# Garfield++ User Guide



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## 1. Introduction

Garfield++ is an object-oriented toolkit for the detailed simulation of particle detectors based on ionisation measurement in gases or semiconductors.

For calculating electric fields, the following 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 [44];
- an interface with the neBEM field solver [20, 21].

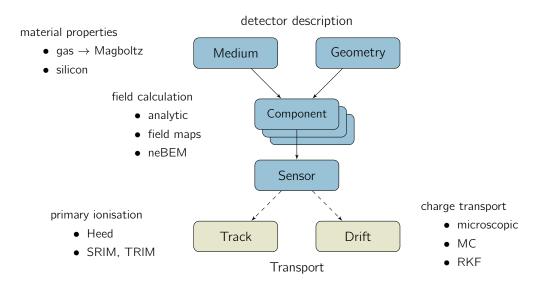
For calculating the transport properties of electrons in gas mixtures, an interface to the Magboltz program [6, 7] is available.

The ionisation pattern produced by relativistic charged particles can be simulated using the program "Heed" [41]. For simulating the ionisation produced by low-energy ions, results calculated using the SRIM software package [48] can be imported.

The present document aims to give an overview of Garfield++, 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 website http://garfieldpp.web.cern.ch/garfieldpp/. If you have questions, doubts, comments etc. about the code or this manual, please do not hesitate to contact the authors.

Fig. 1.1 gives an overview of the different types of classes and their interplay. Readers familiar with the structure of (Fortran) Garfield [46] 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.

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 ROOT framework [9].



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

## 2. Getting started

## 2.1. Prerequisites

To build Garfield++, and a project or application that depends on it, you need to have the following software correctly installed and configured on your machine.

- ROOT 6 (preferably ROOT 6.20 or higher),
- GSL<sup>1</sup> (GNU Scientific Library),
- CMake<sup>2</sup> (version 3.9 or or later),
- a C++ compiler compatible with the same C++ standard with which ROOT was compiled,
- a Fortran compiler,
- (optionally) OpenMP<sup>3</sup> to enable some additional parallel computations.

For ROOT installation instructions, see

- https://root.cern.ch/building-root or
- https://root.cern.ch/downloading-root.

Declare the ROOTSYS environment variable to point to the base folder of the ROOT installation. This operation is typically performed by the ROOT initialization script, called thisroot.sh. Executing that script will also correctly initialize the right environment variables to install Garfield.

## 2.2. Downloading the source code

The Garfield++ source code is managed by a git repository hosted on the CERN GitLab<sup>4</sup> server, https://gitlab.cern.ch/garfield/garfieldpp.

Choose a folder where the source code is to be downloaded. Note that the chosen folder must be empty or non-existing. We will identify this folder with an environment variable named GARFIELD\_HOME. Note that this is not strictly required and you can simply replace the chosen path in all the following commands where that variable appears. To define that variable in the bash shell family type

export GARFIELD\_HOME=/home/git/garfield

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

For (t)csh-type shells, type

<sup>&</sup>lt;sup>1</sup>https://www.gnu.org/software/gsl/

<sup>&</sup>lt;sup>2</sup>https://cmake.org/

<sup>&</sup>lt;sup>3</sup>https://openmp.org

<sup>&</sup>lt;sup>4</sup>https://gitlab.cern.ch/help/gitlab-basics/start-using-git.md

setenv GARFIELD\_HOME /home/git/garfield

Download the code from the repository, either using SSH access<sup>5</sup>

git clone ssh://git@gitlab.cern.ch:7999/garfield/garfieldpp.git \$GARFIELD\_HOME

or HTTPS access

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

To update the source code with the latest changes, run the following command from the GARFIELD\_HOME folder:

git pull

## 2.3. Building the project

Garfield++ uses the CMake build generator to create the actual build system that is used to compile the binaries of the programs we want to build. CMake is a cross-platform scripting language that allows one to define the rules to build and install a complex project and takes care of generating the low-level files necessary for the build system of choice. On Linux systems that build system typically defaults to the GNU Make program. We will therefore assume that GNU Make is used to build Garfield++.

The process is divided in two phases. During the build phase, the source files will be used to generate the necessary binaries, along with a large quantities of temporary files, used in the intermediate phases of the build. In the install phase only the necessary files are copied to the final destination.

First we will create a build directory, and move into it to execute the first phase. This can be any folder on the user filesystem. For simplicity we will use a subfolder of the place where the source code was downloaded.

mkdir \$GARFIELD\_HOME/build
cd build

Inside the build directory we can run CMake to generate the build system.

cmake \$GARFIELD\_HOME

The build can be customized in several ways through CMake by defining a set of internal variables that modify the output accordingly. To set a new value for a CMake variable one can use the -D<var>=<value> syntax at the command line. The most relevant parameters that a user may want to customize are described below.

<sup>&</sup>lt;sup>5</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.

**Installation folder** By default Garfield is installed in the folder pointed to by the environment variable GARFIELD\_INSTALL or, if that variable is missing, in a subfolder of the source directory, that is \$GARFIELD\_HOME/install. To install it elsewhere define the CMAKE\_INSTALL\_PREFIX variable, using a similar command with an appropriate target folder:

cmake -DCMAKE\_INSTALL\_PREFIX=/home/mygarfield \$GARFIELD\_HOME

**Debug and optimization mode** This is controlled by the CMake variable CMAKE\_BUILD\_TYPE which can have one of the following values:

Release Enables all the compiler optimizations to achieve the best performance

**Debug** Disables all the compiler optimizations and add the debug symbols to the binary to be able to use an external debugger on the code

**RelWithDebInfo** Enables all the compiler optimization but stores the debug symbols in the final binaries. This increases the binary size and may reduce the performances

**MinSizeRel** Enables all the compiler optimization necessary to obtain the smaller executable possible

By default Garfield++ is built in *Release* mode. To add the debugging symbol use the following command before building

cmake -DCMAKE\_BUILD\_TYPE=RelWithDebInfo \$GARFIELD\_HOME

Those variables and many other can be set through a textual or graphical user interface, ccmake or cmake-gui respectively, that needs to be installed separately.

Once CMake has generated the build system, you can execute the following to compile and install Garfield++.

make && make install

Once the installation is done, Garfield requires the definition of an environment variable named HEED\_DATABASE to identify the location of the Heed cross-section database, located in the subfolder share/Heed/database of the installation path. Additionally, to build applications that make use of Garfield it may be convenient to append the installation path to an environment variable named CMAKE\_PREFIX\_PATH. To simplify all this, the build procedure generates a shell script, named setupGarfield.sh, located in the subfolder share/Garfield of the installation path, which correctly defines all those variables. You can append the execution of that script to your shell initialization script (e. g. .bashrc for the Bash shell) to setup Garfield automatically.

After updating the source code you can run the make command from the build folder to update the build. Sometimes it may be necessary to restart from a clean slate, in which case one can remove the build folder completely and restart the procedures of this section.

## 2.4. Building an application

The recommended way to build a Garfield++-based application is using CMake. Let us consider as an example the program gem.C (see Sec. 2.5.2) which together with the corresponding

CMakeLists.txt can be found in the directory Examples/Gem of the source tree. As a starting point, we assume that you have built Garfield++ using the instructions above and set up the necessary environment variables.

• To keep the source tree clean, and since you will probably want to modify the program according to your needs, it is a good idea to copy the folder to another location.
cp -r \$GARFIELD_HOME/Examples/Gem .
Create a build directory.
mkdir Gem/build; cd Gem/build
Setup the environment.
<pre>source \$GARFIELD_HOME/install/share/Garfield/setupGarfield.sh</pre>
• Run CMake,
cmake
followed by
make
• In addition to the executable (gem), the build folder should now also contain the field map (*.lis) files which have been copied there during the CMake step.

•	10	run	the	app	lica	tion,	type
---	----	-----	-----	-----	------	-------	------

./gem

## 2.5. Examples

Section 2.5.1 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 introduced in Sec. 2.5.2.

Section 2.5.3 presents an example of the simulation of drift lines and induced signals in a silicon sensor.

Further examples can be found on the webpage (http://garfieldpp.web.cern.ch/garfieldpp/Examples) and in the directory Examples of the source tree.

#### 2.5.1. Drift tube

In this example, we consider a drift tube with an outer diameter of  $15 \, \text{mm}$  and a wire diameter of  $50 \, \mu \text{m}$ , similar to the ATLAS small-diameter muon drift tubes (sMDTs).

#### 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;
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 a 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;
gas.GenerateGasTable(ncoll);
```

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");
```

Once we have saved the transport parameters to file we can skip the steps above, and simply import the table in our program using

```
gas.LoadGasFile("ar_93_co2_7.gas");
```

In order to make sure the calculation of the gas table was successful, it is a good idea to plot, for instance, the drift velocity as a function of the electric field.

```
ViewMedium mediumView;
mediumView.SetMedium(&gas);
mediumView.PlotElectronVelocity('e');
```

#### **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;

We first set the medium inside the active region.

```
cmp.SetMedium(&gas);
```

Next we add the elements defining the electric field, i.e. the wire and the tube.

```
// Wire radius [cm]
const double rWire = 25.e-4;
// Outer radius of the tube [cm]
const double rTube = 0.71;
// Voltages
const double vWire = 2730.;
const double vTube = 0.;
// Add the wire in the centre.
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 ComponentAnalyticField to prepare the solution for the weighting potential and 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;

// 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");
```

We further need to set the time interval within which the signal is recorded and the granularity (bin width). In this example, we use use 1000 bins with a width of 0.5 ns.

```
const double tstep = 0.5;
const double tmin = -0.5 * tstep;
const unsigned int nbins = 1000;
sensor.SetTimeWindow(tmin, tstep, nbins);
```

#### Drift lines from a track

We use Heed (Sec. 5.1) to simulate the ionisation produced by a charged particle crossing the tube (a 170 GeV muon in our example).

```
TrackHeed track;
track.SetParticle("muon");
track.SetEnergy(170.e9);
track.SetSensor(&sensor);
```

The drift lines of the electrons created along the track are simulated along the track are calculated using Runge-Kutta-Fehlberg (RKF) integration, implemented in the class DriftLineRKF. This method uses the previously computed tables of transport parameters to calculate drift lines and multiplication.

```
DriftLineRKF drift;
drift.SetSensor(&sensor);
// Switch on signal calculation.
drift.EnableSignalCalculation();
```

Let us consider a track that passes at a distance of 3 mm from the wire centre. After simulating the passage of the charged particle, we loop over the "clusters" (*i.e.* the ionizing collisions of the primary particle) along the track and calculate a drift line for each electron produced in the cluster.

```
const double rTrack = 0.3;
const double x0 = rTrack;
const double y0 = -sqrt(rTube * rTube - rTrack * rTrack);
track.NewTrack(x0, y0, 0, 0, 0, 1, 0);
// Loop over the clusters along the track.
double xc = 0., yc = 0., zc = 0., tc = 0., ec = 0., extra = 0.;
int nc = 0;
while (track.GetCluster(xc, yc, zc, tc, nc, ec, extra)) {
  // Loop over the electrons in the cluster.
  for (int k = 0; k < nc; ++k) {
    double xe = 0., ye = 0., ze = 0., te = 0., ee = 0.;
    double dx = 0., dy = 0., dz = 0.;
    track.GetElectron(k, xe, ye, ze, te, ee, dx, dy, dz);
    drift.DriftElectron(xe, ye, ze, te);
 }
}
```

As a check whether the simulation is doing something sensible, it can be useful to visualize the drift lines. Before simulating the charged particle track and the electron drift lines, we have to instruct TrackHeed and DriftLineRKF to pass the coordinates of the clusters and the points along the drift line to a ViewDrift object which then takes care of plotting them.

```
// Create a canvas.
cD = new TCanvas("cD", "", 600, 600);
ViewDrift driftView;
driftView.SetCanvas(cD);
drift.EnablePlotting(&driftView);
```

```
track.EnablePlotting(&driftView);
```

We use the class ViewCell to draw the outline of the tube and the position of the wire on the same plot as the drift lines.

```
ViewCell cellView;
cellView.SetCanvas(cD);
cellView.SetComponent(&cmp);
```

After we've simulated all drift lines from a charged particle track, we create a plot using

```
cellView.Plot2d();
constexpr bool twod = true;
constexpr bool drawaxis = false;
driftView.Plot(twod, drawaxis);
```

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

```
ViewSignal signalView;
signalView.SetSensor(&sensor);
signalView.PlotSignal("s");
```

#### Ion tail

So far we have only considered the electron contribution to the induced signal. If we want to include the contribution from the ions produced in the avalanche we need to import a table of ion mobilities

```
auto installdir = std::getenv("GARFIELD_INSTALL");
const std::string path = installdir;
gas.LoadIonMobility(path + "/share/Garfield/Data/IonMobility_Ar+_Ar.txt");
and we need to call
drift.EnableIonTail();
```

before simulating the drift lines.

