COMSOL interface with Garfield++

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This document gives a brief overview over the creation of a model in COMSOL Multiphsics, as well as the import of a COMSOL model to Garfield++.

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1. CREATE A MODEL AND GEOMETRY IN COMSOL

COMSOL Multiphysics is a simulation software that allows the user to create a geometry and define physics in order to model different experiments. It covers a wide range of physics applications, in this example solely the AC DC package is used for illustration purposes. More information on COMSOL Multiphysics can be found at `www.comsol.com` [Accessed 2.09.2020].

These instructions and screenshots are based on COMSOL Multiphysics V5.5.

1.1 Creating a new COMSOL project

The first steps in creating a new COMSOL project are:

1. Open COMSOL V5.5
2. Select "Model Wizard" on the start page to create a new model.
3. Select the space dimension, for example 3D.
4. Select physics. Only add one physic type to start with, more physics can be added later on. For this example only "Electrostatics (es)" by the AC DC module was selected. Add the physics type and continue.
5. Select study. A general stationary study is recommended. More studies can be added later on.
6. Select done.

The initialization steps are now completed. The COMSOL default view can be seen in figure 1.1. On the left hand side under the tab "Model Builder" an overview over the entire project and its components can be seen. COMSOL executes commands in a top down manner. Hence the first thing to define is Geometry, then Materials, Physics and after a mesh is created. The next step is the computation of a study, which can then be analysed in results and exported.

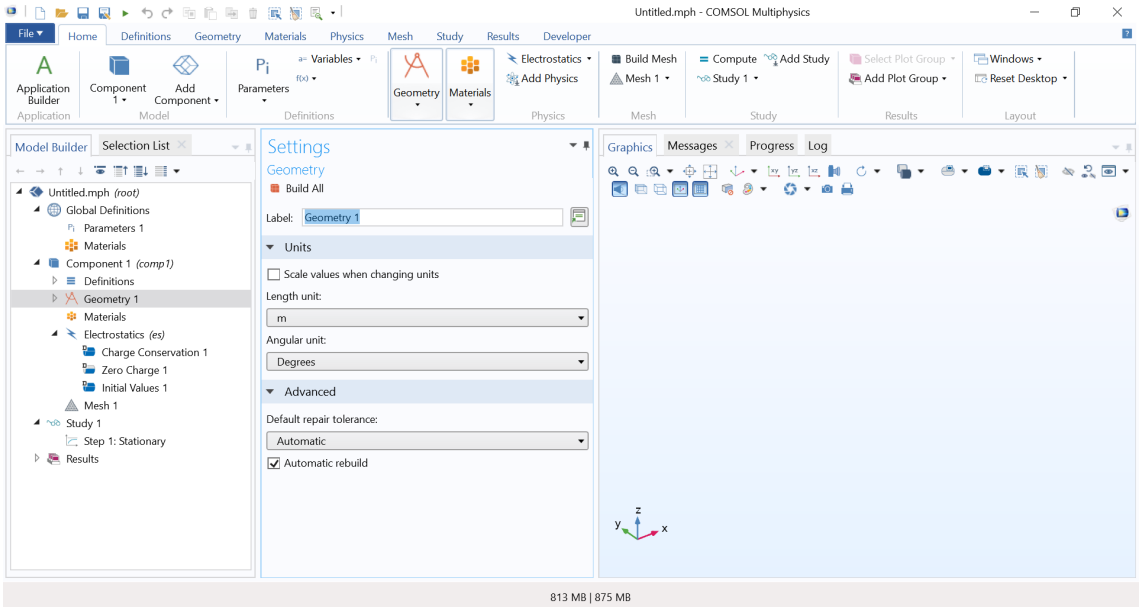

Fig. 1.1: Screenshot of COMSOL V5.5 window after creation of a new project.

1.2 Creation of Geometry

The next step in building a model within COMSOL is to create a geometric representation of the experiment. For this example a simplified version of a thick gas electron multiplier (GEM) was used.

New geometry parts can either be created directly inside Component 1 or be defined more generally as Global Definitions. To define a part as a global definition right click on global definitions, then select "Geometry Parts", then "3D Part". A new part has now been created called "Part 1" per default. Under the Settings window at Units, different units can be chosen for lengths and angles. Choose a unit that represents your order of magnitude of the experimental dimensions, otherwise rounding errors could occur. For this experiment the unit "cm" was chosen. Right click on "Part 1" to add 3D Components, such as boxes, cylinders, spheres and many more. You can rename "Part 1" to GEM by changing its label.

To create a more complex part it will be necessary to combine and subtract different sub parts. An example of this is the GEM itself. For this component, 3 cylinders are required: One for the top part of the GEM, one for the smaller bottom part and finally a cylinder which will be subtracted to created a hole. Create the 3 cylinders with their respective dimensions and choose their positions with respect to each other. Check the positions of all objects by building them ("Build All") and checking the different views, see figure 1.2 for an example.

