# Garfield++ User Guide



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# 1. Introduction

Garfield++ is an object-oriented toolkit for the detailed simulation of particle detectors that use a gas mixture or a semiconductor material as sensitive medium.

For calculating electric fields, three techniques are currently being offered:

- solutions in the thin-wire limit for devices made of wires and planes;
- interfaces with finite element programs, which can compute approximate fields in nearly arbitrary two- and three-dimensional configurations with dielectrics and conductors;
- an interface with the Synopsys Sentaurus device simulation program [19].

In the future, an interface to the neBEM field solver [11, 12] (which already exists for Garfield [21]), should be made available.

For calculating the transport properties of electrons in gas mixtures, an interface to the "Magboltz" program [2, 3] is available.

The ionization pattern produced along the track of relativistic charged particles can be simulated using the program "Heed" [18]. For simulating the ionization produced by low-energy ions, an interface for importing results calculated using the SRIM software package [23] is available.

The present document aims to provide an overview of the Garfield++ classes and their key functionalities, but does not provide an exhaustive description of all classes and functions. A number of examples and code snippets are included which may serve as a basis for the user's own programs. Further examples and information can be found on the webpage http://garfieldpp.web.cern.ch/garfieldpp/ If you have questions, doubts, comments etc. about the code or this manual, please don't hesitate to contact the authors. Any kind of constructive feedback is highly welcome.

### 1.1. Class Structure

An overview of the different types of classes is given in Fig. 1.1. Two main categories can be distinguished: classes for describing the detector (material properties, geometry, fields), and transport classes which deal with tracing particles through the device. The two class types are linked by the class Sensor.

The individual classes are explained in detail in the following chapters.

Readers familiar with the structure of (Fortran) Garfield [21] will recognize a rough correspondence between the above classes and the sections of Garfield. Medium classes, for instance, can be regarded as the counterpart of the &GAS section; Component classes are similar in scope to the &CELL section.

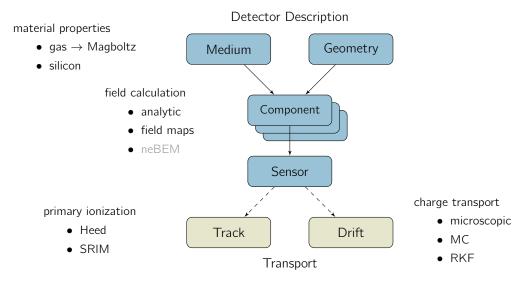


Figure 1.1. Overview of the main classes in Garfield++ and their interplay.

Garfield++ also includes a number of classes for visualization purposes, e. g. for plotting drift lines, making a contour plot of the electrostatic potential or inspecting the layout of the detector. These classes rely extensively on the graphics classes of the ROOT framework [4].

# 2. Getting Started

## 2.1. Installation

 $The source code is hosted on a $\operatorname{GitLab}^1$ repository, $\operatorname{https://gitlab.cern.ch/garfield/garfieldpp.} \\$ 

The following instructions describe how to download and build Garfield++ from source.

- Make sure that ROOT is installed. For installation instructions see https://root.cern.ch/building-root or https://root.cern.ch/downloading-root.
- Define an environment variable GARFIELD\_HOME pointing to the directory where the Garfield++ classes are to be located. In the following, we assume that we want to install Garfield in a directory /home/mydir/garfield. If you are using bash, type

export GARFIELD\_HOME=/home/mydir/garfield

(replace /home/mydir/garfield by the path of your choice).

For (t)csh-type shells, type

setenv GARFIELD\_HOME /home/mydir/garfield

Include the above lines also in the .bashrc (or .cshrc) file in your home directory. If unsure which shell you are using, type echo \$SHELL.

• Download the code from the repository, either using SSH access<sup>2</sup>

 $\verb|git| \verb|clone| ssh://git@gitlab.cern.ch:7999/garfield/garfieldpp.git $$GARFIELD\_HOME$ | Constraints for the constraints of t$ 

or HTTPS access

git clone https://gitlab.cern.ch/garfield/garfieldpp.git \$GARFIELD\_HOME

- Change to the \$GARFIELD\_HOME directory (cd \$GARFIELD\_HOME).
- There are two options for building the library: (1) using directly the makefile in \$GARFIELD\_HOME, or (2) using CMake.
  - If necessary, adapt the makefile according to your configuration. By default, gfortran is used as Fortran compiler. In order to use a different compiler you can modify the definition of the variable \$FC in the makefile accordingly.

<sup>&</sup>lt;sup>1</sup>https://gitlab.cern.ch/help/gitlab-basics/start-using-git.md

<sup>&</sup>lt;sup>2</sup>See https://gitlab.cern.ch/help/gitlab-basics/create-your-ssh-keys.md for instructions how to create and upload the SSH keys for gitlab.

- Compile the classes by giving the command make.
- 2. Create a build directory and make it your work directory, e. g.

mkdir \$GARFIELD\_HOME/build; cd \$GARFIELD\_HOME/build).

- Type cmake \$GARFIELD\_HOME.
- Alternatively, if you want to switch on debugging and switch off optimisation, type
   cmake -DCMAKE\_BUILD\_TYPE=Debug \$GARFIELD\_HOME)
- Type make, followed by make install.
- Delete the build folder.
- Heed requires an environment variable HEED\_DATABASE to be defined.

export HEED\_DATABASE=\$GARFIELD\_HOME/Heed/heed++/database/

Add this line also to your .bashrc/.cshrc as well.

After the initial download,

git pull

followed by make (in case of trouble: try make clean; make), can be used for downloading the latest version of the code from the repository.

# 2.2. Examples

Section 2.2.1 discusses the calculation of transport parameters with Magboltz, the use of analytic field calculation techniques, "macroscopic" simulation of electron and ion drift lines, and the calculation of induced signals.

Microscopic transport of electrons and the use of finite element field maps are dealt with in Sec. 2.2.2.

Sample macros and further examples can be found on the webpage (http://garfieldpp.web.cern.ch/garfieldpp/).

#### 2.2.1. Drift Tube

#### Gas Table

First, we prepare a table of transport parameters (drift velocity, diffusion coefficients, Townsend coefficient, and attachment coefficient) as a function of the electric field  $\bf E$  (and, in general, also the magnetic field  $\bf B$  as well as the angle between  $\bf E$  and  $\bf B$ ). In this example, we use a gas mixture of 93% argon and 7% carbon dioxide at a pressure of 3 atm and room temperature.

```
MediumMagboltz* gas = new MediumMagboltz();
gas->SetComposition("ar", 93., "co2", 7.);
// Set temperature [K] and pressure [Torr].
gas->SetPressure(3 * 760.);
gas->SetTemperature(293.15);
```

We also have to specify the number of electric fields to be included in the table and the electric field range to be covered. Here we use 20 field points between  $100\,\mathrm{V}/\mathrm{cm}$  and  $100\,\mathrm{kV}/\mathrm{cm}$  with logarithmic spacing.

```
gas->SetFieldGrid(100., 100.e3, 20, true);
```

Now we run Magboltz to generate the gas table for this grid. As input parameter we have to specify the number of collisions (in multiples of  $10^7$ ) over which the electron is traced by Magboltz.

```
const int ncoll = 10;
const bool verbose = true;
gas->GenerateGasTable(ncoll, verbose);
```

This calculation will take a while, don't panic. After the calculation is finished, we save the gas table to a file for later use.

```
gas->WriteGasFile("ar_93_co2_7.gas");
```

#### **Electric Field**

For calculating the electric field inside the tube, we use the class ComponentAnalyticField which can handle (two-dimensional) arrangements of wires, planes and tubes.

```
ComponentAnalyticField* cmp = new ComponentAnalyticField();
```

The Component requires a description of the geometry, that is a list of volumes and associated media.

```
// Wire radius [cm]
const double rWire = 25.e-4;
// Outer radius of the tube [cm]
const double rTube = 1.46;
// Half-length of the tube [cm]
const double lTube = 10.;
GeometrySimple* geo = new GeometrySimple();
// Make a tube
// (centered at the origin, inner radius: rWire, outer radius: rTube).
SolidTube* tube = new SolidTube(0., 0., 0., rWire, rTube, lTube);
// Add the solid to the geometry, together with the medium inside.
geo->AddSolid(tube, gas);
// Pass a pointer to the geometry class to the component.
cmp->SetGeometry(geo);
```

Next we setup the electric field.

```
// Voltages
const double vWire = 3270.;
const double vTube = 0.;
// Add the wire in the center.
cmp->AddWire(0., 0., 2 * rWire, vWire, "s");
// Add the tube.
cmp->AddTube(rTube, vTube, 0, "t");
```

We want to calculate the signal induced on the wire. Using

```
cmp->AddReadout("s");
```

we tell the Component to prepare the solution for the weighting field of the wire (which we have given the label "s" before).