#### 2.5.2. GEM

In this example, we will simulate the drift of electrons and ions in a standard GEM [38], which consists of a  $50\,\mu m$  thick kapton foil coated on both sides with a  $5\,\mu m$  layer of copper, with a hexagonal pattern of holes (outer hole diameter:  $70\,\mu m$ , inner hole diameter:  $50\,\mu m$ , pitch:  $140\,\mu m$ ) etched into the foil.

#### Field map

As a first step, we need to calculate the electric field in the GEM. Currently this calculation has to be performed using an external field solver like Ansys [4], Elmer [15], or Comsol [11]. In this example, we use Ansys, but the steps for importing field maps from other programs are very similar.

In the following we assume that the output files resulting from the Ansys run are located in the current working directory. 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;
// Load the field map.
fm.Initialise("ELIST.lis", "NLIST.lis", "MPLIST.lis", "PRNSOL.lis", "mm");
// Set the periodicities
fm.EnableMirrorPeriodicityX();
fm.EnableMirrorPeriodicityY();
// Print some information about the cell dimensions.
fm.PrintRange();
```

We need to apply mirror periodicity in x and y in ComponentAnsys123 since we had exploited the symmetry of the geometry and modelled only half a hole in Ansys.

Using the class ViewField, we do a visual inspection of the field map to make sure it makes sense. We first make a plot of the potential along the hole axis (z axis).

```
ViewField fieldView;
fieldView.SetComponent(&fm);
// Plot the potential along the hole axis.
fieldView.PlotProfile(0., 0., 0.02, 0., 0., -0.02);
```

We also make a contour plot of the potential in the x-z plane.

```
const double pitch = 0.014;
// Set the normal vector (0, -1, 0) of the viewing plane.
fieldView.SetPlane(0., -1., 0., 0., 0.);
fieldView.SetArea(-pitch / 2., -0.02, pitch / 2., 0.02);
fieldView.SetVoltageRange(-160., 160.);
fieldView.PlotContour();
```

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

```
Sensor sensor;
sensor.AddComponent(&fm);
```

Normally, particles are transported until they exit the mesh. To speed up the calculation we restrict the drift region to  $-100\mu m < z < +250\mu m$ .

```
sensor.SetArea(-5 * pitch, -5 * pitch, -0.01, 5 * pitch, 5 * pitch, 0.025);
```

#### Gas

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

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

**Electron collision rates** In this example, we will simulate electron avalanches using a "microscopic" Monte Carlo method, based on the electron-atom/molecule cross-sections in the database of the Magboltz program. As discussed in more detail in Sec. 6.3, the algorithm takes as input the collision rates (as function of the electron's kinetic energy) for each scattering mechanism that can take place in the gas. The preparation of the tables of collision rates and the interpolation in these tables is done by the class MediumMagboltz, which — as the name suggests — provides an interface to Magboltz.

In MediumMagboltz the collision rates are stored on an evenly spaced energy grid. The max. energy can be set by the user. For avalanche calculations,  $50 - 200 \, \text{eV}$  is usually a reasonable choice.

```
gas.SetMaxElectronEnergy(200.);
gas.Initialise();
```

**Penning transfer** Argon includes a number of excitation levels with an excitation energy exceeding the ionisation potential of  $CO_2$  (13.78 eV). These excited states can contribute to the gain, since (part of) the excitation energy can be transferred to a  $CO_2$  molecule through collisions or by photo-ionisation.

In the simulation, this so-called Penning effect can be described in terms of a probability r that an excitation is converted to an ionising collision (Sec. 3.2.3).

```
// Penning transfer probability.
const double rPenning = 0.57;
// Mean distance from the point of excitation.
const double lambdaPenning = 0.;
gas.EnablePenningTransfer(rPenning, lambdaPenning, "ar");
```

**lon transport properties** Unlike electrons, ions cannnot be tracked microscopically in Garfield++. Moreover, there is no program like Magboltz that can compute the macroscopic transport properties (such as the drift velocity), so we have to provide these data ourselves. In this example, we use the mobility of  $Ar^+$  ions in Ar as an approximation because there is no literature data for drift in the mixture. Example files with mobility data for various pure gases are located in the Data

directory of the project. Note that the LoadIonMobility method does not prefix the file name with a directory. If your mobility file is not located in your current working directory, then you have to specify a fully qualified file name.

```
const std::string path = std::getenv("GARFIELD_INSTALL");
gas.LoadIonMobility(path + "/share/Garfield/Data/IonMobility_Ar+_Ar.txt");
```

Associating the gas to a field map region In order to track a particle through the detector we have to tell ComponentAnsys123 which field map material corresponds to which Medium. The gas can be distinguished from the other materials (here: kapton and copper) by its dielectric constant, in our case  $\varepsilon = 1$ .

```
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();</pre>
```

#### **Electron transport**

Microscopic tracking is handled by the class AvalancheMicroscopic (Sec. 6.3).

```
AvalancheMicroscopic aval; aval.SetSensor(&sensor);
```

We are now ready to simulate an electron avalanche in the GEM. We place the initial electron  $200\,\mu m$  above centre of the GEM hole and set its initial energy to a typical energy in the electric field of the drift gap.

```
// 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);
```

After the calculation, we can extract information such as the number of electrons/ions produced in the avalanche and the start- and endpoints of all electron trajectories.

```
int ne, ni;
// Get the number of electrons and ions in the avalanche.
aval.GetAvalancheSize(ne, ni);
```

**Ion transport** For tracking the ions, we use the class AvalancheMC, which takes as input the macroscopic drift velocity as function of the electric field and simulates drift lines using a Monte Carlo technique (Sec. 6.2).

```
AvalancheMC drift;
drift.SetSensor(sensor);
drift.SetDistanceSteps(2.e-4);
```

After simulating an electron avalanche, we loop over all the electron trajectories, and calculate an ion drift line starting from the same initial point as the electron.

We can subsequently retrieve the endpoint of the ion drift line using

#### Visualizing the drift lines

To plot the electron and ion drift lines together with the geometry, we use the classes ViewDrift and ViewFEMesh. When setting up the AvalancheMicroscopic and AvalancheMC objects, we need to switch on the storage of the drift line points and attach a pointer to a ViewDrift object.

```
ViewDrift driftView;
```

```
aval.EnablePlotting(&driftView);
drift.EnablePlotting(&driftView);
```

After having calculated the electron avalanche and ion drift lines, we create a plot using the snippet of code below.

#### 2.5.3. Silicon sensor

In this example, we will simulate the signal in a 100  $\mu$ m thick planar silicon sensor due to the passage of a charged particle. We will adopt a coordinate system where the back side of the sensor is at y=0 and the front side (*i.e.* the strip or pixel side) is at  $y=100 \,\mu$ m.

#### **Transport properties**

We start by creating a MediumSilicon object, which provides the transport parameters (e.g. drift velocity and diffusion coefficients) of electrons and holes as function of the electric field (and, in general, also the magnetic field, but we will assume that it is zero in this example).

```
MediumSilicon si;
// Set the temperature [K].
si.SetTemperature(293.15);
```

Unless the user overrides the default behaviour (by providing a table of velocities at different electric fields), MediumSilicon calculates the drift velocities according to analytic parameterizations. A description of the mobility models is given in Sec. 3.3.1. In this example, we will use the default parameterizations, which correspond to the default models in Sentaurus Device [44]. The diffusion coefficients are calculated according to the Einstein relation.

#### Geometry

As a next step, we define the active volume, which in our case is simply a box with a length of  $d=100\,\mu\text{m}$  along y, centred at  $y=50\,\mu\text{m}$ , and made of silicon. To describe the shape of our detector, we therefore create a SolidBox object.

```
// Thickness of the silicon [cm]
constexpr double d = 100.e-4;
SolidBox box(0, 0.5 * d, 0, 2 * d, 0.5 * d, 2 * d);
```

We then create a GeometrySimple object, and attach the box to it (*i.e.* we pass it a pointer to the SolidBox object), together with the medium inside (*i.e.* a pointer to the MediumSilicon object).

```
// Set up the geometry.
GeometrySimple geo;
geo.AddSolid(&box, &si);
```

#### Electric field

For accurate calculations of the electric field in a segmented silicon sensor, one normally uses TCAD device simulation programs such as Synopsys Sentaurus Device [44]. In the present example, we will follow a simplified approach and approximate the electric field by that of an overdepleted pad sensor. In that case, the x and z components of the electric field vanish, and the y component varies linearly between

$$E_y = \frac{V_{\text{bias}} - V_{\text{dep}}}{d}$$

at the back side of the sensor (y = 0) and

$$E_y = \frac{V_{\text{bias}} + V_{\text{dep}}}{d}$$

at the front side of the sensor (y=d), where  $V_{\rm dep}$  is the depletion voltage of the sensor and  $V_{\rm bias}$  is the applied bias voltage. In this example, we will use  $V_{\rm dep}=-20\,{\rm V}$  and  $V_{\rm bias}=-50\,{\rm V}$ .

In order to use this expression for the electric field in our simulation, we need to write a small function

and set up a ComponentUser object which delegates the calculation of the electric field to this function.

```
ComponentUser linearField;
linearField.SetGeometry(&geo);
linearField.SetElectricField(eLinear);
```

A pointer to this Component is then passed to a Sensor which acts as an interface to the transport classes.

```
Sensor sensor;
sensor.AddComponent(&linearField);
```

#### Weighting field

For signal simulations, we need to know not only the actual electric field in the sensor, but also the weighting field of the electrode for which we want to calculate the induced current (Chapter 7).

In this example, we will use an analytic expression for the weighting field of a strip, as implemented in the class ComponentAnalyticField. We thus create a ComponentAnalyticField object, define the equipotential planes (y=0 and y=d) and set the voltages at these planes to ground and  $V=V_{\text{bias}}$ . We will not use this class to calculate the "real" electric field in the sensor though, so the voltage settings don't actually matter for our purposes.

```
ComponentAnalyticField wField;
wField.SetGeometry(&geo);
wField.AddPlaneY(0, vbias, "back");
wField.AddPlaneY(d, 0, "front");
```

We now define a strip (55  $\mu$ m width, centred at x = 0) on the front side of the sensor and request the calculation of its weighting field (which we label "strip").

```
constexpr double pitch = 55.e-4;
constexpr double halfpitch = 0.5 * pitch;
wField.AddStripOnPlaneY('z', d, -halfpitch, halfpitch, "strip");
wField.AddReadout("strip");
```

Similarly we could have set up the weighting field of a pixel electrode.

```
wField.AddPixelOnPlaneY(d, -halfpitch, halfpitch, -halfpitch, halfpitch, "pixel");
wField.AddReadout("pixel");
```

Finally, we need to instruct the Sensor to use the strip weighting field we just prepared for computing the induced signal

```
// Request signal calculation for the electrode named "strip",
// using the weighting field provided by the Component object wField.
sensor.AddElectrode(&wField, "strip");
```

and we need to set the granularity with which we want to record the signal (in our example: 1000 bins between 0 and 10 ns).