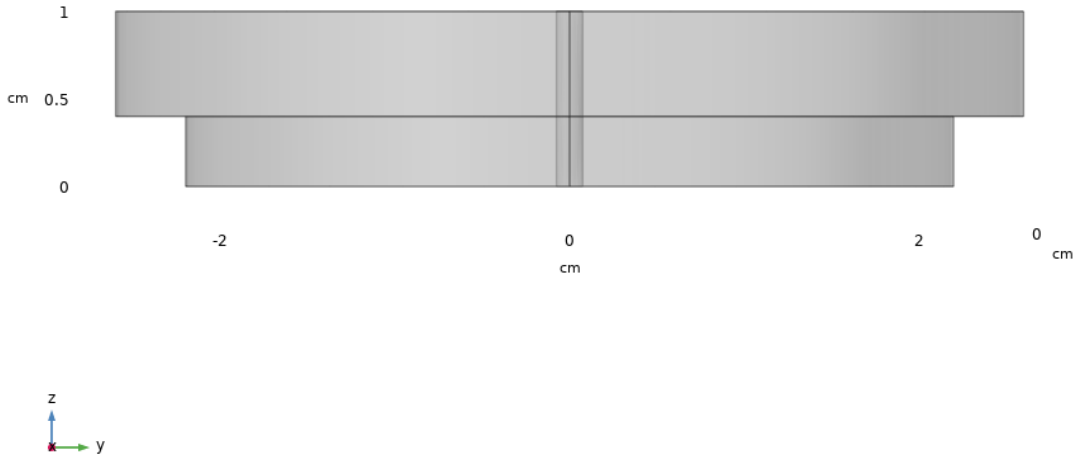

Fig. 1.2: Screenshot of COMSOL V5.5: Side view of GEM part consisting of 3 individual cylinders aligned.

After creating the 3 cylinders, we want to compose a new object "GEM" which consists of the two cylinders minus the hole cylinder. For this right click on Part 1 and select "Booleans and Partitions", then select "Compose". A new command line "compose" under the 3 cylinders has appeared. Select "Compose". As Input objects select all 3 cylinders. Select Keep Input Objects [1]. Select "Keep Interior Boundaries" [2].

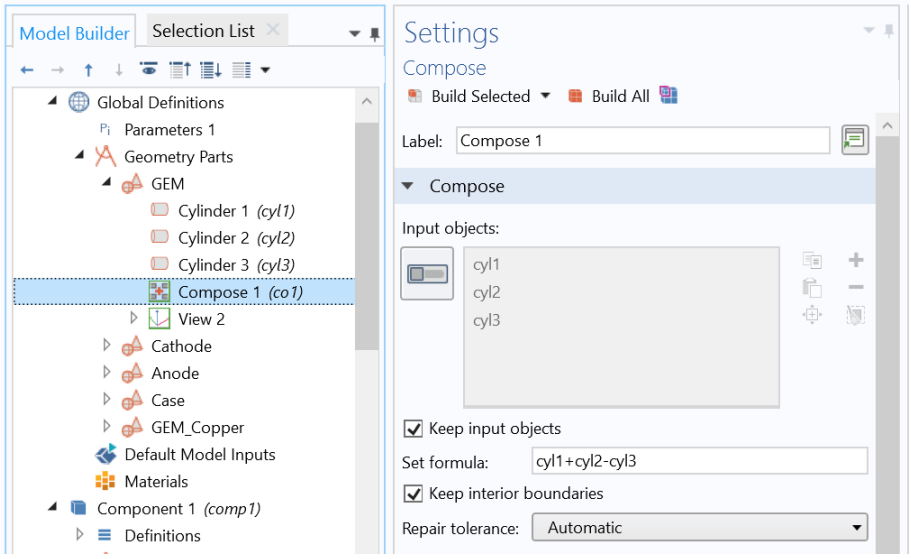

Fig. 1.3: Screenshot of COMSOL V5.5: "Compose" settings for subtraction of the hole from the GEM part.

[1] By selecting "Keep Input Objects" the cylinder which is subtracted will remain a domain, which we can set to gas later.

[2] By selecting "Keep interior boundaries", the boundaries between the top and bottom layer are not deleted, this will be helpful for the mesh creation later.

In order to add a part created as a global definition to a specific component of the experiment right click on Geometry 1 under Component 1 and select "Parts", then select the part you wish to import, for example GEM. Repeat this for all parts you wish to have in your experiment.

By continuing to import and create all individual components a 3D model of the experiment is build step by step. Always check whether the positions of the coordinates match. Make sure the units are consistent. The final geometry of the simplified setup can be seen in figure 1.4 as 3D view and as a side view in figure 1.5. The components used are: GEM, cathode, anode, case and a thin copper layer on the GEM.

1.3 Define Materials

After creating the geometry the next step is to assign a material to each domain. For this first materials must be added by right clicking on "Materials", then select "Add Material from Library". Select your materials or define custom materials. Select a material, for example copper, and then select all the domains from geometry which should be made out of this material. Continue until all domains are assigned. You can find an overview over all the elements and which domain is assigned to what by clicking on "Materials". For this experiment the materials copper, glass (quartz), propane, aluminium and FR4 (circuit board) were used.

1.4 Define Physics

In order to define the physics the user must specify which voltages are applied to which boundaries. From top to bottom the commands are executed, hence first per default charge conservation is applied to all domains. Then zero charge is applied to all domains and the initial values are set to 0 V per default for all domains. Now the user can add additional physical constraints, such as the cathode voltage, anode voltage and which sections are grounded (metal casing and copper layer).