Finally we assemble a Sensor object which acts as an interface to the transport classes discussed below.

```
Sensor* sensor = new Sensor();
// Calculate the electric field using the Component object cmp.
sensor->AddComponent(cmp);
// Request signal calculation for the electrode named "s",
// using the weighting field provided by the Component object cmp.
sensor->AddElectrode(cmp, "s");
```

In this (not very realistic) example, we want to calculate only the electron signal. We set the time interval within which the signal is recorded by the sensor to 2 ns, with a binning of 0.02 ns.

```
const double tMin = 0.;
const double tMax = 2.;
const double tStep = 0.02;
const int nTimeBins = int((tMax - tMin) / tStep);
sensor->SetTimeWindow(0., tStep, nTimeBins);
```

#### **Avalanche**

For simulating the electron avalanche we use the class AvalancheMC which uses the previously computed tables of transport parameters to calculate drift lines and multiplication.

```
AvalancheMC* aval = new AvalancheMC();
aval->SetSensor(sensor);

// Switch on signal calculation.
aval->EnableSignalCalculation();

// Do the drift line calculation in time steps of 50 ps.
aval->SetTimeSteps(0.05);

// Starting position [cm] and time [ns] of the initial electron.
// The electron is started at 100 micron above the wire.
const double x0 = 0.;
```

```
const double y0 = rWire + 100.e-4;
const double z0 = 0.;
const double t0 = 0.;
// Simulate an avalanche.
aval->AvalancheElectron(x0, y0, z0, t0);
```

Using the class ViewSignal, we plot the current induced on the wire by the avalanche simulated in the previous step.

```
ViewSignal* signalView = new ViewSignal();
signalView->SetSensor(sensor);
signalView->PlotSignal("s");
```

#### 2.2.2. GEM

#### Field Map

The initialisation of ComponentAnsys123 consists of

- loading the mesh (ELIST.lis, NLIST.lis), the list of nodal solutions (PRNSOL.lis), and the material properties (MPLIST.lis);
- specifying the length unit of the values given in the .LIS files;
- setting the appropriate periodicities/symmetries.

```
ComponentAnsys123* fm = new ComponentAnsys123();
// Load the field map.
fm->Initialise("ELIST.lis", "NLIST.lis", "MPLIST.lis", "PRNSOL.lis", "mm");
// Set the periodicities
fm->EnableMirrorPeriodicityX();
fm->EnableMirorPeriodicityY();
// Print some information about the cell dimensions.
fm->PrintRange();
```

Next we create a Sensor and add the field map component to it

```
Sensor* sensor = new Sensor();
sensor->AddComponent(fm);
```

#### Gas

We use a gas mixture of 80% argon and 20%  $CO_2$ .

```
MediumMagboltz* gas = new MediumMagboltz();
gas->SetComposition("ar", 80., "co2", 20.);
// Set temperature [K] and pressure [Torr].
gas->SetTemperature(293.15);
gas->SetPressure(760.);
```

In this example, we will calculate electron avalanches using "microscopic" Monte Carlo simulation, based directly on the electron-atom/molecule cross-sections in the Magboltz database.

In order to track a particle through the detector we have to tell ComponentAnsys123 which field map material corresponds to which Medium.

```
const unsigned int nMaterials = fm->GetNumberOfMaterials();
for (unsigned int i = 0; i < nMaterials; ++i) {
  const double eps = fm->GetPermittivity(i);
  if (fabs(eps - 1.) < 1.e-3) fm->SetMedium(i, gas);
}
// Print a list of the field map materials (for information).
fm->PrintMaterials();
```

#### **Avalanche**

Microscopic tracking is handled by the class AvalancheMicroscopic.

```
AvalancheMicroscopic* aval = new AvalancheMicroscopic();
aval->SetSensor(aval);
```

We are now ready to track an electron through the GEM.

```
// Initial position [cm] and starting time [ns]
double x0 = 0., y0 = 0., z0 = 0.02;
double t0 = 0.;
// Initial energy [eV]
double e0 = 0.1;
// Initial direction
// In case of a null vector, the initial direction is randomized.
double dx0 = 0., dy0 = 0., dz0 = 0.;
// Calculate an electron avalanche.
aval->AvalancheElectron(x0, y0, 0, t0, e0, dx0, dy0, dz0);
```

# 3. Media

Media are derived from the abstract base class Medium.

The name (identifier) of a medium can be read by the function

```
const std::string& GetName();
```

For compound media (e. g. gas mixtures), the identifiers and fractions of the constituents are available via

```
unsigned int GetNumberOfComponents();
void GetComponent(const unsigned int i, std::string& label, double& f);
```

# 3.1. Transport Parameters

Medium classes provide functions for calculating the macroscopic transport parameters of electrons, holes, and ions as a function of the electric and magnetic field:

```
bool ElectronVelocity(const double ex, const double ey, const double ez,
                     const double bx, const double by, const double bz,
                     double& vx, double& vy, double& vz);
bool ElectronDiffusion(const double ex, const double ey, const double ez,
                      const double bx, const double by, const double bz,
                      double& dl, double& dt);
bool ElectronTownsend(const double ex, const double ey, const double ez,
                     const double bx, const double by, const double bz,
                     double& alpha);
bool ElectronAttachment(const double ex, const double ey, const double ez,
                       const double bx, const double by, const double bz,
                       double& eta);
ex, ey, ez electric field (in V / cm)
bx, by, bz magnetic field (in T)
vx, vy, vz drift velocity (in cm / ns)
dl, dt longitudinal and transverse diffusion coefficients (in \sqrt{\text{cm}})
alpha Townsend coefficient (in cm^{-1})
eta attachment coefficient (in cm<sup>-1</sup>)
```

transport parameter	scaling
drift velocity	v vs. E/p
diffusion	$\sigma\sqrt{p}$ vs. $E/p$
Townsend coefficient	lpha/p vs. $E/p$
attachment coefficient	$\eta/p$ vs. $E/p$

**Table 3.1.** Pressure scaling relations for gases.

The above functions return true if the respective parameter is available at the requested field.

Analogous functions are available for holes (albeit of course not meaningful for gases), and also for ions (except for the Townsend and attachment coefficients). A function specific to ions is

It returns the dissociation coefficient (in  $cm^{-1}$ ).

The components of the drift velocity are stored in a coordinate system which is aligned with the electric and magnetic field vectors. More precisely, the axes are along

- the electric field **E**,
- the component of the magnetic field **B** transverse to **E**,
- **E** × **B**.

The longitudinal diffusion is measured along **E**. The transverse diffusion is the average of the diffusion coefficients along the two remaining axes.

## 3.1.1. Transport Tables

The transport parameters can either be stored in a one-dimensional table (as a function of the electric field only) or in a three-dimensional table (as a function of **E**, **B**, and the angle  $\theta$  between **E** and **B**). If only a one-dimensional table is present and the drift velocity at  $B \neq 0$  is requested, the Laue-Langevin equation

$$\mathbf{v} = \frac{\mu}{1 + \mu^2 B^2} \left( \mathbf{E} + \mu \mathbf{E} \times \mathbf{B} + \mu^2 \mathbf{B} \left( \mathbf{E} \cdot \mathbf{B} \right) \right), \qquad \mu = v/E.$$

is used.

In the present version of the code, all transport parameters share the same grid of electric fields, magnetic fields, and angles. By default, the field and angular ranges are

- 20 electric field points between 100 V / cm and 100 kV / cm, with logarithmic spacing
- **B** = 0,  $\theta$  = 0

For specifying the field grid, two functions are available:

emin, emax min. and max. value of the electric field range to be covered by the tables

ne number of electric field grid points

**logE** flag specifying whether the *E*-field grid points should be evenly spaced (false), or logarithmically spaced (true)

bmin, bmax, ne magnetic field range and number of values

amin, amax, na angular range and number of angles

**efields, bfields, angles** lists of E, B, and  $\theta$  (in ascending order)

Electric fields have to be supplied in V / cm, magnetic fields in Tesla, and angles in rad.

The gas tables are interpolated using Newton polynomials. The order of the interpolation polynomials can be set by means of

```
void SetInterpolationMethodVelocity(const unsigned int intrp);
void SetInterpolationMethodDiffusion(const unsigned int intrp);
void SetInterpolationMethodTownsend(const unsigned int intrp);
void SetInterpolationMethodAttachment(const unsigned int intrp);
void SetInterpolationMethodIonMobility(const unsigned int intrp);
void SetInterpolationMethodIonDissociation(const unsigned int intrp);
```

**intrp** order of the interpolation polynomial

The interpolation order must be between 1 and the smallest of the two numbers: 10 and number of table entries - 1. Orders larger than 2 are not recommended.

The method for extrapolating to E values smaller and larger than those present in the table can be set using

extrLow, extrHigh extrapolation method to be used ("constant", "exponential", or "linear")

Similar functions are available for the other transport parameters. The extrapolation method set using this function has no effect on extrapolation in three-dimensional tables. In such tables, polynomial extrapolation is performed with the same order as for the interpolation.

The default settings are

- quadratic interpolation,
- constant extrapolation towards low values,
- linear extrapolation towards high values.

For plotting the transport parameters, the class ViewMedium can be used.

collision type	index
collision type	muex
elastic collision	0
ionisation	1
attachment	2
inelastic collision	3
excitation	4
superelastic collision	5
virtual ("null") collision	6

**Table 3.2.** Classification of electron collision processes.

# 3.2. Electron Scattering Rates

For calculating electron drift lines using "microscopic tracking" (see Sec. 6.3), the preparation of an electron transport table is not necessary, since this method is based directly on the electron-atom/molecule scattering rates.

The following functions which are meant to be called from within the class AvalancheMicroscopic are available in Medium:

```
double GetElectronCollisionRate(const double e, const int band = 0);
```

returns the total scattering rate of an electron with energy e (in eV) in the Medium. The band index is relevant only for semiconducting media.

e electron energy prior to the collision

**type** category of the collision process (see Tab. 3.2)

level index of the collision process

e1 electron energy after the collision

dx, dy, dz incoming and outgoing direction

**secondaries** list of "ionisation products" (*i. e.* electrons and ions) created in the collision. The first (integer) number in the pair is a flag indicating whether it is an ion or an electron. The second number corresponds to the kinetic energy.

ndxc number of "deexcitation products" created in the collision

**band** band index (irrelevant for gases)

## **3.3.** Gases

There are currently two classes implemented which can be used for the description of gaseous media: MediumGas and its daughter class MediumMagboltz. While MediumGas deals only with the interpolation of gas tables and the import of gas files, MediumMagboltz — owing to an interface to the Magboltz program [3] — can be used for the calculation of transport parameters. In addition, the latter class provides access to the electron-molecule scattering cross-sections used in Magboltz and is thus suitable for microscopic tracking (chapter 6).