```
// Set the time bins.
const unsigned int nTimeBins = 1000;
```

```
const double tmin = 0.;
const double tmax = 10.;
const double tstep = (tmax - tmin) / nTimeBins;
sensor.SetTimeWindow(tmin, tstep, nTimeBins);
```

#### Primary ionization and charge carrier transport

We use Heed (Sec. 5.1) to simulate the electron/hole pairs produced by a  $180 \,\text{GeV} \,/\, c$  charged pion traversing the sensor.

```
TrackHeed track;
track.SetSensor(&sensor);
// Set the particle type and momentum [eV/c].
track.SetParticle("pion");
track.SetMomentum(180.e9);
```

For transporting the electrons and holes, we use the class AvalancheMC. When setting up the AvalancheMC object, we need to set the step size used for the drift line calculation to a reasonable value. In this example, we use steps of  $1\,\mu m$ . This means that at each step, the electron/hole will be propagated by  $1\,\mu m$  in the direction of the drift velocity at the local field, followed by a random step based on the diffusion coefficient.

```
AvalancheMC drift;
drift.SetSensor(&sensor);
// Set the step size [cm].
drift.SetDistanceSteps(1.e-4);
drift.EnableSignalCalculation();
```

We are now ready to run the simulation. In the snippet below, we simulate a perpendicularly incident charged particle track passing through the centre of the strip (x = 0), loop over the electron/hole pairs produced by the particle, and simulate a drift line for each electron and hole.

```
double x0 = 0., y0 = 0., z0 = 0., t0 = 0.;
double dx = 0., dy = 1., dz = 0.;
track.NewTrack(x0, y0, z0, t0, dx, dy, dz);
double xc = 0., yc = 0., zc = 0., tc = 0., ec = 0., extra = 0.;
int ne = 0;
// Retrieve the clusters along the track.
while (track.GetCluster(xc, yc, zc, tc, ne, ec, extra)) {
  // Loop over the electrons in the cluster.
 for (int j = 0; j < ne; ++j) {
    double xe = 0., ye = 0., ze = 0., te = 0., ee = 0.;
    double dxe = 0., dye = 0., dze = 0.;
    track.GetElectron(j, xe, ye, ze, te, ee, dxe, dye, dze);
    // Simulate the electron and hole drift lines.
    drift.DriftElectron(xe, ye, ze, te);
    drift.DriftHole(xe, ye, ze, te);
}
```

To check whether the results are sensible, it can be instructive to visualize the drift lines using the class ViewDrift.

```
ViewDrift driftView;
driftView.SetArea(-0.5 * d, 0, -0.5 * d, 0.5 * d, d, 0.5 * d);
track.EnablePlotting(&driftView);
drift.EnablePlotting(&driftView);
```

With the plotting option switched on, AvalancheMC will pass the coordinates of all drift line points to a ViewDrift object. After having simulated all drift lines from a track, we can create a plot using

```
constexpr bool twod = true;
driftView.Plot(twod);
```

Plotting the drift lines can slow down the execution time quite a bit, so it is advisable to switch it off when simulating a large number of tracks.

#### Retrieving the signal

After having simulated the charge carrier drift lines, we can plot the induced current using the class ViewSignal.

```
ViewSignal signalView;
signalView.SetSensor(&sensor);
constexpr bool plotTotalSignal = true;
constexpr bool plotElectronSignal = false;
constexpr bool plotHoleSignal = false;
signalView.PlotSignal("strip", plotTotalSignal, plotElectronSignal, plotHoleSignal);
```

To post-process the induced current pulse, one can convolute it with a transfer function that describes the response of the front-end electronics.

Often it can also be useful to save the signal to a file. An example for doing so is given in the code snippet below.

```
std::ofstream outfile;
outfile.open("signal.txt", std::ios::out);
for (unsigned int i = 0; i < nTimeBins; ++i) {
   const double t = (i + 0.5) * tstep;
   const double f = sensor.GetSignal(label, i);
   const double fe = sensor.GetElectronSignal(label, i);
   const double fh = sensor.GetIonSignal(label, i);
   outfile << t << "___" << f << "___" << fe << "___" << fh << "\n";
}</pre>
```

## 3. Media

Media are derived from the abstract base class Medium.

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

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

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 the following functions for calculating macroscopic electron transport parameters 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 coefficients	$\sigma\sqrt{p}$ vs. $E/p$
Townsend coefficient	$\alpha/p$ vs. $E/p$
attachment coefficient	$\eta/p$ vs. $E/p$

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).

The components of the drift velocity are stored in a right-handed coordinate system that 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**,  $\mathbf{B}_t = (\mathbf{E} \times \mathbf{B}) \times \mathbf{E}$ ,
- **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 parameter 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 Langevin equation [8]

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

is used.

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,  $\theta = \pi/2$

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 radian.

The electron drift velocity components at a specific point in the table can be set and retrieved using

ie index in the list of electric fields.

ib index in the list of magnetic fields,

ia index in the list of angles,

v velocity

Analogous functions are available for the other transport parameters. For the Townsend coefficient  $\alpha$  and the attachment coefficient  $\eta$ , the logarithms  $\ln \alpha$ ,  $\ln \eta$  and not the actual values are stored in the tables.

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.

#### 3.1.2. Visualization

For plotting the transport parameters, the class ViewMedium can be used. In the following example the drift velocities of electrons and holes in silicon are plotted as a function of the electric field.

```
MediumSilicon si;
ViewMedium view;
view.SetMedium(&si);
view.PlotElectronVelocity('e');
view.PlotHoleVelocity('e', true);
```

The following functions for visualizing transport parameters are currently implemented in ViewMedium.

```
void PlotElectronVelocity(const char xaxis, const bool same = false);
void PlotHoleVelocity(const char xaxis, const bool same = false);
void PlotElectronDiffusion(const char xaxis, const bool same = false);
void PlotHoleDiffusion(const char xaxis, const bool same = false);
void PlotIonDiffusion(const char xaxis, const bool same = false);
void PlotElectronTownsend(const char xaxis, const bool same = false);
void PlotHoleTownsend(const char xaxis, const bool same = false);
void PlotElectronAttachment(const char xaxis, const bool same = false);
void PlotHoleAttachment(const char xaxis, const bool same = false);
void PlotHoleAttachment(const char xaxis, const bool same = false);
void PlotElectronLorentzAngle(const char xaxis, const bool same = false);
```

**xaxis** quantity to plot on the x-axis ('e': electric field, 'b': magnetic field, 'a': angle),

same flag whether to start a new plot (false) or to add the plot to the existing ones.

By default, ViewMedium will try to determine the range of the x axis based on the grid of electric fields, magnetic fields, and angles, and the range of the y axis based on the minima and maxima of the function to be plotted. This feature can be switched on or off using the functions

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

The ranges can be set explicitly using

```
void SetRangeE(const double emin, const double emax, const bool logscale);
void SetRangeB(const double bmin, const double bmax, const bool logscale);
void SetRangeA(const double amin, const double amax, const bool logscale);
void SetRangeY(const double ymin, const double ymax, const bool logscale);
```

The (ROOT) colours with which to draw the graphs/curves and the labels to be used to identify them can be customized using

```
void SetLabels(const std::vector<std::string>& labels);
void SetColours(const std::vector<short>& cols);
```

If the function

```
void EnableExport(const std::string& txtfile);
```

txtfile name of the output text file

is called before one of the Plot.. functions, the plot data will be saved to a text file.

#### **3.2. Gases**

There are currently two classes implemented that 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 [7] — 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

```
bool SetComposition(const std::string& gas1, const double f1 = 1.,

const std::string& gas2 = "", const double f2 = 0.,

const std::string& gas3 = "", const double f3 = 0.,

const std::string& gas4 = "", const double f4 = 0.,

const std::string& gas5 = "", const double f5 = 0.,

const std::string& gas6 = "", const double f6 = 0.);
```

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

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

A valid gas mixture comprises at least one and at most six different species.

The function

```
void PrintGases();
```

prints out a list of the available gases and their identifiers (see also Table B.1).

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 (in Torr) and temperature (in K)

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

and 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;
// 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).

#### 3.2.1. W values and Fano factors

MediumGas has default settings for the W value (average energy to create an electron-ion pair) and the Fano factor of each gas available in Magboltz. Where available, measurements of the W value reported in Refs. [1, 28, 31] and measurements of the Fano factor reported in Refs. [2, 28, 42] were used.

For gases for which there no experimental data could be found in the literature, the W values were calculated based on the set of cross-sections implemented in Magboltz and the Fano factor was calculated using the empirical relation [18]

$$F = 0.188 \frac{W}{I} - 0.15$$

where *I* is the ionisation potential of the gas.

#### 3.2.2. Ion transport

The Data directory of the project includes a number of text files (e. g. IonMobility\_Ar+\_Ar.txt for Ar<sup>+</sup> ions in argon) with ion mobility data. More precisely, the files contain a table of reduced electric fields E/N and reduced mobilities. The reduced electric fields are given in units

of  $Td^1$  (Townsend) and the mobility values in  $cm^2 V^{-1} s^{-1}$ . 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. [12–14, 47].

#### 3.2.3. Magboltz

Magboltz, written by Steve Biagi, is a program for the calculation of electron transport properties in gas mixtures using semi-classical Monte Carlo simulation [7]. It includes a database of electronatom/molecule cross-sections for a large number of detection gases.

The function

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

runs Magboltz for all values of **E**, **B**, and  $\theta$  included in the current field grid.

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.

By default, the max. energy of the cross-section table is chosen automatically by Magboltz. This feature can be enabled or disabled using

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

If it is switched off, the program uses the upper energy limit set using

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

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 at 0 K.

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

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

```
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.

Gas files for the same gas composition and the same temperature and pressure can be merged using

```
bool MergeGasFile(const std::string& filename, const bool replaceOld);
```

filename name of the gas file to be loaded and merged with the present gas table,

replaceOld flag indicating whether new (replaceOld = true) or existing values should be used
in case of overlaps between the two tables.

Suppose we have two gas files for  $Ar/CO_2$ , one for a B field of 1 T and one for B=2 T. We can combine the two tables with the following snippet of code.

```
MediumMagboltz gas;
gas.LoadGasFile("ar_co2_1T.gas");
gas.MergeGasFile("ar_co2_2T.gas");
// Save the merged table.
gas.WriteGasFile("ar_co2_merged.gas");
```

#### **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 table of scattering rates extends from 0 to  $40\,\text{eV}$ . The max. energy to be included in the table can be set using

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

```
e max. electron energy (in eV).
```

<b>Table 3.2.</b> Classification of electron collision pro-
---

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

Up to an upper limit of  $400\,\text{eV}$ , equidistant energy steps are used. If the max. energy exceeds this value, logarithmically spaced energy steps are used for the high-energy part (>  $400\,\text{eV}$ ) of the cross-section table.

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 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

r value of the transfer efficiency

**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 first function, which takes no arguments, calculates the Penning transfer probability for the current gas mixture using pre-implemented parameterisations taken from literature [34–37], if available.

The second function sets the Penning transfer probability for a specific gas component in the mixture.

The third function (without the gasname parameter) activates 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 ( $\epsilon_i > \epsilon_{\rm ion}$ ).