1.5 Create Mesh

The next step is to create a mesh. The mesh is a representation of the geometry and during the meshing step the geometry is subdivided into finite elements. Per default a free tetrahedral mesh is applied over the modelling space by the meshing algorithm, however this might require a lot of memory [3]. ify the model and reduce the mesh size.

[3] For more information in regard to the meshing process, see `https://www.comsol.com/blogs/much-memory-needed-solve-large-comsol-models/` [Accessed 2.09.2020]

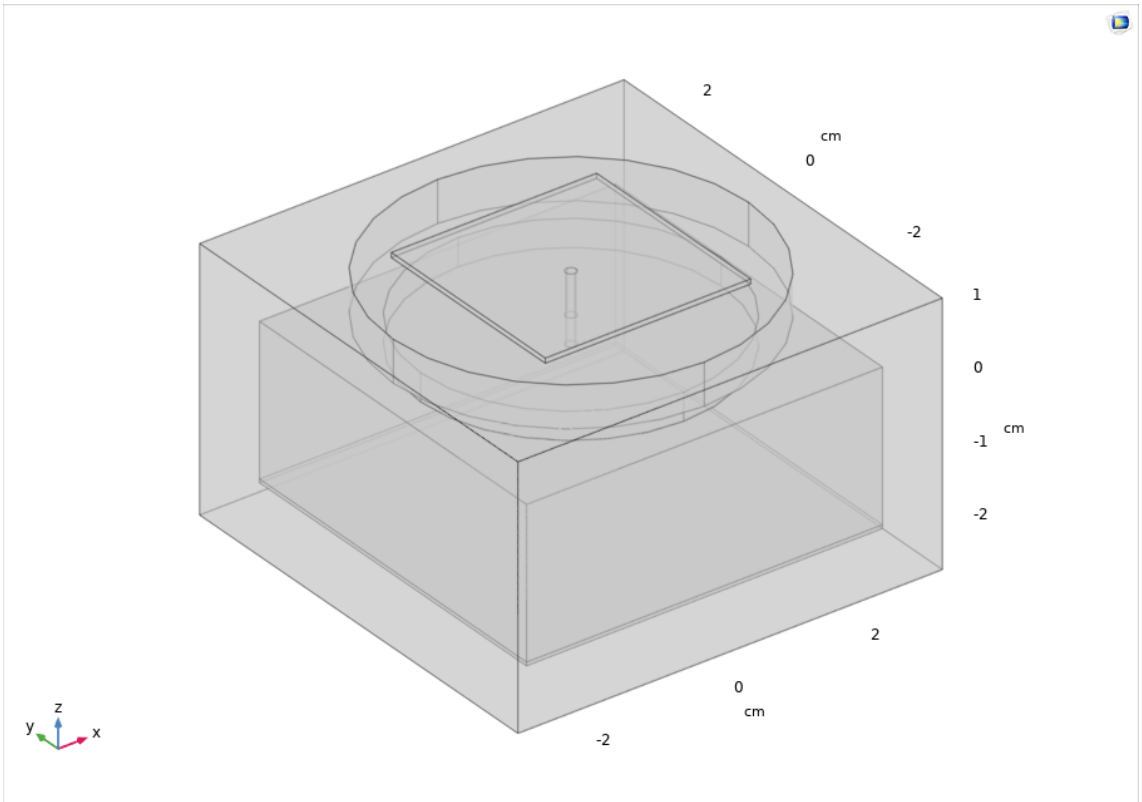

Fig. 1.4: Screenshot of COMSOL V5.5: Final geometry for experimental setup in 3D view.