The composition of the gas mixture is specified using

gas1, ..., gas6 identifier of the molecule/atom

**f1**, ..., **f6** fraction of the respective molecule/atom

A valid gas mixture comprises at least one and at most six different species. A list of the presently available gases and their identifiers can be found in the appendix. The fractions have to be strictly positive and may add up to any non-zero value; internally they will be normalized to one.

The gas density is specified in terms of pressure (Torr) and temperature (K):

```
void SetPressure(const double p);
void SetTemperature(const double t);
```

Note that the density is calculated using the ideal gas law.

In the following example the gas mixture is set to Ar/CH<sub>4</sub> (80/20) at atmospheric pressure and  $20^{\circ}$  C.

```
MediumMagboltz* gas = new MediumMagboltz();
// Set the composition
gas->SetComposition("ar", 80., "ch4", 20.);
gas->SetTemperature(293.15);
gas->SetPressure(760.);
```

The function

```
void PrintGas();
```

prints information about the present transport parameter tables and cross-section terms (if available).

#### 3.3.1. Ion Transport

The  $GARFIELD_HOME/Data$  directory includes a few files (e. g. IonMobility\_Ar+\_Ar.txt for Ar<sup>+</sup> ions in argon) which contain ion mobility data in form of a table of reduced electric fields E/N (in  $Td^1$ ) vs. mobilities (in cm<sup>2</sup> V<sup>-1</sup> s<sup>-1</sup>). These mobility files can be imported using

```
bool MediumGas::LoadIonMobility(const std::string& filename);
```

filename path and filename of the mobility file

Extensive compilations of ion mobilities and diffusion coefficients can be found in Refs. [6–8, 22].

## 3.3.2. Magboltz

Magboltz, written by Steve Biagi, is a program [3] for the calculation of electron transport properties in gas mixtures using semi-classical Monte Carlo simulation. It includes a database of electron-atom/molecule cross-sections for a large number of detection gases.

In order to run Magboltz via the MediumMagboltz interface class given electric field, magnetic field and field angle, the following function is provided:

e, b, btheta E field, B field, and angle

**ncoll** number of collisions (in multiples of 10<sup>7</sup>) over which the electron is tracked

verbose flag switching on/off full output from Magboltz

```
vx, vy, vz drift velocity along E (vz), along B<sub>t</sub> (vy), and along E × B (vy)
```

dl, dt diffusion coefficients

**alpha, eta** Townsend and attachment coefficient calculated using the SST technique or, at low fields, the ionization/loss rate

lor Lorentz angle, calculated from the components of the drift velocity

```
vxerr, vyerr, ..., etaerr statistical error of the calculation in %
```

**alphatof** alternative estimate of the effective Townsend coefficient  $\alpha-\eta$  based on the Time-Of-Flight method

**difftens** components of the diffusion tensor  $(\sigma_{zz}, \sigma_{xx}, \sigma_{yy}, \sigma_{xz} = \sigma_{zx}, \sigma_{yz} = \sigma_{zy}, \sigma_{xy} = \sigma_{yx})$ 

 $<sup>^{1}1 \</sup>text{ Td} = 10^{-17} \text{ V cm}^{2}$ 

The max. energy of the cross-section table is chosen automatically by Magboltz. For inelastic gases, setting nColl = 2...5 should give an accuracy of about 1%. An accuracy better than 0.5% can be achieved by nColl > 10. For pure elastic gases such as Ar, nColl should be at least 10.

Recent versions of Magboltz allow the thermal motion of the gas atoms/molecules to be taken into account in the simulation. This feature can be enabled or disabled using

```
void EnableThermalMotion(const bool on);
```

By default the option is switched off, i. e. the gas is assumed to be 0 K.

In order to calculate the electron transport parameters for all values of  $\mathbf{E}$ ,  $\mathbf{B}$ , and  $\theta$  included in the current field grid, the function

```
void GenerateGasTable(const int numCollisions, const bool verbose);
```

can be used. In addition to the transport parameters, this function also retrieves the rates calculated by Magboltz for each excitation and ionisation level, and stores them in the gas table. These can be used later to adjust the Townsend coefficient based on the Penning transfer probabilities set by the user.

Electron transport parameter tables can be saved to file and read from file by means of

```
bool WriteGasFile(const std::string& filename);
bool LoadGasFile(const std::string& filename);
```

The format of the gas file used in Garfield++ is compatible with the one used in Garfield 9.

## **Scattering Rates**

As a prerequisite for "microscopic tracking" a table of the electron scattering rates (based on the electron-atom/molecule cross-sections included in the Magboltz database) for the current gas mixture and density needs to be prepared. This can be done using the function

```
bool Initialise(const bool verbose);
```

If the flag verbose is set to true, some information (such as gas properties, and collision rates at selected energies) is printed during the initialisation.

lf

```
void EnableCrossSectionOutput();
```

is called prior to Initialise, a table of the cross-sections (as retrieved from Magboltz) is written to a file cs.txt in the current working directory.

By default, the scattering rates table extends from 0 to 40 eV. The max. energy to be included in the scattering rates table can be set using

```
SetMaxElectronEnergy(const double e);
```

e max. electron energy (in eV)

The parameters of the cross-section terms in the present gas mixture can be retrieved via

```
int GetNumberOfLevels();
bool GetLevel(const unsigned int i, int& ngas, int& type, std::string& descr, double& e);
```

i index of the cross-section term

ngas index of the gas in the mixture

**type** classification of the cross-section term (see Table 3.2)

descr description of the cross-section term (from Magboltz)

e energy loss

It is sometimes useful to know the frequency with which individual levels are excited in an avalanche (or along a drift line). For this purpose, MediumMagboltz keeps track of the number of times the individual levels are sampled in GetElectronCollision. These counters are accessible through the functions

The first function returns total number of electron collisions (*i. e.* calls to GetElectronCollisions) since the last reset. The second function additionally provides the number of collisions of each cross-section category (elastic, ionising etc.). The third function returns the number of collisions for a specific cross-section term. The counters can be reset using

```
void ResetCollisionCounters();
```

#### **Excitation Transfer**

Penning transfer can be taken into account in terms of a transfer efficiency  $r_i$ , i.e. the probability for an excited level i with an excitation energy  $\epsilon_i$  exceeding the ionisation potential  $\epsilon_{\text{ion}}$  of the mixture to be "converted" to an ionisation. The simulation of Penning transfer can be switched on/off using

	electrons $\mu_L \ [10^{-6} \ {\rm cm^2  V^{-1}  ns^{-1}}]$	β	holes $\mu_L \ [10^{-6} \ {\rm cm^2  V^{-1}  ns^{-1}}]$	β
Sentaurus [10]	1.417	-2.5	0.4705	-2.5
Minimos [17]	1.43	-2.0	0.46	-2.18
Reggiani [14]	1.32	-2.0	0.46	-2.2

**Table 3.3.** Lattice mobility parameter values.

**lambda** distance characterizing the spatial extent of Penning transfers; except for special studies, this number should be set to zero

**gasname** name of the gas the excitation levels of which are to be assigned the specified transfer efficiency

The functions without the gasname parameter switch on/off Penning transfer globally for all gases in the mixture. Note that r is an average transfer efficiency, it is assumed to be the same for all energetically eligible levels ( $\epsilon_i > \epsilon_{\rm ion}$ ).

If the gas table includes excitation and ionisation rates as function of the electric and magnetic fields, the Townsend coefficient is updated accordingly when calling EnablePenningTransfer (or DisablePenningTransfer). More precisely, the adjusted Townsend coefficient is given by

$$\alpha = \alpha_0 \frac{\sum_i \operatorname{exc}, i + \sum_i \operatorname{ion}, i}{\sum_i \operatorname{ion}, i},$$

where  $\alpha_0$  is the Townsend coefficient calculated without Penning transfers,  $r_{\text{exc},i}$  is the rate of an excited level i with an excitation energy above the ionisation potential of the gas mixture, and  $r_{\text{ion},i}$  is the rate of an ionization level i.

### 3.4. Semiconductors

MediumSilicon is the only semiconductor-type Medium class implemented so far.

### 3.4.1. Transport Parameters

Like for all Medium classes the user has the possibility to specify the transport parameters in tabulated form as function of electric field, magnetic field, and angle. If no such tables have been entered, the transport parameters are calculated based on empirical parameterizations (as used, for instance, in device simulation programs). Several mobility models are implemented. For the mobility  $\mu_0$  at low electric fields, the following options are available:

#### Using

```
void SetLowFieldMobility(const double mue, const double mh);
```

**mue** electron mobility (in  $cm^2/(V ns)$ )

**muh** hole mobility (in cm<sup>2</sup>/(V ns))

the values of low-field electron and hole mobilities can be specified explicitly by the user.

• The following functions select the model to be used for the mobility due to phonon scattering:

```
void SetLatticeMobilityModelMinimos();
void SetLatticeMobilityModelSentaurus();
void SetLatticeMobilityModelReggiani();
```

In all cases, the dependence of the lattice mobility  $\mu_L$  on the temperature  $\mathcal T$  is described by

$$\mu_L(T) = \mu_L(T_0) \left(\frac{T}{T_0}\right)^{\beta}, \qquad T_0 = 300 \text{ K}.$$

The values of the parameters  $\mu_L(T_0)$  and  $\beta$  used in the different models are shown in Table 3.3. By default, the "Sentaurus" model is activated.

 The parameterization to be used for modelling the impact of doping on the mobility is specified using

```
void SetDopingMobilityModelMinimos();
void SetDopingMobilityModelMasetti();
```

The first function activates the model used in Minimos 6.1 (see Ref. [17]). Using the second function the model described in Ref. [13] is activated (default setting).