Penning transfer can be switched off, globally or for a specific component, using

```
void DisablePenningTransfer();
void DisablePenningTransfer(std::string gasname);
```

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

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

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.

	electrons		holes		
	$\mu_L \ [10^{-6} \ {\rm cm^2  V^{-1}  ns^{-1}}]$	$\beta$	$\mu_L \ [10^{-6} \ {\rm cm^2  V^{-1}  ns^{-1}}]$	β	
Sentaurus [19]	1.417	-2.5	0.4705	-2.5	
Minimos [39]	1.43	-2.0	0.46	-2.18	
Reggiani [27]	1.32	-2.0	0.46	-2.2	

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

#### 3.3. Semiconductors

#### 3.3.1. Silicon

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, MediumSilicon calculates the electron and hole transport parameters 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<sup>2</sup>/(V ns))
```

**muh** hole mobility (in  $cm^2/(V ns)$ )

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 T is described by

$$\mu_L(T) = \mu_L(T_0) \left(\frac{T}{T_0}\right)^{\beta}, \qquad T_0 = 300 \text{ K.}$$
 (3.1)

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. [39]). Using the second function the model described in Ref. [22] 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 [10], 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. [27, 30].

• 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

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

$$\mu^{e,h}\left(E\right) = \frac{\mu_{0}^{e,h}}{\left(1 + \left(\frac{\mu_{0}^{e,h}E}{v_{\text{sat}}}\right)^{\beta^{e,h}}\right)^{\frac{1}{\beta^{e,h}}}}, \qquad \text{(Canali [10])}$$

$$\mu^{e}\left(E\right) = \frac{\mu_{0}^{e}}{\left(1 + \left(\frac{\mu_{0}^{e}E}{v_{\text{sat}}^{e}}\right)^{3/2}\right)^{2/3}}, \qquad \mu^{h}\left(E\right) = \frac{\mu_{0}^{h}}{\left(1 + \left(\frac{\mu_{0}^{h}E}{v_{\text{sat}}^{h}}\right)^{2}\right)^{1/2}}, \qquad \text{(Reggiani [27])}$$

By default, the Canali model is used.

For the impact ionization coefficient, the user has currently the choice between the models of Grant [17], van Overstraeten and de Man [45], Okuto and Crowell [26], and Massey [23].

void SetImpactIonisationModelVanOverstraetenDeMan();

- void SetImpactIonisationModelMassey();
- void SetImpactIonisationModelOkutoCrowell();

By default, the model by van Overstraeten and de Man is used.

#### 3.3.2. Gallium arsenide

By default, MediumGaAs uses Eq. (3.1) for calculating the low-field lattice mobility, with

$$\mu_L (T = 300 \text{ K}) = 8 \times 10^{-6} \text{ cm}^2 \text{ V}^{-1} \text{ ns}^{-1}, \qquad \beta = -1$$

for electrons and

$$\mu_L (T = 300 \,\mathrm{K}) = 0.4 \times 10^{-6} \,\mathrm{cm}^2 \,\mathrm{V}^{-1} \,\mathrm{ns}^{-1}, \beta = -2.1$$

for holes. Alternatively, the low-field mobilities can be set explicitly using

SetLowFieldMobility(const double mue, const double muh);

For the dependence of the mobility on the electric field E, the parameterizations [5]

$$\mu^{e}\left(E\right) = \frac{\mu_{0}^{e} + \frac{v_{\text{sat}}}{E} \left(\frac{E}{E_{c}}\right)^{4}}{1 + \left(\frac{E}{E_{c}}\right)^{4}}, \qquad \mu^{h}\left(E\right) = \frac{\mu_{0}^{h} + \frac{v_{\text{sat}}}{E_{c}}}{1 + \frac{E}{E_{c}}}, \qquad E_{c} = 4000 \,\text{V}/\text{cm}$$

are used, and the saturation velocity is calculated using

$$v_{\text{sat}}^{e,h} = 1.13 \times 10^{-2} - 3.6 \times 10^{-3} \left(\frac{T}{T_0}\right) \text{ cm/ns.}$$

The Townsend (impact ionization) coefficient as a function of the electric field E is calculated using

$$\alpha^e = a \exp\left(-\left(\frac{b}{E}\right)^{1.75}\right), \qquad \alpha^h = a \exp\left(-\left(\frac{b}{E}\right)^{1.82}\right).$$

#### 3.3.3. Diamond

Unless the low-field mobility values are set explicitly by the user, MediumDiamond calculates them using

$$\mu_0\left(T\right) = \left(\frac{T}{T_0}\right)^{-1.5} \mu_0\left(T_0\right),\,$$

where  $T_0 = 300 \,\mathrm{K}$  and  $\mu_0 \,(T_0) = 4.551 \times 10^{-6} \,\mathrm{cm}^2 \,\mathrm{V}^{-1} \,\mathrm{ns}^{-1}$  for electrons and  $\mu_0 \,(T_0) = 2.750 \,\mathrm{X}$  $10^{-6}\,\mathrm{cm^2\,V^{-1}\,ns^{-1}}$  for holes [29]. The mobility as function of the electric field E is calculated using

$$\mu\left(E\right) = \frac{\mu_0}{1 + \frac{\mu_0 E}{V_{\text{cat}}}}$$

with default values of  $v_{\rm sat}=2.6 \times 10^{-2}\,{\rm cm\,/\,ns}$  for electrons and  $v_{\rm sat}=1.6 \times 10^{-2}\,{\rm cm\,/\,ns}$  for holes. These default values can be overriden using

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

void SetSaturationVelocity(const double vsate, const double vsath);

# 4. Components

The calculation of electric fields is done by classes derived from the abstract base class Component. 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 object (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 analytic fields, the geometry is, in general, given by the cell layout.

For other components (e.~g. 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

	3
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,
- SolidHole,
- SolidRidge,
- SolidExtrusion.
- SolidWire, and
- SolidSphere.

A description of these classes is given in Appendix C.

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;
// Create the geometry.
GeometrySimple geo;
// Dimensions of the tube
double rMax = 0.5, halfLength = 10.;
SolidTube tube(0., 0., 0., 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);
              medVacuum = new TGeoMedium("Vacuum", 1, matVacuum);
TGeoMedium*
// 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);
\ensuremath{//} 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(Geometry* geo);
```

#### 4.1.1. Visualizing the geometry

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

```
MediumMagboltz gas;
// Create and setup the geometry.
GeometrySimple geo;
const double r1 = 0.4;
const double r2 = 0.6;
SolidHole hole(0, 0, 0, r1, r2, 1, 1, 1);
hole.SetSectors(4);
geo.AddSolid(&hole, &gas);

// Create a viewer.
ViewGeometry geoView;
geoView.SetGeometry(&geo);
geoView.Plot3d();
```

The snippet above will produce a three-dimensional impression of the geometry. The function ViewGeometry::Plot2d() draws a cut through the solids at the current viewing plane, e.~g. using again the geometry defined above,

```
// ...
ViewGeometry geoView;
geoView.SetPlaneXZ();
geoView.Plot2d();
```

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;
....
// Create a viewer.
ViewCell view;
// 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.

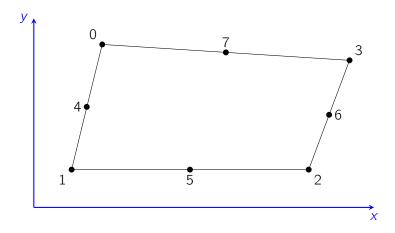
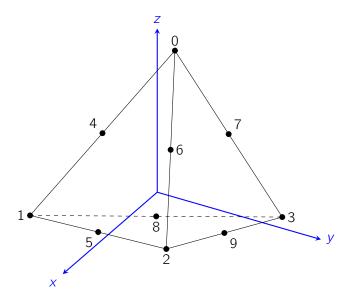


Figure 4.1. Eight-node quadrilateral element used in 2D Ansys field maps.



**Figure 4.2.** Ten-node tetrahedral element used in 3D Ansys field maps. The node numbering scheme shown here is the one used in Ansys and differs slightly from the one used internally in ComponentAnsys123.

## 4.2. Field maps

### 4.2.1. Ansys

The interpolation of FEM field maps created with the program Ansys [4] is dealt with by the classes ComponentAnsys121 and ComponentAnsys123. The class names refer to the type of mesh element used by Ansys:

- ComponentAnsys121 reads two-dimensional field maps with eight-node curved quadrilaterals (Fig. 4.1), known as "plane121" in Ansys).
- ComponentAnsys123 reads three-dimensional field maps with quadratic curved tetrahedra (Fig. 4.2), known as "solid123" in Ansys).

The field map is imported with the function

```
std::string mplist, std::string prnsol, std::string unit);
```

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

**nlist** 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")

unit length unit used in the calculation (default: "cm",

```
other recognized units are "mum"/"micron"/"micrometer", "mm"/"millimeter" and "m"/"meter").
```

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

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.
size_t GetNumberOfMaterials();
// Associate a material with a Medium class.
void SetMedium(const size_t 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 size_t imat);
double GetConductivity(const size_t imat);
```

By default, mesh elements in conductors, *i.e.* materials with resistivity equal to zero, are eliminated. This feature can be switched on or off using

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

**on** flag to delete mesh elements in conductors (true) or keep them (false)

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 means that odd periodic copies of the basic cell are mirror images of even periodic copies. 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(const bool on);
void EnableAxialPeriodicityX(const bool on);
void EnableAxialPeriodicityX(const bool on);
void EnableRotationSymmetryX(const bool on);
```

**on** flag to enable (true) or disable (false) periodicity.

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 size_t 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 size_t nel = fm->GetNumberOfElements();
// Loop over the elements.
double volume, dmin, dmax;
for (size_t 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();
```

Since Ansys uses curved elements, an iterative procedure is used for determining the local coordinates of a point within an element. This search can sometimes fail to achieve the requested

precision. In this case, the first-order approximation is used, and (by default) a warning message is printed out. These messages can be switched on or off using

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

#### 4.2.2. Synopsys TCAD

Electric fields calculated using the device simulation program Synopsys Sentaurus [44] can be imported with the classes ComponentTcad2d and ComponentTcad3d (derived from the base class ComponentTcadBase).

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 .grd 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
size_t GetNumberOfRegions();
// Associate a region with a Medium class
void SetMedium(const size_t 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 size_t 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();
```

Using TCAD, the weighting field and potential are typically determined by first computing the electric field  $\mathbf{E}_0$  and potential  $V_0$  with all electrodes set at the nominal potentials. The potential at the electrode to be read out is then increased by a small voltage  $\Delta V$  and the corresponding electric field  $E_+$  and potential  $V_+$  are calculated. The weighting field and potential are then given by

$$\mathbf{E}_{w} = rac{1}{\Delta V} \left( \mathbf{E}_{+} - \mathbf{E}_{0} \right), \qquad V_{w} = rac{1}{\Delta V} \left( V_{+} - V_{0} \right).$$

In ComponentTcad2d and ComponentTcad3d the weighting field and potential loaded using

**datfile1** .dat file containing the solution  $\mathbf{E}_0$ ,  $V_0$ ,

**datfile2** .dat file containing the solution  $\mathbf{E}_+, V_+,$ 

**dv** potential difference  $\Delta V$ ,

label identifier of the electrode.

The mesh is assumed to be the same as the one for the drift field (imported using Initialise).

Using the function

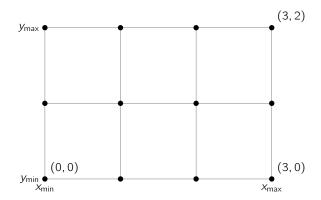
one can set an offset to be applied to the map of weighting fields and potentials imported from TCAD.

#### 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 [15] and the mesh tool Gmsh [16]. 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.



**Figure 4.3.** Example of a two-dimensional regular mesh (as used in ComponentGrid) with  $4 \times 3$  grid points, corresponding to  $n_X = 4$ ,  $n_V = 3$ .

#### 4.2.5. **COMSOL**

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

header COMSOL Multiphysics text file (.mphtxt) containing the mesh data,

mplist file containing the material properties,

**field** file containing the exported field data.

The materials file (second argument) is a simply ASCII file containing

- the number of materials in the field map,
- the relative dielectric constants of each of the materials,
- the number of "domains",
- a list of domain numbers and indices of the corresponding materials.