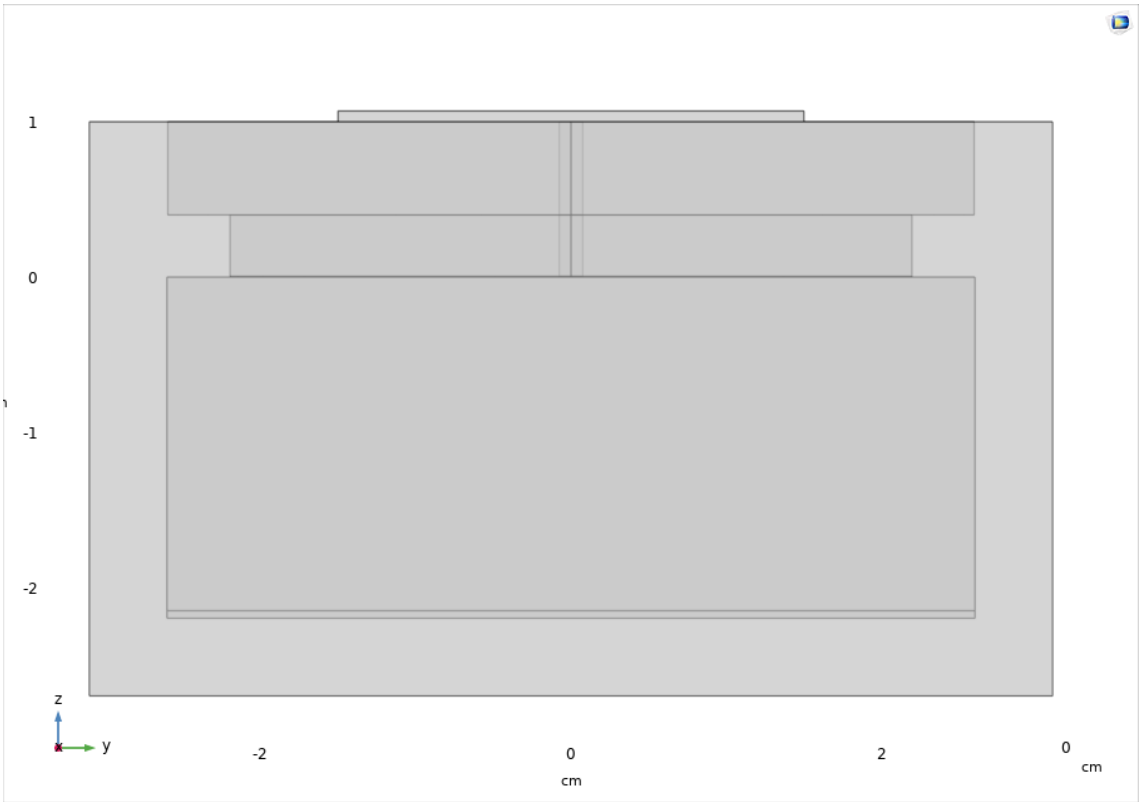

Fig. 1.5: Screenshot of COMSOL V5.5: Final geometry for experimental setup in 2D side view.

Select the mesh tab. Under "Mesh Settings" the sequence type can be selected to be either "User-controlled mesh" or "Physics-controlled mesh". The physics-controlled mesh is an automated meshing sequence designed to create a mesh in regard to the physics. However any automated meshing process can run into problems if the geometry is complicated, as is the case in this example.

The automated meshing runs into problems when attempting to mesh the very thin copper layer which is 0.005 cm thick. The change between a very thin layer and surrounding larger layers causes errors, such as generated some elements of low quality, shorter than the specified minimum element size and many more. To get rid of such errors the user can try to define a very fine physics-controlled mesh, resulting in finely meshing all areas and creating more nodes than necessary, or alternatively, by creating a user-controlled mesh manually.

The creation of a user-controlled mesh is a time intensive and tricky task. The optimization of a mesh is far from straightforward, hence only a basic systematic example is shown here. By selecting user-controlled meshing as the sequence type a new sub layer shows up consisting of the elements "Size" and "Free Tetrahedral".

The size command allows the user to define how finely the meshing based on physics should be. The user can choose between a variety of options ranging from extremely fine over normal to extremely coarse as predefined settings. By changing the element size to "Custom", the user can manually adjust even more details, such as minimum/maximum element size, maximum element growth rate, curvature factor and resolution of narrow regions.

The free tetrahedral command is per default set to the geometric entity level "Remaining", meaning that it will be applied to all domains who have not previously been assigned a different mesh.

The goal of a user created mesh is to create a mesh that fulfils the following properties:

- Coarse meshing as default.
- Finer meshing for regions where interesting physics might take place (in this example: GEM hole and surrounding area).
- Create a mesh fine enough to correctly represent the geometry (in this example: hole must be detailed enough to be meshed as a circle, not a square).

An example of such a mesh for the GEM can be seen in figure 1.6, where the element size is shown as red for small elements and blue for larger elements.