For modelling the velocity as function of the electric field, the following options are available:

• The method for calculating the high-field saturation velocities can be set using

```
void SetSaturationVelocity(const double vsate, const double vsath);
void SetSaturationVelocityModelMinimos();
void SetSaturationVelocityModelCanali();
void SetSaturationVelocityModelReggiani();
```

The first function sets user-defined saturation velocities (in cm/ns) for electrons and holes. The other functions activate different parameterizations for the saturation velocity as function of temperature. In the Canali model [5], which is activated by default,

$$v_{\text{sat}}^{e} = 0.0107 \left(\frac{T_{0}}{T}\right)^{0.87} \text{ cm/ns,}$$
 $v_{\text{sat}}^{h} = 0.00837 \left(\frac{T_{0}}{T}\right)^{0.52} \text{ cm/ns,}$ 

where  $T_0 = 300$  K. The expressions for the other two implemented models can be found in Refs. [14, 15].

• The parameterization of the mobility as function of the electric field to be used can be selected using

```
void SetHighFieldMobilityModelMinimos();
void SetHighFieldMobilityModelCanali();
void SetHighFieldMobilityModelReggiani();
void SetHighFieldMobilityModelConstant();
```

The last function requests a constant mobility (i. e. linear dependence of the velocity on the electric field). The models activated by the other functions used the following expressions

$$\mu^{e}(E) = \frac{2\mu_{0}^{e}}{1 + \sqrt{1 + \left(\frac{2\mu_{0}^{e}E}{v_{\text{sat}}^{e}}\right)^{2}}}, \qquad \mu^{h}(E) = \frac{\mu_{0}^{h}}{1 + \frac{\mu_{0}}{v_{\text{sat}}^{h}}}, \qquad \text{(Minimos)}$$

$$\mu^{e,h}(E) = \frac{\mu_{0}^{e,h}}{\left(1 + \left(\frac{\mu_{0}^{e,h}E}{v_{\text{sat}}e,h}\right)^{\beta^{e,h}}\right)^{\frac{1}{\beta^{e,h}}}}, \qquad \text{(Canali [5])}$$

$$\mu^{e}(E) = \frac{\mu_{0}^{e}}{\left(1 + \left(\frac{\mu_{0}^{e}E}{v_{\text{sat}}^{e}}\right)^{3/2}\right)^{2/3}}, \qquad \mu^{h}(E) = \frac{\mu_{0}^{h}}{\left(1 + \left(\frac{\mu_{0}^{h}E}{v_{\text{sat}}^{h}}\right)^{2}\right)^{1/2}}, \qquad \text{(Reggiani [14])}$$

By default, the Canali model is used.

For the impact ionization coefficient, the user has currently the choice between the model of Grant [9] and the model of van Overstraeten and de Man [20].

```
void SetImpactIonisationModelGrant();
void SetImpactIonisationModelVanOverstraetenDeMan();
```

The latter model is used by default.

On an experimental basis, electron collision rates for use with microscopic tracking are also included.

# 4. Components

The calculation of electric fields is done by classes derived from the abstract base class ComponentBase. The key functions are

x, y, z position where the electric field (medium) is to be determined

ex, ey, ez, v electric field and potential at the given position

**m** pointer to the medium at the given position; if there is no medium at this location, a null pointer is returned

**status** status flag indicating where the point is located (see Table 4.1)

# 4.1. Defining the Geometry

As mentioned above, the purpose of Component classes is to provide, for a given location, the electric (and magnetic) field and a pointer to the Medium (if available). For the latter task, it is obviously necessary to specify the geometry of the device. In case of field maps, the geometry is already defined in the field solver. It is, therefore, sufficient to associate the materials of the field map with the corresponding Medium classes.

For other components (e. g. analytic or user-parameterized fields), the geometry has to be defined separately.

Simple structures can be described by the native geometry (GeometrySimple), which has only a very restricted repertoire of shapes (solids). At present, the available solids are

value	meaning
0	inside a drift medium
> 0	inside a wire
-14	on the side of a plane where no wires are
-5	inside the mesh, but not in a drift medium
-6	outside the mesh

**Table 4.1.** Status flags for electric fields.

- SolidBox,
- SolidTube, and
- SolidSphere.

As an example, we consider a gas-filled tube with a diameter of 1 cm and a length of 20 cm (along the z-axis), centred at the origin:

```
// Create the medium.
MediumMagboltz* gas = new MediumMagboltz();
// Create the geometry.
GeometrySimple* geo = new GeometrySimple();
// Dimensions of the tube
double rMin = 0., rMax = 0.5, halfLength = 10.;
SolidTube* tube = new SolidTube(0., 0., 0., rMin, rMax, halfLength);
// Add the solid to the geometry, together with the gas inside.
geo->AddSolid(tube, gas);
```

Solids may overlap. When the geometry is scanned (triggered, for instance, by calling GetMedium), the first medium found is returned. The sequence of the scan is reversed with respect to the assembly of the geometry. Hence, the last medium added to the geometry is considered the innermost.

For more complex structures, the class GeometryRoot can be used which provides an interface to the ROOT geometry (TGeo). Using GeometryRoot, the above example would look like this:

```
// Create the ROOT geometry.
TGeoManager* geoman = new TGeoManager("world", "geometry");
// Create the ROOT material and medium.
// For simplicity we use the predefined material "Vacuum".
TGeoMaterial* matVacuum = new TGeoMaterial("Vacuum", 0, 0, 0);
TGeoMedium* medVacuum = new TGeoMedium("Vacuum", 1, matVacuum);
// Dimensions of the tube
double rMin = 0., rMax = 0.5, halfLength = 10.;
// In this simple case, the tube is also the top volume.
TGeoVolume* top = geoman->MakeTube("TOP", medVacuum, rMin, rMax, halfLength);
geoman->SetTopVolume(top);
geoman->CloseGeometry();
// Create the Garfield medium.
MediumMagboltz* gas = new MediumMagboltz();
// Create the Garfield geometry.
GeometryRoot* geo = new GeometryRoot();
// Pass the pointer to the TGeoManager.
geo->SetGeometry(geoman);
// Associate the ROOT medium with the Garfield medium.
geo->SetMedium("Vacuum", gas);
```

In either case (GeometrySimple and GeometryRoot), after assembly the geometry is passed to the Component as a pointer:

```
void SetGeometry(GeometryBase* geo);
```

## 4.1.1. Visualizing the Geometry

Geometries described by GeometrySimple can be viewed using the class ViewGeometry.

```
// Create and setup the geometry.
GeometrySimple* geo = new GeometrySimple();
...
// Create a viewer.
ViewGeometry* view = new ViewGeometry();
// Set the pointer to the geometry.
view->SetGeometry(geo);
view->Plot();
```

ROOT geometries can be viewed by calling the Draw() function of TGeoManager.

The layout of an arrangement of wires, planes and tubes defined in ComponentAnalyticField can be inspected using the class ViewCell.

```
// Create and setup the component.
ComponentAnalyticField* cmp = new ComponentAnalyticField();
...
// Create a viewer.
ViewCell* view = new ViewCell();
// Set the pointer to the component.
view->SetComponent(cmp);
// Make a two-dimensional plot of the cell layout.
view->Plot2d();
```

Similarly, the function ViewCell::Plot3d() paints a three-dimensional view of the cell layout.

# 4.2. Field Maps

## 4.2.1. Ansys

The interpolation of FEM field maps created with the program Ansys [1] is dealt with by the classes ComponentAnsys121 and ComponentAnsys123. The class names refer to the type of mesh element used by Ansys:

- ComponentAnys121 reads two-dimensional field maps with 8-node curved quadrilaterals (known as "plane121" in Anys).
- ComponentAnsys123 reads three-dimensional field maps with quadric curved tetrahedra (known as "solid123" in Ansys).

The field map is imported with the function

elist name of the file containing the list of elements (default: "ELIST.lis")

```
mlist name of the file containing the list of nodes (default: "NLIST.lis")
mplist name of the file containing the list of materials (default: "MPLIST.lis")
```

prnsol name of the file containing the nodal solutions (default: "PRNSOL.lis")

The return value is true if the map was successfully read.

In order to enable charge transport and ionization, the materials in the map need to be associated with Medium classes.

```
// Get the number of materials in the map.
unsigned int GetNumberOfMaterials();
// Associate a material with a Medium class.
void SetMedium(const unsigned int imat, Medium* medium);
```

**imat** index in the list of (field map) materials

medium pointer to the Medium class to be associated with this material

The materials in the field map are characterized by the relative dielectric constant  $\varepsilon$  and the conductivity  $\sigma$ . These parameters are accessible through the functions

```
double GetPermittivity(const unsigned int imat);
double GetConductivity(const unsigned int imat);
```

A weighting field map can be imported using

```
bool SetWeightingField(std::string prnsol, std::string label);
```

prnsol name of the file containing the nodal solution for the weighting field configuration

label arbitrary name, used for identification of the electrode/signal

The weighting field map has to use the same mesh as the previously read "actual" field map.

For periodic structures, e. g. GEMs, one usually models only the basic cell of the geometry and applies appropriate symmetry conditions to cover the whole problem domain. The available symmetry operations are:

- simple periodicities,
- mirror periodicities,
- axial periodicities, and
- rotation symmetries.

Mirror periodicity and simple periodicity as well as axial periodicity and rotation symmetry are, obviously, mutually exclusive. In case of axial periodicity, the field map has to cover an integral fraction of  $2\pi$ .

Periodicities can be set and unset using

```
void EnablePeriodicityX(); void DisablePeriodicityX();
void EnableMirrorPeriodicityX(); void DisableMirrorPeriodicityX();
void EnableAxialPeriodicityX(); void DisableAxialPeriodicityX();
void EnableRotationSymmetryX(); void DisableRotationSymmetryX();
```

Analogous functions are available for y and z.