The domain numbers can be found in the section # Geometric entity indices of the mesh data file (mesh.mphtxt). For a field map with two materials, one with a dielectric constant of  $\varepsilon=1$  (domain number 1) and the other one with a dielectric constant of  $\varepsilon=4$  (domain number 2), the file should look like the following.

```
2
1. 4.
2
1 0
2 1
```

#### 4.2.6. Regular grids

Electric field values on a regular two-dimensional or three-dimensional grid can be imported from a text file using the class ComponentGrid. The electric field values (and potential) for each point on the grid 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 indicating whether the point is in an active medium (1) or not (0).

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

The file should contain one line for each grid point. 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 determines the closest grid point and assigns the electric field and potential accordingly. In case of IJ (IJK) the indices of the grid point along x, y (and z) are specified directly. The file can include comments (lines starting with # or //).

Prior to reading the electric field, the limits and spacing of the grid can be set using the function

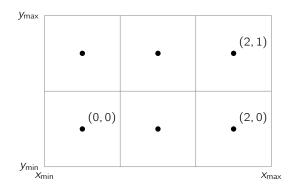
**nx, ny, nz** number of grid lines along x, y, z

**xmin, xmax, ...** boundaries of the grid in x, y, z

An example illustrating the parameters defining the mesh and the numbering of the grid nodes is shown in Fig. 4.3. Alternatively, the grid parameters can be read from the file that contains the electric field/potential. For instance, to specify the limits and number of grid lines along z, a line like

```
\# ZMIN = -1., ZMAX = 1., NZ = 3
```

should be included at the beginning of the file. If the user has not specified the grid explicitly (using SetMesh) and the information given in the comment lines is incomplete, the class will try to



**Figure 4.4.** Example of a two-dimensional regular mesh (as used in ComponentVoxel) with  $3 \times 2$  cells, corresponding to  $n_X = 3$ ,  $n_V = 2$ .

determine the remaining grid parameters from the table of coordinates and corresponding electric fields itself.

When retrieving the field/potential at a given point (x, y, z) the class performs a trilinear interpolation between the values at the grid nodes surrounding this point. The medium in the domain covered by the mesh is set using

```
void SetMedium(Medium* m);
```

A point (x, y, z) is considered in an active region (*i.e.* associated to the medium) if all surrounding grid nodes are flagged as active.

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 active medium flag). Prompt and delayed weighting fields/potentials can be imported using

The class ComponentVoxel is similar to ComponentGrid but uses a different definition of the mesh. An example illustrating the parameters of the mesh and the numbering of the voxels/cells is shown in Fig. 4.4. As a first step, the mesh needs to be defined using the function

```
const double zmax);
```

**nx, ny, nz** number of rows/columns of cells along x, y, z

**xmin, xmax,...** boundaries of the grid in x, y, z

The electric field values (and potential) for each voxel are imported using

filename name of the ASCII file

format description of the file format (see ComponentGrid)

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 medium to be associated with a given region can be set using

```
void SetMedium(const unsigned int i, Medium* m);
```

i index of the region

If the regions are not assigned explicitly when importing the electric field, all voxels are assumed to belong to the same region (index 0).

By default, the field and potential are assumed to be constant within 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->SetFillMesh(false);
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

The medium to be associated with the active region of the cell is set using

```
SetMedium(Medium* medium);
```

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

```
void AddPlaneX(const double x, const double v, const std::string& label);
// Add a plane at constant y
void AddPlaneY(const double y, const double v, const std::string& label);
```

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();
```

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. Cylindrical geometries

By default, the wire coordinates are specified in Cartesian coordinates and the planes are parallel to the x or y axis. Calling

```
void SetPolarCoordinates();
```

switches to a polar coordinate system. This can be useful for certain types of cells which are more conveniently described in polar coordinates  $(r, \phi)$ , for instance because of the presence of a circular plane.

Internally, the class uses log-polar coordinates  $(\rho, \phi)$ , where the angular coordinate  $\phi$  is the same as in polar coordinates, and  $\rho = \ln r$ . The transformation<sup>2</sup>

$$(x, y) = e^{\rho} (\cos \phi, \sin \phi)$$

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

<sup>&</sup>lt;sup>2</sup> Using complex numbers, the transformation can be written as  $x + iy = \exp(\rho + i\phi)$ .

is a conformal mapping<sup>3</sup> which translates circles to lines at constant  $\rho$ . After calculating the field in internal coordinates, it is transformed back to Cartesian coordinates using

$$\begin{pmatrix} E_x \\ E_y \end{pmatrix} = \mathrm{e}^{\rho} \begin{pmatrix} \cos \phi & -\sin \phi \\ \sin \phi & \cos \phi \end{pmatrix} \begin{pmatrix} E_\rho \\ E_\phi \end{pmatrix}.$$

By calling

```
void SetCartesianCoordinates();
```

one can change back to Cartesian coordinates. Mixed coordinates are not permitted; when switching from Cartesian to polar coordinates or vice versa the description of the cell is reset.

In order to add a wire to the cell, the same function is used for both Cartesian and polar coordinates. In the latter case, the first coordinate corresponds to the radius of the wire (in cm), and the second coordinate corresponds to the angle (in degrees). A wire may not be positioned at the origin if polar coordinates are being used.

Planes at constant radius or at constant angle are specified using

```
void AddPlaneR(const double r, const double voltage, const std::string& label);
void AddPlanePhi(const double phi, const double voltage, const std::string& label);
```

r radius of the plane (in cm),

**phi** angle of the plane (in degrees).

The following simple example generates a pie wedge with a wire inside.

```
ComponentAnalyticField cmp;
cmp.SetPolarCoordinates();
const double r = 2.;
cmp.AddPlaneR(r, 0., "r");
cmp.AddPlanePhi( 0., 0., "phi1");
cmp.AddPlanePhi(60., 0., "phi2");
cmp.AddWire(0.5 * r, 30., 50.e-4, 500., "w");
```

#### 4.3.3. Periodicities

The class supports simple periodicity in x and y direction. The periodic lengths are set using

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

When working in polar coordinates, one can set the  $\phi$  periodicity using

```
void SetPeriodicityPhi(const double s);
```

<sup>&</sup>lt;sup>3</sup>This implies that the Laplace equation in log-polar coordinates has the same form as in Cartesian coordinates.

s angular period (in degrees).

If the  $\phi$  periodicity is not set explicitly by the user, a cyclic boundary condition with a period of  $2\pi$  is imposed.

Radial periodicity is not supported since the internal coordinate  $\rho$  is not linear in r.

#### 4.3.4. 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();
```

#### 4.3.5. Dipole moments

By default, ComponentAnalyticField uses the thin-wire approximation for computing the electric field and potential. In this approach, dipole and higher-order terms are neglected which is usually a good approximation if the wire spacing is large compared to the diameter. One can request dipole terms to be included in the calculation using

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

Dipole terms are currently implemented only for cell types A, B1X, B1Y, B2X and B2Y. To investigate whether dipole and higher order terms are significant, one can use the function

iw index of the wire for which the multipole decomposition should be done,

order order of the highest multipole moment to be taken into account,

**print** flag to request verbose output during the minimisation step,

**plot** flag to create a plot of the result of the multipole fit,

rmult distance (in units of the wire radius) at which the potential is to be calculated,

eps "small number" used by the minimisation function to calculate the derivative matrix,

**nMaxIter** max. number of iteration in the minimisation.

#### 4.3.6. Weighting fields

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

```
const double zmin, const double zmax,
const std::string& label, const double gap = -1.,
const double rot = 0.);
```

The last (optional) parameter specifies the rotation angle (in rad) of the pixel in the plane. Pixel weighting fields are calculated using the expressions given in Ref. [32].

When working in polar coordinates, strips and pixels are defined using

Valid strip directions are 'p' ( $\phi$ ) or 'z' for circular planes and 'r' or 'z' for  $\phi$  planes.

#### 4.4. neBEM

The nearly exact Boundary Element Method (neBEM) solver discretizes the boundary of the domain in triangular and rectangular elements and computes the surface charge density on each of these elements that is required to satisfy the applied boundary conditions. Once the charge density distribution has been obtained, the potential and field can be evaluated at any point in the domain. A detailed description of the technique can be found in Refs. [20, 24, 25].

The ComponentNeBem3d interface class requires as input a GeometrySimple object with its list of solids and associated media.

```
void ComponentNeBem3d::SetGeometry(Geometry* geo);
```

The boundary conditions to be applied to each solid can be set using

```
void Solid::SetBoundaryPotential(const double v);
```

in case of a conductor at fixed potential (Dirichlet boundary conditions) or

```
void Solid::SetBoundaryDielectric();
```

in case of a dielectric-dielectric interface. In the latter case (Neumann boundary conditions), the normal component of the displacement field  $\mathbf{D} = \varepsilon \mathbf{E}$  is required to be continuous at the boundary of the solid,

$$\mathbf{n} \cdot \left( \varepsilon^+ \mathbf{E}^+ - \varepsilon^- \mathbf{E}^- \right)$$
 .

During initialisation, ComponentNeBem3d

- retrieves the surface panels from the Solid objects present in the geometry,
- searches for and eliminates overlaps between the panels,
- and splits the resulting polygons into rectangular and triangular "primitives".

These "primitives" are then passed on to neBEM, where they are further subdivided into "elements" (rectangles and right-angled triangles). A special case are SolidWire objects which are represented as one-dimensional straight line primitives and elements (corresponding to the thin-wire approximation used also in ComponentAnalyticField). The elements should be small enough such that the distribution of the charge density on them be approximated as uniform. The size of the elements can be controlled using the functions

```
void SetTargetElementSize(const double length);
void SetMinMaxNumberOfElements(const unsigned int nmin, const unsigned int nmax);
```

length preferred linear size of the elements, measured along their edges.

**nmin,nmax** smallest and largest number of elements produced along either axis of a single primitive.

One can also request different target element sizes for each Solid object, using

```
void Solid::SetDiscretisationLevel(const double dis);
```

After splitting the primitives into elements, neBEM determines the influence matrix K and the right-hand side vector<sup>4</sup> of the system of equations

$$K \boldsymbol{\rho} = \mathbf{b}$$
,

inverts the matrix and computes the surface charge density  $\rho_i$  of every element,

$$\rho_i = K_{ij}^{-1} b_j.$$

#### 4.4.1. Weighting fields

If a Solid object has been given a label using

```
void Solid::SetLabel(const std::string& label);
```

neBEM will compute its weighting field at the same time as the electric field. One can assign the same label to multiple Solid objects. The weighting field corresponding to this label will then be computed by setting the potential of all elements associated to solids with this label to 1V (and grounding all other conducting elements).

<sup>&</sup>lt;sup>4</sup>In a system with only Dirichlet boundary conditions, the right-hand side vector is given by the potentials at the elements,  $b_i = V_i$ .

### 4.5. 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

```
void SetElectricField(const double ex, const double ey, const double ez);
void SetPotential(const double x, const double p, const double z, const double v);
```

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 and potential can be set using

wx,wy,wz components of the weighting field

label identifier of the weighting field/electrode

x, y, z coordinates where the weighting potential is specified

v weighting potential at the given position

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

f user function

Similar functions are available to set the weighting field and potential, and the magnetic field.

As an example, let us consider the electric 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.

	3 11 1 1 1
Quantity	option
Electrostatic potential Magnitude of the electric field ( $ \mathbf{E} $ ) $x$ -component of the electric field ( $E_x$ ) $y$ -component of the electric field ( $E_y$ ) $z$ -component of the electric field ( $E_z$ )	"v", "p", "phi" "e", "emag", "norm" "ex" "ey" "ez"
Magnitude of the magnetic field ( $ \mathbf{B} $ ) x-component of the magnetic field ( $B_x$ ) y-component of the magnetic field ( $B_y$ ) z-component of the magnetic field ( $B_z$ )	"bmag" "bx" "by" "bz"

**Table 4.2.** ViewField option strings and corresponding quantities.

```
const double d = 0.1;

ey = ez = 0.;
ex = (v - vdep) / d + 2 * x * vdep / (d * d);
};
ComponentUser cmp;
cmp.SetElectricField(efield);
```

### 4.6. Visualizing the field

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

The functions

```
void PlotContour(const std::string& option = "v");
void Plot(const std::string& option = "v", const std::string& drawopt = "");
```

create a contour plot or another two-dimensional plot in the chosen viewing plane. The quantity to be plotted is set using the parameter option (see Table 4.2). The parameter drawopt is passed on to the function Draw() of the ROOT TF2 class and sets the plotting options. For instance,

```
ViewField view;
view.Plot("v", "SURF4");
```

will create a surface plot of the potential.