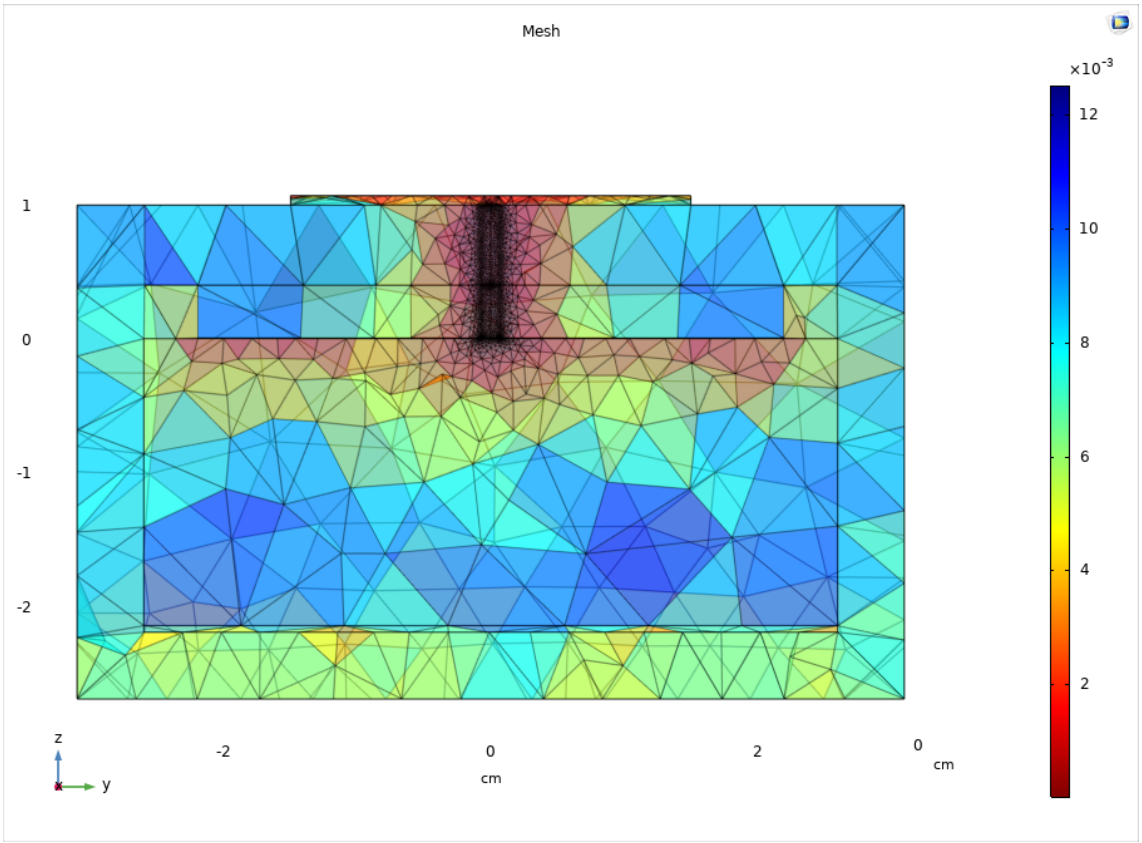

Fig. 1.6: Screenshot of COMSOL V5.5: Mesh view at x=0 plane with color coded elements for size.

A typical method to create manual meshing is to follow this procedure:

1. Start with regions, where fine meshing will be required and find a domain to be meshed.
2. Check geometry of this domain: What shape is it? Which side/boundary of this domain should be meshed most precisely? Should the mesh be square or triangular?
3. After deciding which boundary shall be meshed in which manner, right click on "Mesh" and select "More Operations", then select "Free Triangular" (or "Free Quad").
4. Open up the newly created "Free Triangular 1" and select "Boundary" as geometric entity level. Select the boundary you chose to mesh.
5. Right click on "Free Triangular 1" and select "Size". In the newly created size command select how large the element size of this mesh should be. If necessary, change certain values manually in custom setting.
6. Click on "Build Selected".

Now a mesh on the selected boundary should appear. In general COMSOL then uses the function of "Swept Meshes" to extend the boundary mesh to a 3D volume. By adding a "Distribution" subcommand to the Swept command the user can define how many steps should be performed along the swept direction.

However, unfortunately Garfield++ is unable to read swept meshes, this is still under investigation. An alternative to using swept meshing is to use different free tetrahedral settings for individual domains. By firstly meshing regions of interest with a fine boundary mesh this will directly force the free tetrahedrals to be fine around said regions. Note that the fine boundary meshes must be created before the remaining domains are filled up with tetrahedral meshes.

The final mesh can be seen in figures 1.7 and 1.8.

1.6 Create Study

In order to create a study and hence compute the physics of the modelling process, the user must select the Study tag "Study 1". As a subcommand of "Study 1" there is the previously selected stationary study, called "Step 1: Stationary". Select the stationary study. In the "Physics and Variables Settings" tab select which physics you are interested in, for example activate electrostatics. Under "Mesh Selection", select the mesh which you would like to use in this calculation. To calculate the study click "Compute", this step can take a while. If your mesh is very fine it will take longer.

1.7 Plot results

After creating and solving our model, the results can be shown in different plot types. Under "Results/Datasets" there should be a command called "Solution 1", which is the solution of Study 1. In datasets the user can manually change the solution to only take into account certain regions of interest and other things. This is also the place to define 2D curves, useful for setting starting points for streamline plots.

In order to define a plane cutting through our experiment, used for 2D plots later on, we define a Cut Plane by right clicking on "Datasets" and selecting "Cut Plane". Under the tab "Data", select the dataset which you want to study. As Plane type choose "Quick" and select a plane of your choice, for example the xz-plane. By clicking on "Plot" the selected plane with respect to the geometry is shown, see figure 1.9.