In order to assess the quality of the mesh, one can retrieve the dimensions of each mesh element using

```
bool GetElement(const unsigned int i, double& vol, double& dmin, double& dmax);
```

i index of the element

vol volume/area of the element

dmin, dmax min./max. distance between two node points

In the following example we make histograms of the aspect ratio and element size.

```
ComponentAnsys123* fm = new ComponentAnsys123();
TH1F* hAspectRatio = new TH1F("hAspectRatio"; "Aspect_Ratio", 100, 0., 50.);
TH1F* hSize = new TH1F("hSize", "Element_Size", 100, 0., 30.);
const unsigned int nel = fm->GetNumberOfElements();
// Loop over the elements.
double volume, dmin, dmax;
for (unsigned int i = 0; i < nel; ++i) {</pre>
  fm->GetElement(i, volume, dmin, dmax);
  if (dmin > 0.) hAspectRatio->Fill(dmax / dmin);
 hSize->Fill(volume);
}
TCanvas* c1 = new TCanvas();
hAspectRatio->Draw();
TCanvas* c2 = new TCanvas();
c2->SetLogy();
hSize->Draw();
```

## 4.2.2. Synopsys TCAD

Electric fields calculated using the device simulation program Synopsys Sentaurus [19] can be imported with the classes ComponentTcad2d and ComponentTcad3d.

The function to import the field map is

gridfilename name of the mesh file, the extension is typically .grd

datafilename name of the file containing the nodal solution; the filename typically typically ends with \_des.dat

Both files have to be exported in DF-ISE format, files in the default TDR format cannot be read. To convert a TDR file to \_.dat and .grid files, the Sentaurus tool tdx can be used

```
tdx -dd fieldToConvert.tdr
```

The classes have been tested with meshes created with the application Mesh which can produce axis-aligned two- and three-dimensional meshes. The only three-dimensional mesh elements ComponentTcad3d can deal with are tetrahedra. A mesh which consists only of simplex elements (triangles in 2D, tetrahedra in 3D), can be generated by invoking Mesh with the option -t.

After importing the files, the regions of the device where charge transport is to be enabled need to be associated with Medium classes.

```
// Get the number of regions in the device
unsigned int GetNumberOfRegions();
// Associate a region with a Medium class
void SetMedium(const unsigned int ireg, Medium* m);
```

ireg index in the list of device regions

medium pointer to the Medium class to be associated with this region

The name of a region can be retrieved with

```
void GetRegion(const unsigned int i, std::string& name, bool& active);
```

**name** label of the region as defined in the device simulation

active flag indicating whether charge transport is enabled in this region

Simple periodicities and mirror periodicities along x, y, and - in case of ComponentTcad3d - z are supported.

```
void EnablePeriodicityX();
void EnableMirrorPeriodicityX();
```

#### 4.2.3. Elmer

The class ComponentElmer (contributed by J. Renner) allows one to import field maps created with the open source field solver Elmer and the mesh tool Gmsh. A detailed tutorial can be found on the webpage.

### 4.2.4. CST

The class ComponentCST (contributed by K. Zenker) reads field maps extracted from CST Studio. More details can be found at http://www.desy.de/zenker/FLC/garfieldpp.html.

#### 4.2.5. **COMSOL**

The class ComponentComsol (contributed by E. Bodnia) can be used for importing field maps computed using COMSOL. The function to import a field map is

**header** COMSOL Multiphysics text field (.mphtxt) containing the mesh data. exported field data.

#### 4.2.6. Regular grids

Electric field values on a regular two-dimensional or three-dimensional grid can be imported using the class ComponentVoxel. As a first step, the grid needs to be defined using the function

```
nx, ny, nz number of cells along x, y, z xmin, xmax, ... boundaries of the grid in x, y, z
```

The electric field values (and potential) for each grid cell are read in using

**filename** name of the ASCII file

**format** description of the file format (see below)

withPotential flag whether the file contains an additional column with the electrostatic potential

withRegion flag whether the file contains an additional column with an integer value corresponding to the region index (each region can be associated with a different medium)

**scaleX, scaleE, scaleP** scaling factors to be applied to the coordinates, electric field values and potentials

The available formats are XY, IJ, XYZ, and IJK, the first two for two-dimensional maps, and the last two for three-dimensional maps. In case of XY (XYZ), the first two (three) columns contain the x, y (and z) coordinates of a given point in the grid, followed by the electric field values (and potential if available) at this point. The class then looks up the grid cell corresponding to this point and assigns the electric field and potential accordingly. In case of IJ (IJK) the indices of the grid cell along x, y (and z) are specified directly.

A magnetic field map can be imported using the function

The available formats are the same as for the electric field (except for the extra columns for potential and region index).

By default, the field and potential are assumed to be constant throughout a voxel. Alternatively, the fields/potentials given in the field map file can be interpreted to be the values at the voxel centres and the fields/potentials at intermediate points be determined by trilinear interpolation. This feature can be activated using the function

```
void EnableInterpolation(const bool on = true);
```

## 4.2.7. Visualizing the Mesh

For visualizing the mesh imported from a FEM field map, the class ViewFEMesh (written by J. Renner) is available. Using

```
void ViewFEMesh::SetViewDrift(ViewDrift* driftView);
```

a ViewDrift object can be attached to the mesh viewer. The function

```
bool ViewFEMesh::Plot();
```

then allows draws a two-dimensional projection of the drift lines stored in the ViewDrift class together with the mesh. The plot can be customized using

```
void SetColor(int matid, int colorid);
void SetFillColor(int matid, int colorid);
void SetFillMesh(bool fill);
```

matid material index in the field map

colorid index of the ROOT color with which all elements of material matid are to be drawn

fill flag indicating whether to draw a wireframe mesh (false) or filled elements

As an illustration consider the following example (suppose that fm is a pointer to a field map component and driftView is a pointer to a ViewDrift class)

```
TCanvas* c1 = new TCanvas();
ViewFEMesh* meshView = new ViewFEMesh();
meshView->SetCanvas(c1);
// Set the component.
meshView->SetComponent(fm);
// Set the viewing plane.
meshView->SetPlane(0, -1, 0, 0, 0, 0);
meshView->SetFillMesh(false);
meshView->SetViewDrift(driftView);
```

```
meshView->SetArea(-0.01, -0.01, -0.03, 0.01, 0.01, 0.01);
meshView->Plot();
```

# 4.3. Analytic Fields

For two-dimensional geometries consisting of wires, planes and tubes, semi-analytic calculation techniques – based essentially on the capacitance matrix method – are implemented.

## 4.3.1. Describing the Cell

Wires, tubes and planes can be added to the cell layout by means of the following functions:

In all of these functions, the potential v (in V) and a label (used for signal calculation) have to be supplied as parameters.

For wires, the center of the wire (x, y) and its diameter (d) need to be specified. Optional parameters are the wire length, the tension (more precisely, the mass in g of the weight used to stretch the wire during the assembly) and the density (in  $g/cm^3$ ) of the wire material. These parameters have no influence on the electric field. The number of wires that can be added is not limited.

Tube-specific parameters are the radius (r) and the number of edges, which determines the shape of the tube:

- n = 0: cylindrical pipe
- $3 \le n \le 8$ : regular polygon

There can be only one tube in a cell. The tube is always centered at the origin (0,0).

Planes are described by their coordinates. A cell can have at most two x and two y planes. Planes and tubes cannot be used together in the same cell.

The geometry can be reset (thereby deleting all wires, planes and tubes) by

```
void Clear();
```

<sup>&</sup>lt;sup>1</sup>For non-circular tubes, this parameter is the distance between the origin and any of the edges.

Before assembling and inverting the capacitance matrix, a check is performed whether the provided geometry matches the requirements. If necessary, the planes and wires are reordered. Wires outside the tube or the planes as well as overlapping wires are removed.

#### 4.3.2. Periodicities

The class supports simple periodicity in x and y direction. The periodic lengths are set by means of

```
void SetPeriodicityX(const double s);
void SetPeriodicityY(const double s);
```

### 4.3.3. Cell Types

Internally, cells are classified as belonging to one of these types:

**A** non-periodic cells with at most one x and one y plane

**B1X** x-periodic cells without x planes and at most one y plane

**B1Y** y-periodic cells without y planes and at most one x plane

**B2X** cells with two x planes and at most one y plane

**B2Y** cells with two y planes and at most one x plane

**C1** doubly periodic cells without planes

**C2X** doubly periodic cells with x planes

**C2Y** doubly periodic cells with y planes

**C3** doubly periodic cells with x and y planes

**D1** round tubes without axial periodicity

D2 round tubes with axial periodicity

D3 polygonal tubes without axial periodicity

After the cell has been assembled and initialized, the cell type can be retrieved by the function

```
std::string GetCellType();
```

## 4.3.4. Weighting Fields

The weighting field calculation for a readout group -i.e. all elements (wires, planes, etc.) with the same label - is activated by the function

```
void AddReadout(const std::string& label);
```

In addition to the weighting fields of the elements used for the calculation of the (actual) electric field, the weighting field for a strip segment of a plane can also be calculated. Strips can be defined using

**direction** orientation of the strip ('y' or 'z' in case of x-planes, 'x' or 'z' in case of y-planes

x, y coordinate of the plane on which the strip is located

**smin, smax** min. and max. coordinate of the strip

The strip weighting field is calculated using an analytic expression for the field between two infinite parallel plates which are kept at ground potential except for the strip segment, which is raised to 1 V. The anode-cathode distance d to be used for the evaluation of this expression can be set by the user (variable gap in AddStripOnPlaneX, AddStripOnPlaneY). If this variable is not specified (or set to a negative value), the following default values are used:

- if two planes are present in the cell, d is assumed to be the distance between those planes;
- if only one plane is present, d is taken to be the distance to the nearest wire.

Similarly, pixels can be defined using

Pixel weighting fields are calculated using the expressions given in Ref. [16].

# 4.4. Other Components

For simple calculations, the class ComponentConstant can be used. As the name implies, it provides a uniform electric field. The electric field and potential can be specified using

ex, ey, ez components of the electric field

x, y, z coordinates where the potential is specified

v voltage at the given position

The weighting field can be set using

The class ComponentUser takes the electric field and potential from a user-defined function.

