function to print a string inside a block.*
- void print_done (std::ostream &=std::cout)

  *Auxiliary function to print a "DONE!" string.*

## Variables

- const Index PARAMS_NO = 26

  *Number of parameters required in input file.*
- const Real PI = M_PI

  $\pi$.
- const Real SQRT_PI = std::sqrt(PI)

  $\sqrt{\pi}$.
- const Real PI_M4 = 0.7511255444649425

  $\pi^{-\frac{1}{4}}$.
- const Real SQRT_2 = std::sqrt(2)

  $\sqrt{2}$.

### 8.19.1 Detailed Description

Typedefs and utility functions.

**Author**

Pasquale Claudio Africa pasquale.africa@gmail.com

**Date**

2014

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Definition in file typedefs.h.

### 8.19.2 Typedef Documentation

#### 8.19.2.1 using VectorX = Matrix<ScalarType, Dynamic, 1>

Template alias for Eigen vectors.

**Template Parameters**

| | |
|---|---|
| *ScalarType* | : the scalar type. |

Definition at line 46 of file typedefs.h.

#### 8.19.2.2 using VectorXpair = VectorX<std::pair<T, Index> >

Template alias for an Eigen vector of pairs: (*ScalarType*, *Index*).

**Template Parameters**

| | |
|---|---|
| *ScalarType* | : the scalar type. |

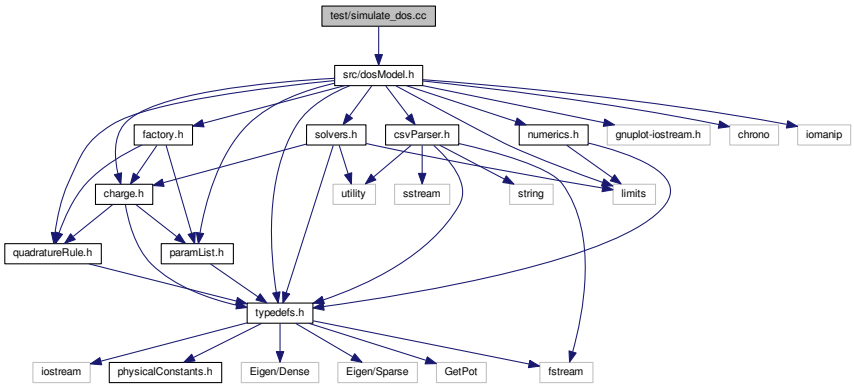
Definition at line 53 of file typedefs.h.

## 8.20 DosExtraction/test/simulate_dos.cc File Reference

A test file.

```
#include "src/dosModel.h"
```

Include dependency graph for simulate_dos.cc:




### Functions

- int main (const int argc, const char *const *argv, const char *const *envp)

  *The **main** function.*

### 8.20.1 Detailed Description

A test file.

**Author**

Pasquale Claudio Africa pasquale.africa@gmail.com

**Date**

2014

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Definition in file simulate_dos.cc.

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