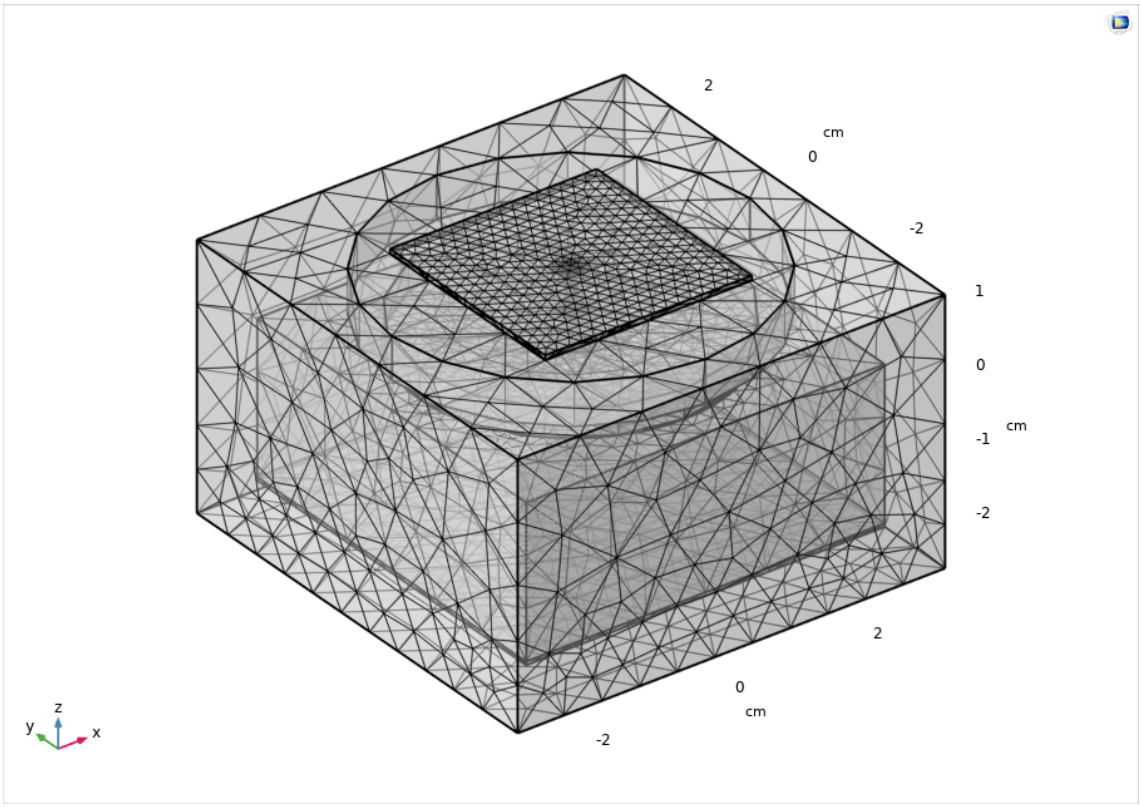

Fig. 1.7: Screenshot of COMSOL V5.5: Final meshed geometry for experimental setup in 3D view.

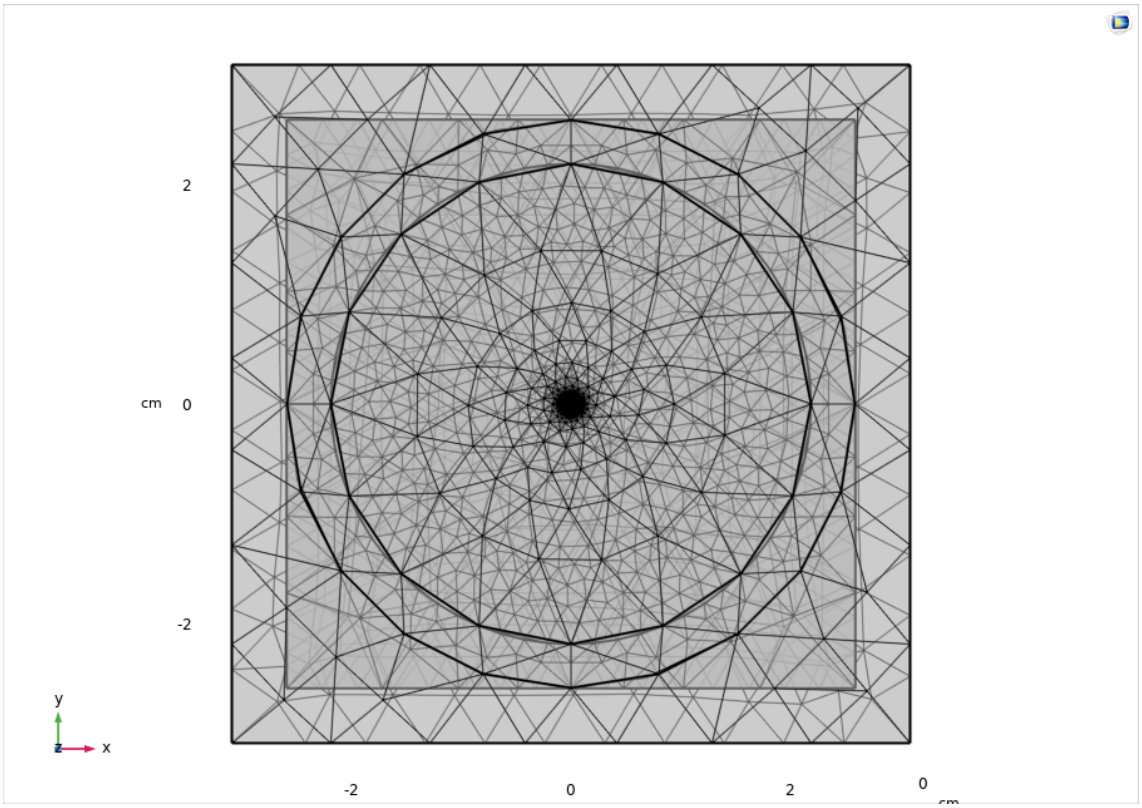

Fig. 1.8: Screenshot of COMSOL V5.5: Final meshed geometry for experimental setup in 2D top view. Note how the center of the GEM is meshed more finely than the surrounding areas.