**f** pointer to the user function

As an example, let us consider the field in the bulk of an overdepleted planar silicon sensor, given by

$$E(x) = \frac{V - V_{\text{dep}}}{d} + 2x \frac{V_{\text{dep}}}{d^2},$$

where V is the applied bias voltage,  $V_{\text{dep}}$  is the depletion voltage, and d is the thickness of the diode.

A user-defined weighting field can be set using

# 4.5. Visualizing the Field

The class ViewField provides a number of functions for plotting the potential and field of a component.

x0, ..., z1 coordinates of the start and end points of the line along which the potential or field should be plotted.

**option** quantity to be plotted: potential ("v"/"p"/"phi"), magnitude of the electric field ("e"/"field"), or individual components of the field ("ex", "ey", "ez").

drawopt option string passed on to the function Draw() of the ROOT TF2 class.

The first three functions create a contour, surface or other two-dimensional plot in the chosen viewing plane. The last function plots the potential/field along the line  $(x_0, y_0, z_0) \rightarrow (x_1, y_1, z_1)$ .

Similar functions are available for visualizing weighting potentials and fields.

**label** identifier of the electrode for which to plot the weighting field/potential.

The component or sensor from which to retrieve the field to be plotted is set by means of

```
void SetComponent(ComponentBase* c);
void SetSensor(Sensor* s);
```

The viewing plane and the region to be drawn can be specified using

xmin, ymin, xmax, ymax plot range in "local coordinates" (in the current viewing plane).

fx, fy, fz normal vector of the plane.

**x0, y0, z0** in-plane point.

angle rotation angle (in radian).

By default, the viewing plane is the x-y plane (at z=0) and the plot range is retrieved from the bounding box of the component/sensor. The default viewing plane can be restored using

```
void SetDefaultProjection();
```

and the feature to determine the plot area from the bounding box can be activated using

```
void SetArea();
```

The density of the plotting grid can be set using

```
void SetNumberOfSamples1d(const unsigned int n);
void SetNumberOfSamples2d(const unsigned int nx, const unsigned int ny);
```

**n, nx, ny** number of points in x and y direction (default for one-dimensional plots: n = 1000; default for two-dimensional plots:  $n_x = n_y = 200$ )

The number of contour levels can be set using

```
void SetNumberOfContours(const unsigned int n);
```

By default, the voltage range is retrieved from the minimum and maximum values of the potential in the component/sensor, and the range of the electric and weighting fields is "guessed" by taking random samples. This feature can be switched on or off using the function

```
void EnableAutoRange(const bool on = true);
```

If the "auto-range" feature is disabled, the range of the function to be plotted needs to be set using

```
void SetVoltageRange(const double vmin, const double vmax);
void SetElectricFieldRange(const double emin, const double emax);
void SetWeightingFieldRange(const double wmin, const double wmax);
```

#### 4.6. Sensor

The Sensor class can be viewed as a composite of components. In order to obtain a complete description of a detector, it is sometimes useful to combine fields from different Component classes. For instance, one might wish to use a field map for the electric field, calculate the weighting field using analytic methods, and use a parameterized B field. Superpositions of several electric, magnetic and weighting fields are also possible.

Components are added using

```
void AddComponent(ComponentBase* comp);
void AddElectrode(ComponentBase* comp, std::string label);
```

While AddComponent tells the Sensor that the respective Component should be included in the calculation of the electric and magnetic field, AddElectrode requests the weighting field named label to be used for computing the corresponding signal.

To reset the sensor, thereby removing all components and electrodes, use

```
void Clear();
```

The total electric and magnetic fields (sum over all components) at a given position are accessible through the functions ElectricField and MagneticField. The syntax is the same as for the corresponding functions of the Component classes. Unlike the fields, materials cannot overlap. The function Sensor::GetMedium, therefore, returns the first valid drift medium found.

The Sensor acts as an interface to the transport classes.

For reasons of efficiency, it is sometimes useful to restrict charge transport, ionization and similar calculations to a certain region of the detector. This "user area" can be set by

**xmin**, ..., **zmax** corners of the bounding box within which transport is enabled.

Calling SetArea() (without arguments) sets the user area to the envelope of all components (if available).

In addition, the Sensor class takes care of signal calculations (Chapter 7).

## 5. Tracks

The purpose of classes of the type Track is to simulate ionization patterns produced by fast charged particles traversing the detector.

The type of the primary particle is set by the function

```
void SetParticle(std::string particle);
```

#### particle name of the particle

Only particles which are sufficiently long lived to leave a track in a detector are considered. A list of the available particles is given in Table 5.1.

The kinematics of the charged particle can be defined by means of a number of equivalent methods:

- the total energy (in eV) of the particle,
- the kinetic energy (in eV) of the particle,
- the momentum (in eV/c) of the particle,
- the (dimension-less) velocity  $\beta = v/c$ , the Lorentz factor  $\gamma = 1/\sqrt{1-\beta^2}$  or the product  $\beta\gamma$  of these two variables.

The corresponding functions are

```
void SetEnergy(const double e);
void SetKineticEnergy(const double ekin);
void SetMomentum(const double p);
void SetBeta(const double beta);
void SetGamma(const double gamma);
void SetBetaGamma(const double bg);
```

A track is initialized by means of

x0, y0, z0 initial position (in cm)

t0 starting time

dx0, dy0, dz0 initial direction vector

particle		mass [MeV/c²]	charge
e	electron, e-	0.510998910	-1
$e^+$	positron, e+	0.510998910	+1
$\mu^-$	muon, mu-	105.658367	-1
$\mu^+$	mu+	105.658367	+1
$\pi^-$	pion, pi, pi-	139.57018	-1
$\pi^+$	pi+	139.57018	+1
$K^-$	kaon, K, K-	493.677	-1
$\mathcal{K}^+$	K+	493.677	+1
p	proton, p	938.272013	+1
$\overline{p}$	anti-proton, antiproton, p-bar	938.272013	-1
d	deuteron, d	1875.612793	+1

**Table 5.1.** Available charged particles.

The starting point of the track has to be inside an ionizable medium. Depending on the type of Track class, there can be further restrictions on the type of Medium. If the specified direction vector has zero norm, an isotropic random vector will be generated.

After successful initialization, the "clusters" produced along the track can be retrieved by

xcls, ycls, zcls, tcls position (and time) of the ionizing collision

- **n** number of electrons produced in the collision
- **e** transferred energy (in eV)

The function returns false if the list of clusters is exhausted or if there is no valid track.

The concept of a "cluster" deserves some explanation. In the present context it refers to the energy loss in a single ionizing collision of the primary charged particle and the secondary electrons produced in this process.

### **5.1.** Heed

The program Heed [18] is an implementation of the photo-absorption ionization (PAI) model. It was written by I. Smirnov. An interface to Heed is available through the class TrackHeed.

After calling GetCluster, one can retrieve details about the electrons in the present cluster using

```
bool GetElectron(const unsigned int i, double& x, double& y, double& z, double& t, double& e, double& dx, double& dy, double& dz);
```

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#### 5.1.1. Delta Electron Transport

Heed simulates the energy degradation of  $\delta$  electrons and the production of secondary ("conduction") electrons using a phenomenological algorithm described in Ref. [18].

The asymptotic W value (eV) and the Fano factor of a Medium can be specified by the user by means of the functions

```
void Medium::SetW(const double w);
void Medium::SetFanoFactor(const double f);
```

If these parameters are not set, Heed uses internal default values. The default value for the Fano factor is F=0.19.

The transport of  $\delta$  electrons can be activated or deactivated using

```
void EnableDeltaElectronTransport();
void DisableDeltaElectronTransport();
```

If  $\delta$  electron transport is disabled, the number of electrons returned by GetCluster is the number of "primary" ionisation electrons, *i. e.* the photo-electrons and Auger electrons. Their kinetic energies and locations are accessible through the function GetElectron.

If  $\delta$  electron transport is enabled (default setting), the function GetElectron returns the locations of the "conduction" electrons as calculated by the internal  $\delta$  transport algorithm of Heed. Since this method does not provide the energy and direction of the secondary electrons, the corresponding parameters in GetElectron are not meaningful in this case.

#### **5.1.2.** Photon Transport

Heed can also be used for the simulation of x-ray photoabsorption.

x0, y0, z0, t0 initial position and time of the photon

e0 photon energy in eV

dx0, dy0, dz0 direction of the photon

**nel** number of photoelectrons and Auger-electrons produced in the photon conversion

### 5.1.3. Magnetic fields

By default, Heed does not take the electric and magnetic field in the sensor into account for calculating the charged-particle trajectory. In order to use the electric and/or magnetic field in the stepping algorithm, the functions

```
EnableElectricField();
EnableMagneticField();
```

need to be called before simulating a track. Depending on the strength of the magnetic field, it might be necessary to adapt the limits/parameters used in the stepping algorithm in order to obtain a smoothly curved trajectory as, for instance, in the example below.

```
// Get the default parameters.
double maxrange = 0., rforstraight = 0., stepstraight = 0., stepcurved = 0.;
track->GetSteppingLimits(maxrange, rforstraight, stepstraight, stepcurved);
// Reduce the step size [rad].
stepcurved = 0.02;
track->SetSteppingLimits(maxrange, rforstraight, stepstraight, stepcurved);
```

### 5.2. **SRIM**

SRIM<sup>1</sup> is a program for simulating the energy loss of ions in matter. It produces tables of stopping powers, range and straggling parameters that can subsequently be imported in Garfield using the class TrackSrim. The function

```
bool ReadFile(const std::string& file)
```

returns true if the SRIM output file was read successfully. The SRIM file contains the following data

- a list of kinetic energies at which losses and straggling have been computed;
- average energy lost per unit distance via electromagnetic processes, for each energy;
- average energy lost per unit distance via nuclear processes, for each energy;
- projected path length, for each energy;
- longitudinal straggling, for each energy;
- transverse straggling, for each energy.