The function

plots the potential or field (depending on the parameter option) along the line  $(x_0, y_0, z_0) \rightarrow (x_1, y_1, z_1)$ . With the flag normalised set to true (default), normalised coordinates [0, 1] are used for the x-axis.

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(Component* 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 SetPlaneXY();
```

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, const bool samplePotential = true);
```

The flag samplePotential indicates whether the range of the potential should be determined by random sampling or if ViewField should first try to retrieve it from the component/sensor.

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);
```

## 4.7. Inspecting the field

Component provides functions for inspecting the field, in particular for determining the electric flux over a surface.

calculates the charge (in fC) enclosed in a sphere of radius r centred at  $(x_c, y_c, z_c)$  using Gauss's law, i.e. by integrating the normal component of the electric field over the surface of the sphere,

$$Q = \varepsilon_0 \oint \mathbf{E} \cdot d\mathbf{A}.$$

Similarly,

calculates the line charge (in fC/cm) contained in a circle of radius r centred at  $(x_c, y_c)$ . The integrations are performed using six-point Gaussian quadrature. The number of integration intervals can be set as a parameter.

The integral of the flux over a parallelogram can be calculated using the function

```
double IntegrateFluxParallelogram(const double x0, const double y0, const double z0, const double dx1, const double dx1, const double dx1, const double dx2, const double dx2, const double dx2, const double dx2, const unsigned int nV = 20);
```

x0,y0,z0 coordinates of one of the corners of the parallelogram,

dx1,dy1,dz1 direction vector from  $(x_0, y_0, z_0)$  to one of the adjacent corners,

dx2,dy2,dz2 direction vector to the other adjacent corner,

**nU,nV** number of integration intervals along the two directions.

The result is given in units of V cm.

#### 4.8. 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(Component* comp);
void AddElectrode(Component* 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 deactivate (or activate) a component after having added it, the function

```
void EnableComponent(const unsigned int i, const bool on);
```

can be used. Components that have been deactivated are not taken into account when calculating the electric field but are not removed from the list. Similarly,

```
void EnableMagneticField(const unsigned int i, const bool on);
```

can be used to deactivate (or activate) the magnetic field of a given component.

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

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 length, an isotropic random vector will be generated.

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
$K^+$	K+	493.677	+1
р	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.

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 [41] 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);
```

#### 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. [41].

TrackHeed retrieves the necessary input parameters - the asymptotic W value (eV) and the Fano factor - from the relevant Medium object. If these parameters are set to zero, 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 simulating 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.

```
TrackHeed track;
// 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**

 $SRIM^1$  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 type therefore does not need to be specified by the user. The user does however need to set the kinetic energy of the projectile.

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,

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

Table	5 2	Fluctuation	models	in	TrackSrim.
Iabic	J. Z.	I IUCLUALION	HIOUCIS	111	II ackot III.

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

• 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.

The generation of Vavilov distributed random numbers is based on a C++ implementation of the CERNLIB G115 procedures for the fast, approximate calculation of functions related to the Vavilov distribution. The description of the algorithm can be found in Ref. [33].

For sampling the energy loss, TrackSrim needs the electron density of the target material. By default it is retrieved from the relevant Medium object (and scaled to the mass density given in the SRIM output file). Alternatively, the user can specify the effective atomic number Z and mass number A of the target using TrackSrim::SetAtomicMassNumbers.

Transverse and longitudinal straggling can be switched on or off using

```
void EnableTransverseStraggling(const bool on);
void EnableLongitudinalStraggling(const bool on);
```

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

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.

To calculate the number of electrons for given amount of deposited energy, TrackSrim needs the work function W (in eV) and the Fano factor of the target material. By default, TrackSrim retrieves these parameters from the relevant Medium object. Altenatively, they can be set explicitly using TrackSrim::SetWorkFunction and TrackSrim::SetFanoFactor.

#### 5.3. TRIM

TRIM<sup>2</sup> is a Monte Carlo simulation program from the same collection of software packages as SRIM. It simulates individual ion trajectories in a target (which can be made of several layers) and the processes following the ion's energy loss (recoil cascades, displacement damage, *etc.*). TRIM typically produces a number of output files. One of them is a file called EXYZ.txt which lists the position and electronic stopping power for each simulated ion at regular steps in the ion's kinetic energy. The energy interval is set by the user.

The class TrackTrim allows one to import these data in Garfield and use them for simulating tracks. The function for reading ion trajectories from an EXYZ.txt file is

**file** name/path of the EXYZ.txt file to be loaded,

**nlons** number of ion trajectories to be loaded from the file,

**nSkip** number of ion trajectories to be skipped at the beginning of the file.

If the value of nIons is zero, TrackTrim will import all ion trajectories included in the file.

When the function NewTrack is called, TrackTrim will generate clusters according to one of the ion trajectories imported from EXYZ.txt (starting with the first one). Each cluster will correspond to one energy interval. The number of clusters along a track and the deposited energy per cluster is therefore controlled by the energy interval specified when running TRIM. The number of electrons in a cluster is sampled using an algorithm that reproduces the requested work function (W value) and Fano factor. At the next call to NewTrack, TrackTrim moves to the next ion trajectory in the list (if it reaches the end of the list, it rewinds to the first one).

<sup>&</sup>lt;sup>2</sup>TRansport of lons in Matter

# 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

$$\dot{\mathbf{r}} = \mathbf{v}_{\mathsf{d}}(\mathbf{E}(\mathbf{r}), \mathbf{B}(\mathbf{r})),$$
 (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, implemented in the class DriftLineRKF, calculates a drift line by iterating over the following steps.

- 1. Given a starting point  $\mathbf{x}_0$ , the velocity at the starting point, and a time step  $\Delta t$ , compute two estimates of the step to the next point on the drift line,
  - $\Delta \mathbf{v}_{l} = \sum_{k=0}^{2} C_{l,k} \mathbf{v}_{d}(\mathbf{x}_{k})$ , accurate to second order, and
  - $\Delta \mathbf{v}_{\text{II}} = \sum_{k=0}^{3} C_{\text{II},k} \mathbf{v}_{d}(\mathbf{x}_{k})$ , accurate to third order.

These two estimates are based on the drift velocity at the starting point and the velocity at three new locations

$$\mathbf{x}_{k} = \mathbf{x}_{0} + \Delta t \sum_{i=0}^{k-1} \beta_{k,i} \mathbf{v}_{d} \left(\mathbf{x}_{i}\right).$$

**Table 6.1.** Coefficients of the Runge-Kutta-Fehlberg formula [43].

	$oldsymbol{eta}_{k,i}$		
k	0	1	2
1	$\frac{1}{4}$		
2	$\frac{-189}{800}$	$\frac{729}{800}$	
3	$ \begin{array}{r} \frac{1}{4} \\ -189 \\ \hline 800 \\ 214 \\ 891 \end{array} $	1 33	650 891

k	$C_{I,k}$	$C_{II,k}$
0	214 891	<u>533</u> 2106
1	1 33 650	
2	650 891	$\frac{800}{1053}$
3	031	$\frac{-1}{78}$

The values of the coefficients are shown in Table 6.1.

2. The time step is updated by comparing the second and third order estimates with the requested accuracy

$$\Delta t' = \sqrt{\frac{\varepsilon \Delta t}{|\Delta v_{\mathsf{I}} - \Delta v_{\mathsf{II}}|}}.$$

- 3. The step is repeated if
  - the time step shrinks by more than a factor five,
  - the step size exceeds the maximum step length allowed (if such a limit is set),
- 4. The position is updated with the second order estimate.
- 5. The velocity is updated according to the end-point velocity of the step, which is one of the three velocity vectors that were computed under 1.

The initial time step is estimated using  $\Delta t = \varepsilon/|\mathbf{v}_d(\mathbf{x}_0)|$ . The parameter  $\varepsilon$  used in this initial estimate and in step 2 of the above algorithm, can be set using

```
void SetIntegrationAccuracy(const double eps);
```

When traversing a large area with a very smooth field, the step size becomes large. If this is not desired, for instance because there is a fine structure behind the smooth area, then one should limit the step size using

```
void SetMaximumStepSize(const double ms);
```

The maximum step size is recommended to be of order 1/10-1/20 of the distance to be traversed. The default behaviour (no limit on the step size) can be reinstated using

```
void UnsetMaximumStepSize();
```

By default, the drift line calculation is aborted if the drift line makes a bend sharper than  $90^{\circ}$ . Such bends rarely occur in smooth fields, the most common case is a drift line that tries to cross a saddle point. This check can be switched on or off using

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

During the evaluation of the velocities  $\mathbf{v}_d(\mathbf{x}_k)$  for the next step, checks are made to ensure that none of the probe points  $\mathbf{x}_k$  are outside the active area and that no wire was crossed. If a wire has been crossed during the step, another algorithm for stepping towards a wire takes over. The stepping towards the wire also starts when the distance between the particle position and a wire is less than n times the wire radius. The factor n ("trap radius") can be set in ComponentAnalyticField when defining the wire. If one of the points along the step is outside the active area, the drift line is terminated by doing a last linear step towards the boundary.

Drift line calculations are started using

```
bool DriftElectron(const double x0, const double y0, const double z0, const double t0); bool DriftHole(const double x0, const double y0, const double z0, const double t0);
```

bool DriftIon(const double x0, const double y0, const double z0, const double t0);

x0, y0, z0, t0 initial position and time

The function

```
bool DriftPositron(const double x0, const double y0, const double z0, const double t0);
```

computes an electron drift line, but assuming that the electron has positive charge (which can be useful for determining isochrons). Analogously, the function

```
bool DriftNegativeIon(const double x0, const double y0, const double z0, const double t0);
```

computes an ion drift line, assuming that the ion has negative charge.

After calculating a drift line, the multiplication and loss factors

$$\exp\left(\int \alpha ds\right)$$
 ,  $\exp\left(-\int \eta ds\right)$ 

along the drift line can be obtained using

```
void GetGain(const double eps = 1.e-4);
void GetLoss(const double eps = 1.e-4);
```

**eps** parameter determining the accuracy of the integration.

Both functions use an adaptive Simpson-style integration.

Similarly, the function

```
void GetArrivalTimeSpread(const double eps = 1.e-4);
```

computes the  $\sigma$  of the arrival time distribution by integrating quadratically the ratio of longitudinal diffusion coefficient and drift velocity over the drift line,

$$\sigma^2 = \int \left( D_L / v_D \right)^2 \, \mathrm{d}s.$$

The points along the most recent drift line are accessible through the functions

```
size_t GetNumberOfDriftLinePoints() const;
void GetDriftLinePoint(const size_t i, double& x, double& y, double& z, double& t) const;
```

i index of the point.

x, y, z, t coordinates and time of the point.

If one is simply interested in the end point and status flag of the current drift line, the function

```
void GetEndPoint(double& x, double& y, double& z, double& t, int& st) const;
```

can be used. A list of the status codes is given in Table 6.2.

By default, the induced current is calculated for each drift line. This can be activated or deactivated using

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

For electron drift lines, multiplication is taken into account in the signal calculation. For this purpose, after calculating a drift line the number of electrons and ions at each point of the line is calculated by integrating the Townsend and attachment coefficient along the line. For a given starting point, the number of electrons at the end of the drift line is thus given by

$$n_e = \exp\left(\int \left(\alpha - \eta\right) \mathrm{d}s\right).$$

The multiplication factor can be set explicitly using