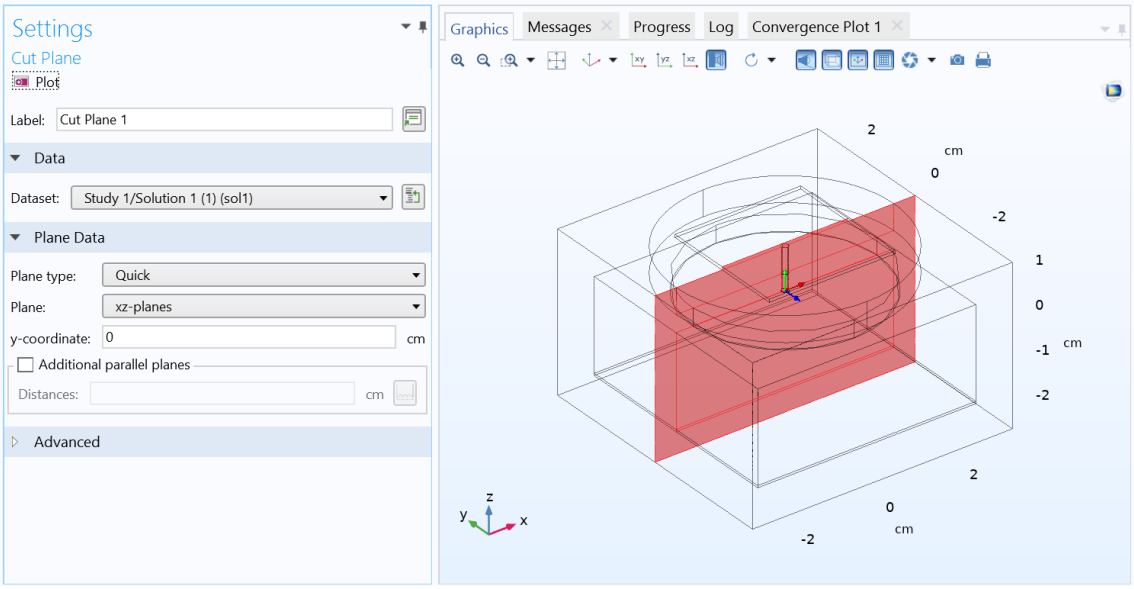

Fig. 1.9: Screenshot of COMSOL V5.5: Cut plane for xz-plane.

1.7.1 Electric potential in 2D

In order to show the electric potential in a 2D plot, right click on Results and add a 2D Plot Group. Open the newly created 2D Plot group. Under dataset choose the cut plane previously set for the 2D view. Right click on the 2D Plot group and add a "Surface" plot. In the surface plot command set the dataset to "From parent" and select the expression "V" in units of "V" to plot the electric potential. In the colouring and style tab, the colour scheme can be adjusted to "Rainbow", for example. In order to create a contour plot the procedure is identical, expect choose a "Contour" plot in the 2D Group instead of the "Surface" Option.

1.7.2 Streamline Plot in 2D

Right click on Results and add a new 2D Plot Group. Select dataset from cut plane. Right click on new 2D Plot group and add a "Streamline" plot. In the streamline plot select dataset "From Parent" and under expression choose the Global Cartesian coordinate system. For the x-component select es.Ex, for y-component es.Ey and for the z-component es.Ez. For the streamline plots the user must define how the streamline should be positioned. In order to have streamlines covering the entire region you might have to overlap different streamline plots.

One option is to create a starting-point controlled stream line plot. For this choose positioning "Starting-point controlled", entry method "Coordinates" and enter the x and y parameters of your coordinates. For example x= range(-0.075, 0.01, 0.075), y=0. This will create a series of points in which the streamlines will be started. In order to color code the streamlines right click on streamline plot and add a color expression.

Another option is to use starting-point controlled positioning and the entry method "Number of Points" along a curve. To define a curve right click on "Datasets", select "More 2D Datasets", select "2D Parametrized curve". In the new 2D Curve dataset tab, see figure 1.10, select parameters and an expression for your curve. In this example a linear curve ranging from x=[-2,+2] and y=-1.1 was used. Use the plot function to check whether your curve is placed where you want it to be with respect to the geometry. In the streamline plot, select this curve and the number of points that should be placed along it.

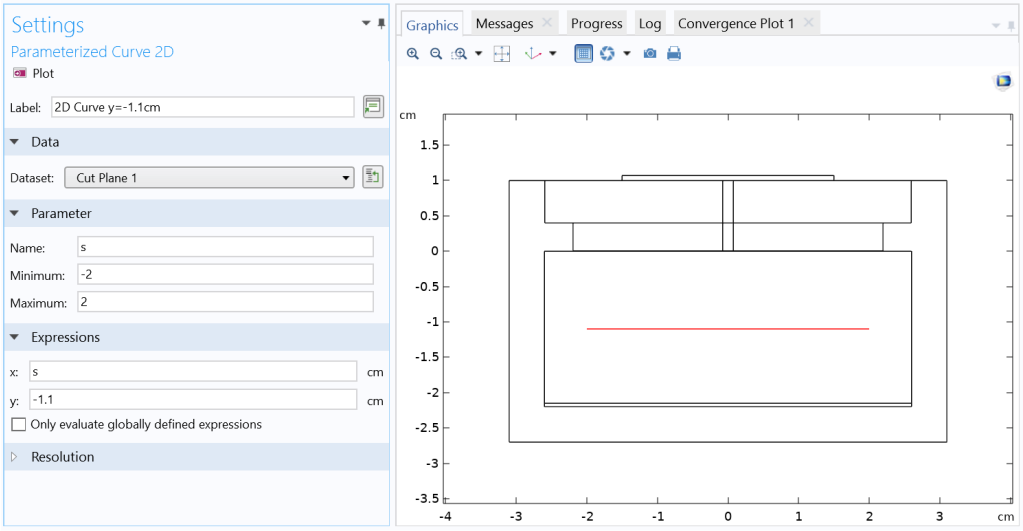

Fig. 1.10: Screenshot of COMSOL V5.5: Settings for 2D parametrized curve.