These can be visualized using the functions

```
void PlotEnergyLoss();
void PlotRange();
void PlotStraggling();
```

and printed out using the function <code>TrackSrim::Print()</code>. In addition to these tables, the file also contains the mass and charge of the projectile, and the density of the target medium. These properties are also imported and stored by <code>TrackSrim</code> when reading in the file. Unlike in case of Heed, the particle therefore does not need to be specified by the user. In addition, the following parameters need to be supplied "by hand" by the user.

<sup>&</sup>lt;sup>1</sup>Stopping and Range of lons in Matter, www.srim.org

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Model	Description
0	No fluctuations
1	Untruncated Landau distribution
2	Vavilov distribution (provided the kinematic parameters are within the range of applicability, otherwise fluctuations are disabled)
3	Gaussian distribution
4	Combination of Landau, Vavilov and Gaussian models, each applied in their alleged domain of applicability

**Table 5.2.** Fluctuation models in SRIM.

- the work function (in eV) of the medium (TrackSrim::SetWorkFunction),
- the Fano factor of the medium (TrackSrim::SetFanoFactor),
- the atomic number Z and mass number A of the medium (TrackSrim::SetAtomicMassNumbers).

Note that in the formulae used by TrackSrim, Z and A only enter in the form of the ratio Z/A. For gas mixtures, these numbers should therefore be chosen such that the average  $\langle Z/A \rangle$  of the mixture is reproduced.

TrackSrim tries to generate individual tracks which statistically reproduce the average quantities calculated by SRIM. Starting with the energy specified by the user, it iteratively

- computes (by interpolating in the tables) the electromagnetic and nuclear energy loss per unit length at the current particle energy,
- calculates a step with a length over which the particle will produce on average a certain number of electrons.
- updates the trajectory based on the longitudinal and transverse scatter at the current particle energy,
- calculates a randomised actual electromagnetic energy loss over the step and updates the particle energy.

This is repeated until the particle has no energy left or leaves the geometry. The model for randomising the energy loss over a step can be set using the function

```
void SetModel(const int m);
```

**m** fluctuation model to be used (Table 5.2); the default setting is model 4.

Transverse and longitudinal straggling can be switchen on or off using

```
void EnableTransverseStraggling();
void DisableTransverseStraggling();
void EnableLongitudinalStraggling();
void DisableLongitudinalStraggling();
```

If energy loss fluctuations are used, longitudinal straggling should be disabled. By default, transverse straggling is switched on and longitudinal straggling is switched off.

Chapter 5. Tracks

SRIM is aimed at low energy nuclear particles which deposit large numbers of electrons in a medium. The grouping of electrons to a cluster is therefore somewhat arbitrary. By default, TrackSrim will adjust the step size such that there are on average 100 clusters on the track. If the user specifies a target cluster size, using

```
void SetTargetClusterSize(const int n);
```

the step size will be chosen such that a cluster comprises on average n electrons. Alternatively, if the user specifies a maximum number of clusters, using

```
void SetClustersMaximum(const int n);
```

the step size will be chosen such that on average there are n / 2 clusters on the track.

## 6. Charge Transport

On a phenomenological level, the drift of charge carriers under the influence of an electric field **E** and a magnetic field **B** is described by the first order equation of motion

$$\dot{\mathbf{r}} = \mathbf{v}_{d}(\mathbf{E}(\mathbf{r}), \mathbf{B}(\mathbf{r})), \tag{6.1}$$

where  $\mathbf{v}_d$  is the drift velocity. For the solution of (6.1), two methods are available in Garfield++:

- Runge-Kutta-Fehlberg integration, and
- Monte Carlo integration (AvalancheMC).

For accurate simulations of electron trajectories in small-scale structures (with characteristic dimensions comparable to the electron mean free path), and also for detailed calculations of ionisation and excitation processes, transporting electrons on a microscopic level – *i. e.* based on the second-order equation of motion – is the method of choice. Microscopic tracking of electrons is dealt with by the class AvalancheMicroscopic.

## 6.1. Runge-Kutta-Fehlberg Integration

This method is implemented in the class DriftLineRKF.

## **6.2. Monte Carlo Integration**

In the class AvalancheMC, Eq. (6.1) is integrated in a stochastic manner:

- a step of length  $\Delta s = v_d \Delta t$  in the direction of the drift velocity  $\mathbf{v}_d$  at the local field is calculated (with either the time step  $\Delta t$  or the distance  $\Delta s$  being specified by the user);
- a random diffusion step is sampled from three uncorrelated Gaussian distributions with standard deviation  $\sigma_L = D_L \sqrt{\Delta s}$  for the component parallel to the drift velocity and standard deviation  $\sigma_T = D_T \sqrt{\Delta s}$  for the two transverse components;
- the two steps are added vectorially and the location is updated.

The functions for setting the step size are

```
void SetTimeSteps(const double d = 0.02);
void SetDistanceSteps(const double d = 0.001);
void SetCollisionSteps(const int n = 100);
```

In the first case the integration is done using fixed time steps (default: 20 ps), in the second case using fixed distance steps (default:  $10 \mu m$ ). Calling the third function instructs the class to do the

integration with exponentially distributed time steps with a mean equal to the specified multiple of the "collision time"

$$\tau = \frac{m v_d}{q E}.$$

The third method is activated by default.

Drift line calculations are started using

#### x0, y0, z0, t0 initial position and time

The trajectory can be retrieved using

The calculation of an avalanche initiated by an electron, a hole or an electron-hole pair is done using

The flags hole and electron specify whether multiplication of holes and electrons, respectively, should be taken into account in the simulation. In case of gas-based detectors, only AvalancheElectron with hole = false is meaningful.

The starting and endpoints of electrons in the avalanche can be retrieved using

i index of the electron

x0, y0, z0, t0 initial position and time of the electron

x1, y1, z1, t1 final position and time of the electron

**status** status code indicating why the tracking of the electron was stopped.

Analogous functions are available for holes and ions.

The functions

```
void EnableMagneticField();
```

instructs the class to consider not only the electric but also the magnetic field in the evaluation of the transport parameters. By default, magnetic fields are not taken into account.

For debugging purposes, attachment and diffusion can be switched off using

```
void DisableAttachment();
void DisableDiffusion();
```

A time interval can be set using

```
void SetTimeWindow(const double t0, const double t1);
```

- t0 lower limit of the time window
- **t1** upper limit of the time window

Only charge carriers with a time coordinate  $t \in [t_0, t_1]$  are tracked. If the time coordinate of a particle crosses the upper limit, it is stopped and assigned the status code -17. Slicing the calculation into time steps can be useful for instance for making a movie of the avalanche evolution or for calculations involving space charge. The time window can be removed using

```
void UnsetTimeWindow();
```

## 6.3. Microscopic Tracking

Microscopic tracking is (at present) only possible for electrons. It is implemented in the class AvalancheMicroscopic. A calculation is started by means of

```
void AvalancheElectron(const double x0, const double y0, const double z0, const double t0, const double e0, const double dx0 = 0., const double dy0 = 0., const double dz0 = 0.);
```

x0, y0, z0, t0 initial position and time

**e0** initial energy (eV)

dx0, dy0, dz0 initial direction

If the norm of the direction vector is zero, the initial direction is randomized.

After the calculation is finished, the number of electrons (ne) and ions (ni) produced in the avalanche can be retrieved using

```
void GetAvalancheSize(int& ne, int& ni);
```

status code	meaning
-1	particle left the drift area
-3	calculation abandoned (error, should not happen)
-5	particle not inside a drift medium
-7	attachment
-16	energy below transport cut
-17	outside the time window

**Table 6.1.** Status codes for the termination of drift lines.

Information about the "history" of each avalanche electron can be retrieved by

i index of the electron

x0, y0, z0, t0, e0 initial position, time and energy of the electron

x1, y1, z1, t1, e1 final position, time and energy of the electron

status status code indicating why the tracking of the electron was stopped.

A list of status codes is given in Table 6.1.

The function

traces only the initial electron but not the secondaries produced along its drift path (the input parameters are the same as for AvalancheElectron).

The electron energy distribution can be extracted in the following way:

```
AvalancheMicroscopic* aval = new AvalancheMicroscopic();

// Make a histogram (100 bins between 0 and 100 eV).

TH1F* hEnergy = new TH1F("hEnergy", "Electron_energy", 100, 0., 100.);

// Pass the histogram to the avalanche class.

aval->EnableElectronEnergyHistogramming(hEnergy);
```

After each collision, the histogram is filled with the current electron energy.

The effect of magnetic fields can be included in the stepping algorithm using the function

```
void EnableMagneticField();
```

By default, magnetic fields are not taken into account in the calculation.

Using

```
void EnableAvalancheSizeLimit(const int size);
```

the size of an electron avalanche can be limited. After the avalanche has reached the specified max. size, no further secondaries are added to the stack of electrons to be transported.

Like in AvalancheMC a time window can be set/unset using

```
void SetTimeWindow(const double t0, const double t1);
void UnsetTimeWindow();
```

An energy threshold for transporting electrons can be applied using

```
void SetElectronTransportCut(const double cut);
```

```
cut energy threshold (in eV)
```

The tracking of an electron is aborted if its energy falls below the transport cut. This option can be useful for  $\delta$  electron studies in order to stop the calculation once the energy of an electron is below the ionization potential of the gas. The transport cut can be removed by setting the threshold to a negative value. By default, no cut is applied.