```
void SetGainFluctuationsFixed(const double gain = -1.);
```

**gain** multiplication factor to be used. If the provided value is < 1, the multiplication factor obtained by integrating  $\alpha - \eta$  along the drift line is used instead (as is the default).

In order to take fluctuations of the avalanche size into account in the signal calculation, the number of electrons in the avalanche can be sampled from a Pólya distribution [3]

$$\overline{n}P_n = \frac{(\theta+1)^{\theta+1}}{\Gamma(\theta+1)} \left(\frac{n}{\overline{n}}\right)^{\theta} e^{-(\theta+1)n/\overline{n}},$$

where  $P_n$  is the probability that the avalanche comprises n electrons,  $\overline{n}$  is the mean avalanche size, and  $\theta$  is a parameter controlling the shape of the distribution. For  $\theta=0$  one obtains an exponential distribution, while with increasing  $\theta$  the distribution becomes more and more "rounded". The simulation of gain fluctuations can be enabled using the function

```
void SetGainFluctuationsPolya(const double theta, const double mean = -1.);
```

**theta** shape parameter  $\theta$  of the Pólya distribution.

**mean** mean avalanche size  $\overline{n}$ . If the provided value is < 1, the multiplication factor obtained by integrating  $\alpha - \eta$  along the drift line is used instead (as is the default).

## 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 electric and magnetic 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 a multiple of the "collision time"

$$\tau = \frac{mv_d}{qE}.$$

The third method is activated by default.

Instead of making simple straight-line steps (using the drift velocity vector at the starting point of a step), the end point of a step can be calculated using a (second-order) Runge-Kutta-Fehlberg method. This feature can be activated using

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

The average velocity  $\mathbf{v}$  over a step  $\Delta t$  is then calculated using

$$\mathbf{v} = \sum_{k=0}^{2} C_{k} \mathbf{v}_{d} (\mathbf{x}_{k}), \quad \mathbf{x}_{1} = \mathbf{x}_{0} + \Delta t \beta_{1,0} \mathbf{v}_{d} (\mathbf{x}_{0}), \quad \mathbf{x}_{2} = \mathbf{x}_{0} + \Delta t (\beta_{2,0} \mathbf{v}_{d} (\mathbf{x}_{0}) + \beta_{2,1} \mathbf{v}_{d} (\mathbf{x}_{1})),$$

where  $\mathbf{x}_0$  is the starting point of the step. The values of the coefficients  $C_k$  and  $\beta_{k,i}$  are given in Table 6.1.

If the electric field or drift speed is zero, the algorithm switches to diffusion-only steps based on the low-field mobility.

Drift line calculations are started using

```
bool DriftElectron(const double x0, const double y0, const double z0, const double t0); bool DriftHole(const double x0, const double y0, const double z0, const double t0); bool DriftIon(const double x0, const double y0, const double z0, const double t0);
```

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

The trajectory can be retrieved using

```
size_t GetNumberOfDriftLinePoints() const;
void GetDriftLinePoint(const size_t i, double& x, double& y, double& z, double& t);
```

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 the drift and multiplication of the holes/ions (electrons) created in the avalanche should be simulated.

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.

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

If a time window is set, 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. Another useful function for that purpose is

```
bool ResumeAvalanche(const bool electron = true, const bool hole = true);
```

electron, hole flags to switch off the electron (hole) component of the avalanche

which instructs AvalancheMC to continue the avalanche simulation from the most recent set of end points.

The time window can be removed using

```
void UnsetTimeWindow();
```

Using the function

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

one can request the Townsend and attachment coefficients to be projected onto the local drift velocity vector when integrating them over drift path segments. By default, this feature is switched on. The function

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

sets an upper limit to the number of electrons in an avalanche can be imposed.

### 6.3. Microscopic tracking

In the microscopic tracking approach – implemented at present only for electrons – a particle is followed from collision to collision. As input, it requires a table of the collision rates  $\tau_i^{-1}\left(\epsilon\right)$  for each scattering process i as function of the electron energy  $\epsilon$ . For gases, these data are provided by the class MediumMagboltz. Between collisions, an electron is traced on a classical vacuum trajectory according to the local electric (and optionally magnetic) field. The duration  $\Delta t$  of a free-flight step is controlled by the total collision rate  $\tau^{-1}\left(\epsilon\right) = \sum_i \tau_i^{-1}\left(\epsilon\right)$ . The sampling of  $\Delta t$  of a free-flight step is done using the "null-collision" method [40], which accounts for the change in electron energy during the step. After the step, the energy, direction, and position of the electron are updated and the scattering process to take place is sampled based on the relative collision rates at the new energy  $\epsilon'$ . The energy and direction of the electron are subsequently updated according to the type of collision.

In Garfield++, the microscopic tracking method 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 length 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);
```

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

```
size_t GetNumberOfElectronEndpoints() const;
void GetElectronEndpoint(const size_t i,
```

**Table 6.2.** Status codes for the termination of drift lines.

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
-8	sharp kink (only for RKF)
-16	energy below transport cut
-17	outside the time window

```
double& x0, double& y0, double& z0, double& t0, double& e0,
double& x1, double& y1, double& z1, double& t1, double& e1,
int& status);
```

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 6.2.

The function

```
bool DriftElectron(const double x0, const double y0, const double z0, const double t0, const double e0, const double dx0, const double dy0, const double dz0);
```

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;

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

TH1F hEnergy("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.

If the sensor has a non-zero magnetic field, AvalancheMicroscopic will by default use a more complicated stepping algorithm which takes the effect of the B field on the electron trajectory into account. In order to explicitly switch using magnetic fields on or off one can use the function

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

```
void EnableAvalancheSizeLimit(const unsigned 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 to retrieve all excitations happening in the avalanche.

## 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 DriftLineRKF::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.

### 6.5. Visualizing isochrons

For drift chambers, it is useful to determine the contours of equal drift time to a wire. These so-called isochrons can be calculated and drawn using the class ViewIsochrons. The component or sensor from which to retrieve the field is set using

```
void SetComponent(Component* c);
```

or

```
void SetSensor(Sensor* s);
```

The function

```
void DriftElectrons(const bool positive = false);
```

instructs the class to compute isochrons using electron drift lines. If the flag positive is set to true, the electrons are drifted with positive charge, which is useful for calculating isochrons of wires that attract electrons.

By calling

```
void DriftIons(const bool negative = false);
```

one requests drift lines of (positive or negative) ions.

The calculation of the drift lines and equal time contours and their visualization is done by the function

```
void PlotIsochrons(const double tstep,
  const std::vector<std::array<double, 3> >& points, const bool reverse = false,
  const bool colour = false, const bool markers = false, const bool plotDriftLines = true);
```

**tstep** time interval between isochron lines,

points list of starting points from which to simulate drift lines,

**reverse** flag to measure the drift time from the end points of the drift lines (true) or from the starting points (false),

colour requests drawing the contour lines using the currently active colour palette,

markers flag to draw markers at the points on the isochrons (true) or draw the isochron as lines (false),

plotDriftLines requests plotting of the drift lines together with the isochrons.

The calculation of the drift lines is done using DriftLineRKF.

The appearance of the isochrons is affected by a number of additional parameters. By default, the algorithm tries to order the points at equal time such that the isochrons appear as reasonably smooth lines. This sorting step can be switched off or on using

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

When an isochron appears to be more or less circular, its points are ordered by increasing angle with respect to the centre of gravity. If the isochron, on the other hand, seems to be more or less linear, the points are ordered along the longest principal axis of the distribution. Whether the set is circular or linear is decided by computing the RMS in the two principal axes of the point distribution. If the ratio of these two numbers exceeds a threshold then the isochron is assumed to be linear, otherwise circular. This parameter (which defaults to 3) can be set using

```
void SetAspectRatioSwitch(const double ar);
```

Isochrons that appear to be circular are closed if the largest distance between two points does not exceed a certain fraction of the total length of the isochron. This threshold (initially set to 0.2) can be modified using

```
void SetLoopThreshold(const double thr);
```

Points on an isochron are only joined if they are less than a certain fraction away from each other on the screen. Points that can not be connected are shown by a marker. This fraction (initial value: 0.2) can be set using

```
void SetConnectionThreshold(const double thr);
```

By default, points on an isochron are also not joined if their connecting line crosses a drift line. This feature can be switched on or off using

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

# 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

$$i(t) = -q\mathbf{v} \cdot \mathbf{E}_{w}(\mathbf{r}), \tag{7.1}$$

where  $\mathbf{E}_w$  is the so-called weighting field for the electrode to be read out and the charge induced by particle moving from  $\mathbf{r}_1$  to  $\mathbf{r}_2$  is given by

$$\int_{t_{1}}^{t_{2}} i(t) dt = q \left[ \phi_{w} \left( \mathbf{r}_{2} \right) - \phi_{w} \left( \mathbf{r}_{1} \right) \right], \tag{7.2}$$

where  $\phi_w$  is the weighting potential.

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

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

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

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

3. Setup the binning for the signal calculation.

```
void Sensor::SetTimeWindow(const double tmin, const double tstep, const int nbins);
```

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();
void DriftLineRKF::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;
fm.SetWeightingField("WPOT.lis", label);
Sensor 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;
aval.SetSensor(&sensor);
aval.EnableSignalCalculation();
// Calculate some drift lines.
// Plot the induced current.
ViewSignal signalView;
signalView.SetSensor(&sensor);
signalView.PlotSignal(label);
```

The algorithms used for calculating the induced current are slightly different for DriftLineRKF, AvalancheMC, and AvalancheMicroscopic.

For drift lines calculated using the RKF method, the times  $t_j$ , coordinates  $\mathbf{r}_j$  and drift velocities  $\mathbf{v}_j$  at each point along the drift line are taken and the induced current

$$i_i = -q\mathbf{E}_w(\mathbf{r}_i)\cdot\mathbf{v}_i$$

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at these points is computed. In order to calculate the average current in each time bin, the array of  $(t_j, i_j)$  is interpolated (linearly) and then integrated using Simpson's rule over  $2n_{\text{avg}} + 1$  points. The parameter  $n_{\text{avg}}$  defaults to 2 and can be set using

```
void DriftLineRKF::SetSignalAveragingOrder(const unsigned int navg);
```

For drift lines simulated using microscopic tracking (AvalancheMicroscopic), the signal between subsequent points along the drift path is assumed to be constant, and can be calculated using either the weighting potential or the weighting field. The method can be selected using

```
void AvalancheMicroscopic::UseWeightingPotential(const bool on = true);
```

By default, the weighting field is evaluated at the mid-point of a drift line segment. Using

```
void AvalancheMicroscopic::EnableWeightingFieldIntegration(const bool on = true);
```

one can request 6-point Gaussian integration of the weighting field over a drift line segment.

The weighting potential method takes  $\phi_w$  at the start and end of each step  $j \to j+1$  along the drift path and calculates the average current  $q\Delta\phi_w/\left(t_{j+1}-t_i\right)$ .

For drift lines simulated using AvalancheMC one also has the choice between using the weighting potential or the weighting field for computing the induced current. The method to be used can be selected using

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

The weighting potential method should be used if one wants to ensure that the integrated current is correct (equal to the collected charge).