In order to extract information from the avalanche on a collision-by-collision basis, so-called "user handles" are available.

```
void SetUserHandleStep(void (*f)(double x, double y, double z,
                               double t, double e,
                               double dx, double dy, double dz,
                               bool hole));
void UnsetUserHandleStep();
void SetUserHandleCollision(void (*f)(double x, double y, double z, double t,
                                   int type, int level, Medium* m,
                                   double e0, double e1,
                                   double dx0, double dy0, double dz0,
                                   double dx1, double dy1, double dz1));
void UnsetUserHandleCollision();
void SetUserHandleAttachment(void (*f)(double x, double y, double z,
                                    double t,
                                    int type, int level, Medium* m));
void UnsetUserHandleAttachment();
void SetUserHandleInelastic(void (*f)(double x, double y, double z,
                                   double t,
                                   int type, int level, Medium* m));
void UnsetUserHandleInelastic();
void SetUserHandleIonisation(void (*f)(double x, double y, double z,
                                    double t,
                                    int type, int level, Medium* m));
void UnsetUserHandleIonisation();
```

The function specified in SetUserHandleStep is called prior to each free-flight step. The parameters passed to this function are

x, y, z, t position and time,

e energy before the step

dx, dy, dz direction,

**hole** flag indicating whether the particle is an electron or a hole.

The "user handle" function set via SetUserHandleCollision is called every time a real collision (as opposed to a null collision) occurs. The "user handle" functions for attachment, ionisation, and inelastic collisions are called each time a collision of the respective type occurs. In this context, inelastic collisions also include excitations. The parameters passed to these functions are

x, y, z, t the location and time of the collision,

**type** the type of collision (see Table 3.2),

**level** the index of the cross-section term (as obtained from the Medium),

m a pointer to the current Medium.

In the function set using SetUserHandleCollision, the energy and the direction vector before and after the collision are available in addition.

In the following example we want all excitations which occur to undergo a special treatment.

## 6.4. Visualizing Drift Lines

For plotting drift lines and tracks the class ViewDrift can be used. After attaching a ViewDrift object to a transport class, e. g. using

```
void AvalancheMicroscopic::EnablePlotting(ViewDrift* view);
void AvalancheMC::EnablePlotting(ViewDrift* view);
void Track::EnablePlotting(ViewDrift* view);
```

ViewDrift stores the trajectories which are calculated by the transport class. The drawing of the trajectories is triggered by the function

```
void ViewDrift::Plot();
```

In case of AvalancheMicroscopic, it is usually not advisable to plot every single collision. The number of collisions to be skipped for plotting can be set using

```
void AvalancheMicroscopic::SetCollisionSteps(const int n);
```

**n** number of collisions to be skipped

Note that this setting does not affect the transport of the electron as such, the electron is always tracked rigorously through single collisions.

## 7. Signals

Signals are calculated using the Shockley-Ramo theorem. The current i(t) induced by a particle with charge q at a position  $\mathbf{r}$  moving at a velocity  $\mathbf{v}$  is given by

$$i(t) = -q\mathbf{v} \cdot \mathbf{E}_w(\mathbf{r})$$
,

where  $\mathbf{E}_{w}$  is the so-called weighting field for the electrode to be read out.

The basic steps for calculating the current induced by the drift of electrons and ions/holes are:

- 1. Prepare the weighting field for the electrode to be read out. This step depends on the field calculation technique (*i. e.* the type of Component) which is used (see Chapter 4).
- 2. Tell the Sensor that you want to use this weighting field for the signal calculation.

```
void Sensor::AddElectrode(ComponentBase* cmp, std::string label);
```

where cmp is a pointer to the Component which calculates the weighting field, and label (in our example "readout") is the name you have assigned to the weighting field in the previous step.

3. Setup the binning for the signal calculation.

The first parameter in this function is the lower time limit (in ns), the second one is the bin width (in ns), and the last one is the number of time bins.

4. Switch on signal calculation in the transport classes using

```
void AvalancheMicroscopic::EnableSignalCalculation();
void AvalancheMC::EnableSignalCalculation();
```

The Sensor then records and accumulates the signals of all avalanches and drift lines which are simulated.

5. The calculated signal can be retrieved using

```
double Sensor::GetSignal(const std::string label, const int bin);
double Sensor::GetElectronSignal(const std::string label, const int bin);
double Sensor::GetIonSignal(const std::string label, const int bin);
```

The functions GetElectronSignal and GetIonSignal return the signal induced by negative and positive charges, respectively. GetSignal returns the sum of both electron and hole signals.

6. After the signal of a given track is finished, call

```
void Sensor::ClearSignal();
```

to reset the signal to zero.

For plotting the signal, the class ViewSignal can be used. As an illustration of the above recipe consider the following example.

```
// Electrode label
const std::string label = "readout";
// Setup the weighting field.
// In this example we use a FEM field map.
ComponentAnsys123* fm = new ComponentAnsys123();
fm->SetWeightingField("WPOT.lis", label);
Sensor* sensor = new Sensor();
sensor->AddComponent(fm);
sensor->AddElectrode(fm, label);
// Setup the binning (0 to 100 ns in 100 steps).
const double tStart = 0.;
const double tStop = 100.;
const int nSteps = 100;
const double tStep = (tStop - tStart) / nSteps;
AvalancheMicroscopic* aval = new AvalancheMicroscopic();
aval->SetSensor(sensor);
aval->EnableSignalCalculation();
// Calculate some drift lines.
// Plot the induced current.
ViewSignal* signalView = new ViewSignal(tStart, tStep, nSteps);
signalView->SetSensor(sensor);
signalView->Plot(label);
```

#### 7.1. Readout Electronics

In order to model the signal-processing by the front-end electronics, the "raw signal" -i.e. the induced current - can be convoluted with a so-called "transfer function". The transfer function to be applied can be set using

in which case the transfer function will be calculated by interpolation of the values provided in the table.

In order to convolute the presently stored signal with the transfer function (specified using the above function), the function

```
bool Sensor::ConvoluteSignal();
```

can be called.

As an example, consider the following transfer function

$$f(t) = e^{\frac{t}{\tau}} e^{1-t/\tau}, \qquad \tau = 25 \text{ ns}$$

```
double transfer(double t) {
  const double tau = 25.;
  return (t / tau) * exp(1 - t / tau);
}
int main(int argc, char* argv[]) {
  // Setup component, media, etc.
  ...
  Sensor* sensor = new Sensor();
  sensor->SetTransferFunction(transfer);
  // Calculate the induced current.
  ...
  // Apply the transfer function.
  sensor->ConvoluteSignal();
  ...
}
```

## A. Units and Constants

The basic units are cm for distances, g for (macroscopic) masses, and ns for times. Particle energies, momenta and masses are expressed in eV, eV/c and eV/ $c^2$ , respectively. For example, the electron mass is given in eV/ $c^2$ , whereas the mass density of a material is given in g/cm<sup>3</sup>. The mass of an atom is specified in terms of the atomic mass number A.

There are a few exceptions from this system of units, though.

- The unit for the magnetic field **B** corresponding to the above system of units  $(10^{-5} \text{ Tesla})$  is impractical. Instead, magnetic fields are expressed in Tesla.
- Pressures are specified in Torr.
- Electric charge is expressed in fC.

A summary of commonly used quantities and their units is given in Table A.1.

The values of the physical constants used in the code are defined in the file FundamentalConstants.hh.

physical quantity	unit
length	cm
mass	g
time	ns
temperature	K
electric potential	V
electric charge	fC
energy	eV
pressure	Torr
electric field	V / cm
magnetic field	Tesla
electric current	fC / ns
angle	rad

 Table A.1. Physical units.

# **B.** Gases

Table B.1 shows a list of the gases available in the current version of Magboltz. The star rating represents an estimate of the reliability of the cross-section data for the respective gas. A rating of "5\*" indicates a detailed, well-validated description of the cross-sections, while "2\*" indicates a low quality, that is a coarse modelling of the cross-sections associated with large uncertainties.

chem. symbol	name	rating
<sup>4</sup> He	helium	 5*
<sup>3</sup> He	helium-3	5*
Ne	neon	5*
Ar	argon	5*
Kr	krypton	4*
Xe	xenon	4*
Cs	cesium	2*
Hg	mercury	2*
$H_2$	hydrogen	5*
para H <sub>2</sub>	para hydrogen	4*
$D_2$	deuterium	5*
$N_2$	nitrogen	5*
$O_2$	oxygen	5*
F <sub>2</sub>	fluorine	2*
CO	carbon monoxide	5*
NO	nitric oxide	2*
H <sub>2</sub> O	water	5*
$CO_2$	carbon dioxide	5*
$N_2O$	nitrous oxide	4*
O <sub>3</sub>	ozone	3*
$H_2S$	hydrogen sulfide	2*
COS	carbonyl sulfide	2*
$CS_2$	carbon disulfide	2*
CH <sub>4</sub>	methane	5*
$CD_4$	deuterated methane	4*
$C_2H_6$	ethane	5*
$C_3H_8$	propane	4*
$nC_4H_{10}$	n-butane	4*
$iC_4H_{10}$	isobutane	4*
$nC_5H_{12}$	n-pentane	4*
$neo-C_5H_{12}$	neopentane	4*
$C_2H_4$	ethene	4*
$C_2H_2$	acetylene	4*

$C_3H_6$	propene	4*
cC <sub>3</sub> H <sub>6</sub>	cyclopropane	4*
CH <sub>3</sub> OH	methanol	4*
$C_2H_5OH$	ethanol	4*
$C_3H_7OH$	isopropanol	3*
$nC_3H_7OH$	n-propanol	3*
$C_3H_8O_2$	methylal	2*
$C_4H_{10}O_2$	DME	4*
CF <sub>4</sub>	tetrafluoromethane	5*
CHF <sub>3</sub>	fluoroform	3*
$C_2F_6$	hexafluoroethane	4*
$C_2H_2F_4$	tetrafluoroethane	3*
$C_3F_8$	octafluoropropane	3*
SF <sub>6</sub>	sulfur hexafluoride	4*
BF <sub>3</sub>	boron trifluoride	4*
CF <sub>3</sub> Br	bromotrifluoromethane	3*
NH <sub>3</sub>	ammonia	4*
$N(CH_3)_3$	TMA	3*
SiH <sub>4</sub>	silane	3*
GeH <sub>4</sub>	germane	4*

**Table B.1.** Gases available in Magboltz 11.7

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