#### 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" (often also referred to as delta response 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. A third option is to use a predefined expression, implemented in the helper class Shaper. Its constructor,

Shaper(const unsigned int n, const double tau, const double g, std::string shaperType);

takes four arguments: n is the order of the shaper,  $\tau$  is the time constant, g is the gain factor, and shaperType is either "unipolar" or "bipolar". In the first case (unipolar shaper), the transfer function is given by

$$f(t) = g \exp(n) \left(\frac{t}{t_p}\right)^n \exp(-t/\tau), \qquad t_p = n\tau,$$

while for a bipolar shaper the expression

$$f(t) = g \frac{\exp(r)}{\sqrt{n}} \left( n - \frac{t}{\tau} \right) \left( \frac{t}{t_p} \right)^{n-1} \exp(-t/\tau), \qquad t_p = r\tau, \qquad r = n - \sqrt{n}.$$

is used. The normalization of these expressions is chosen such that the value of the transfer function at the peaking time  $t=t_p$  is unity. In order to use a transfer function provided by a Shaper class, one should call

Sensor::SetTransferFunction(Shaper& shaper);

The presently stored signal can be convoluted with the transfer function (specified using one of the methods above) using

```
bool Sensor::ConvoluteSignal(const std::string& label);
```

label name of the electrode

The function

```
bool Sensor::ConvoluteSignals();
```

convolutes the signals of all electrodes with the transfer function.

As an example, consider the following transfer function

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

*i.e.* a unipolar shaper with n=1. The two code snippets below illustrate different methods for applying this transfer function to the induced signal. In the first one, we pass a pointer to a C-style function to the Sensor.

```
double transfer(double t) {
  constexpr double tau = 25.;
  return (t / tau) * exp(1 - t / tau);
}
int main(int argc, char* argv[]) {
  // Setup component, media, etc.
  // ...
  Sensor sensor;
  sensor.SetTransferFunction(transfer);
```

```
// Calculate the induced current.
// ...
// Apply the transfer function.
sensor.ConvoluteSignals();
// ...
}
```

In the second one, we use a Shaper object.

```
int main(int argc, char* argv[]) {
    // ...
    Shaper shaper(1, 25., 1., "unipolar");
    Sensor sensor;
    sensor.SetTransferFunction(shaper);
    // ...
    sensor.ConvoluteSignals();
    // ...
}
```

#### 7.1.1. Noise

Prior to convoluting the induced current with a transfer function, one can add a random noise component to the signal using

```
void AddWhiteNoise(const double enc, const bool poisson = true, const double q0 = 1.);
```

**enc** desired equivalent noise charge (ENC) of the convoluted signal,

**poisson** flag whether to sample the number of noise pulses from a Poisson distribution, or to sample the noise charge in each bin from a Gaussian distribution,

**q0** amplitude of the noise delta pulses (in electrons).

The algorithm is based on the fact that white current noise is equivalent to a random sequence of delta current pulses with large frequency  $\nu$  and with constant amplitude  $q_0$ . When processing this signal by an amplifier with transfer function f(t), with a peak normalized to unity, the variance of the output signal becomes

$$\nu q_0^2 \int f(t)^2 dt.$$

We want this to be equivalent to the ENC<sup>2</sup>, which defines

$$\nu = \frac{1}{q_0^2} \frac{\mathsf{ENC}^2}{\int f(t)^2 \, \mathrm{d}t}.$$

The total number of current delta pulses in a period of time  $\Delta t$  is Poisson distributed with a mean  $\nu \Delta t$  and a standard deviation  $\sqrt{\nu \Delta t}$ . With the flag poisson set to true, a Poisson-distributed number of current pulses is added to the signal in the time window.

For large frequencies, the Poisson distribution becomes a Gaussian distribution, so the standard deviation of charge in a time bin  $\Delta t$  is

$$\sigma_q = q_0 \sqrt{\nu \Delta t}$$
.

With the flag poisson set to false, a Gaussian-distributed noise charge is added to each signal bin.

## 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.

 Table A.1. Physical units.

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	

# **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* 5*
Ne	neon	5* 5*
Ar	argon	5*
Kr	krypton	4*
Xe	xenon	4*
Cs	caesium	2*
Hg	mercury	2*
$H_2$	hydrogen	5*
para H <sub>2</sub>	para hydrogen	5*
$D_2$	deuterium	5*
ortho $D_2$	ortho deuterium	4*
$N_2$	nitrogen	5*
$O_2$	oxygen	5*
$F_2$	fluorine	2*
СО	carbon monoxide	5*
NO	nitric oxide	2*
H <sub>2</sub> O	water	 5*
$CO_2$	carbon dioxide	5*
$N_2O$	nitrous oxide	4*
$O_3$	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 <sub>4</sub> H <sub>10</sub>	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	5*
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	4*
SF <sub>6</sub>	sulfur hexafluoride	4*
$BF_3$	boron trifluoride	4*
CF₃Br	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*
CCI <sub>4</sub>	carbon tetrachloride	4*

Table B.1. Gases available in Magboltz 11.14.

## C. Solids

The constructors of the Solid classes usually come in two versions: one where the solid is kept in its default orientation (i.e. the local frame of the solid and the global frame are identical except for a translation), and one where the solid's orientation is set explicitly. This is done by specifying the direction of the solid's local z axis in the global frame.

#### C.1. Box

SolidBox describes a rectangular cuboid (Fig. C.1). The simplest version of the constructor creates a box the edges of which are aligned with the axes of the coordinate system.

```
SolidBox(const double cx, const double cy, const double cz, const double lx, const double ly, const double lz);
```

**cx,cy,cz** Coordinates of the centre of gravity of the box.

**Ix,ly,lz** Half-widths of the box along x, y, and z.

A box with a non-default orientation in space is created using

```
SolidBox(const double cx, const double cy, const double cz, const double lx, const double ly, const double lz, const double dx, const double dy, const double dz);
```

#### C.2. Tube

SolidTube describes a cylinder. The simplest constructor requires the location of the centre, the (outer) radius and the half-length.

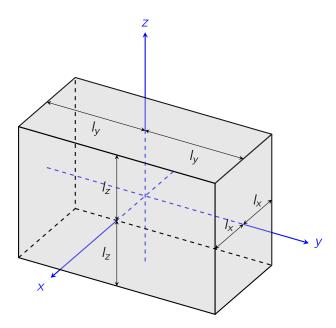
```
SolidTube(const double cx, const double cy, const double cz, const double r, const double lz);
```

**cx,cy,cz** Coordinates of the centre of gravity of the cylinder.

r Outer radius of the cylinder.

Iz Half-length of the cylinder.

By default, the central axis of the cylinder is collinear with the z-axis, as illustrated in Fig. C.2. To create a cylinder with a different orientation, the constructor



**Figure C.1.** SolidBox centred at (0,0,0), defined by its half-widths  $I_x$ ,  $I_y$ ,  $I_z$ .

```
SolidTube(const double cx, const double cy, const double cz, const double r, const double lz, const double dx, const double dy, const double dz);
```

can be used.

When determining the surface panels (e.g. for use in neBEM), the cylinder is approximated as a polygon with a finite number of panels. The type of polygon to be used can be set using

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

The number of corners of the polygon equals 4(n-1). Thus, n=2 will produce a square, n=3 an octagon. By default, the polygon used for approximating the cylinder is inscribed in a circle of the specified radius. If the "average-radius" flag is activated using

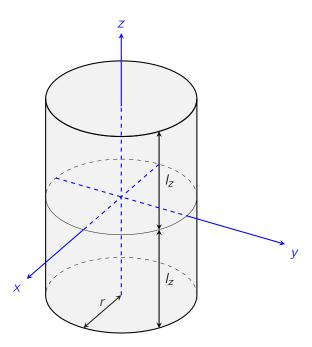
```
void SetAverageRadius(const bool average);
```

the radius will be interpreted as the mean radius of the polygon that approximates the cylinder. By default, the list of surface panels will include the "lids" at  $\pm z$ . This can be switched off using the functions

```
void SetTopLid(const bool closed);
void SetBottomLid(const bool closed);
```

## C.3. Sphere

SolidSphere has two constructors. The first one takes the location of the centre and the outer radius of the sphere.



**Figure C.2.** SolidTube centred at (0, 0, 0).

**cx,cy,cz** Coordinates of the centre of the sphere.

r Radius of the sphere.

The second one takes the coordinates of the centre and the inner and outer radii.

When calculating surface panels (e.g. for use in neBEM), the sphere is approximated by a set of parallelograms. The parameter n, set using

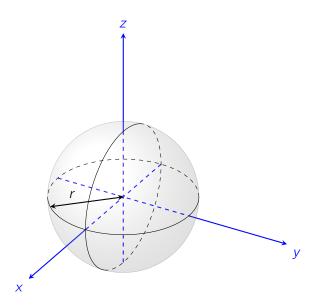
```
void SetMeridians(const unsigned int n);
```

specifies the number of meridians and also the number of parallels.

#### C.4. Hole

SolidHole describes an, optionally tapered, cylindrical hole in a box. Mandatory parameters are the location of the centre, the radii and the dimensions of the box (see Fig. C.4 for an illustration of the parameters).

```
SolidHole(const double cx, const double cy, const double cz, const double rup, const double rlow, const double lx, const double ly, const double lz);
```



**Figure C.3.** SolidSphere centred at (0,0,0).

**cx,cy,cz** Location of the point that is on the central axis of the hole, half-way between the two planes of the box perpendicular to the central axis of the hole.

rup,rlow Radius of the hole as measured at the "upper" and at the "lower" surface of the box.

**Ix,ly,lz** Half-lenghts of the box.

The central axis of the hole is collinear with the z-axis. To create a hole with a non-default orientation, the constructor

```
SolidHole(const double cx, const double cy, const double cz, const double rup, const double rlow, const double lx, const double ly, const double lz, const double dx, const double dy, const double dz);
```

is available.

Like in SolidTube, the type of polygon used for approximating the hole when calculating the surface panels can be specified using

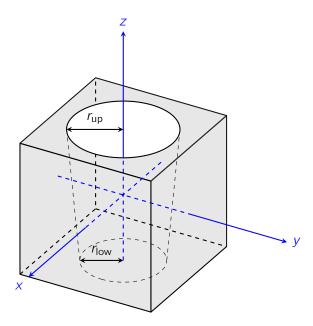
```
void SetSectors(const unsigned int n);
```

## C.5. Ridge

SolidRidge describes a ridge, similar to a Toblerone bar. The constructor takes the location of the centre and size of the floor, and the position of the ridge proper.

```
SolidRidge(const double cx, const double cy, const double cz, const double lx, const double ly, const double hz, const double hx);
```

**cx,cy,cz** Centre of the floor of the ridge in the (x, y) plane at z = 0.



**Figure C.4.** SolidHole centred at (0,0,0).

**Ix,ly** Half-lenghts of the floor.

**hz** Height of the ridge measured from the floor.

**hx** Offset in the x-direction of the ridge. If the offset is set to 0, then the ridge will be symmetric.

An illustration is given in Fig. C.5. By default, the ridge is taken to be parallel with the y-axis.

### C.6. Extrusion

SolidExtrusion (illustrated in Fig. C.6) describes a volume generated by extruding a polygon along its normal axis (default: z-axis). The constructor takes the half-length along z, and the x, y coordinates of the polygon defining the extrusion.

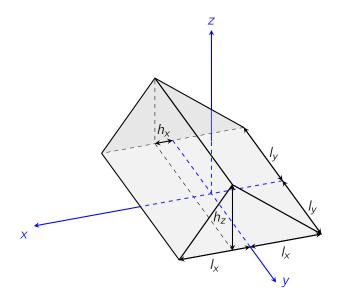
```
SolidExtrusion(const double lz,
const std::vector<double>& xp, const std::vector<double>& yp);
```

**Iz** Half-length of the extrusion along z.

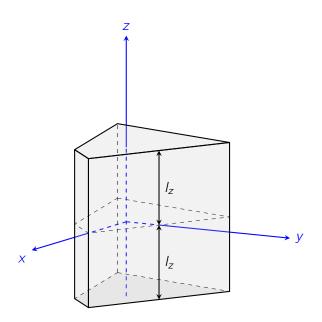
**xp,yp** x, y coordinates of the point defining the extrusion profile.

To create an extrusion with an orientation or offset different from the default one, the constructor

can be used.



**Figure C.5.** SolidRidge in its default orientation, centred at (0,0,0).



**Figure C.6.** SolidExtrusion in its default orientation.

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