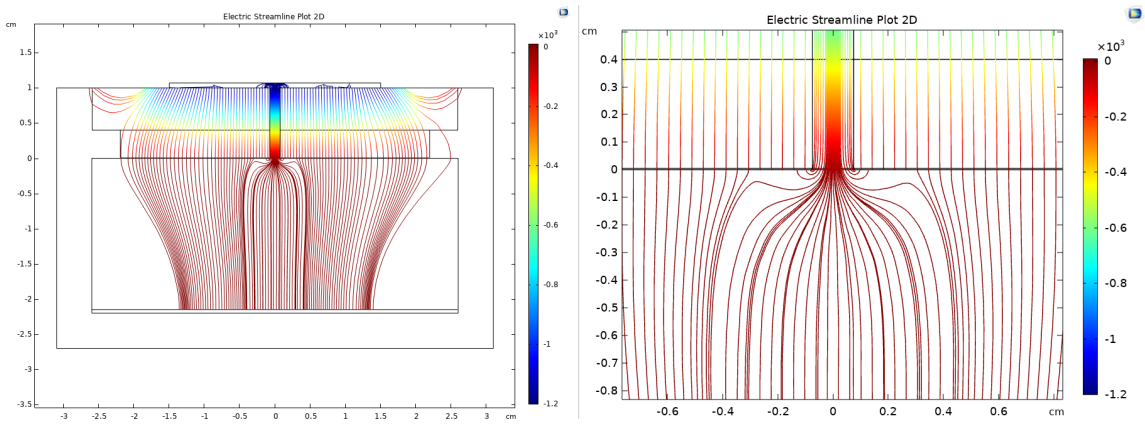

Fig. 1.11: Screenshot of COMSOL V5.5: Streamline Plot

1.7.3 Mesh Plot

In order to create a plot of the mesh used in the simulations create a 3D Plot group and add a "Mesh" plot to it. Select the Solution 1 dataset for this plot group. In the mesh plot select dataset "From parent" and under the settings tab "Level" select

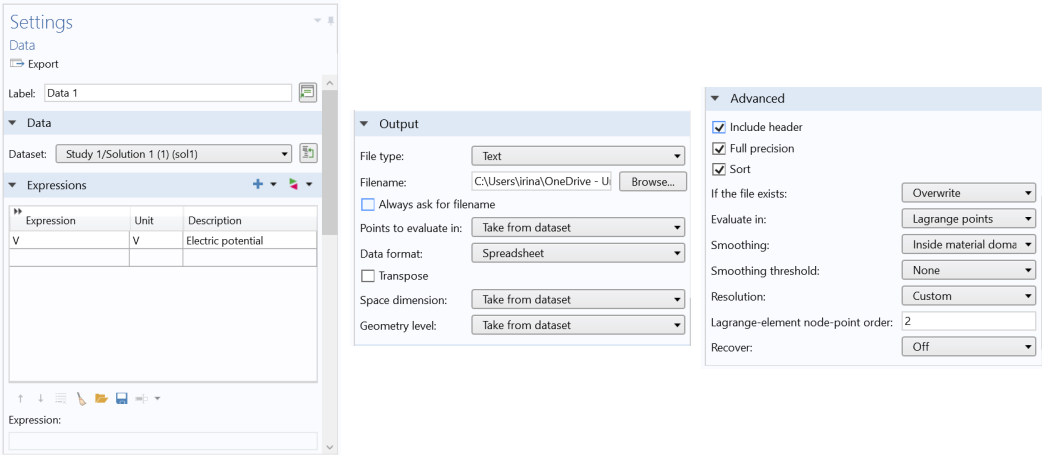

Fig. 1.12: Screenshot of COMSOL V5.5: Settings for export of electric potential data.

level "Volume" and element type "All". Under element color the user can choose between quality, size and others.

If the user wants to visualize the mesh inside the experiment the easiest way to do so is to add a filter. Right click on the mesh plot and add "Filter". In the settings tab "Element Selection" choose the logical expression for inclusion, for example x<0. This results in the plot seen in figure 1.6.

1.8 Export Electric Field and Mesh to Garfield++

Garfield++ requires mesh files and a data file containing the electric field potential. In order to create these exports right click on export and add a data export and a mesh export.

In the data export select solution 1 as dataset. Under Expressions select "V" as the electric potential to be exported. In the tab "Output" select the file type "txt" and filename. Under the "Advanced" tab select include header, full precision and sort, change evaluate in "Lagrange points" and resolution "custom" with Lagrange-element node-point order "2". See figure 1.12 for all settings. For the mesh export choose solution 1 as dataset, the file type "mphtxt" and a file name, see figure 1.13.

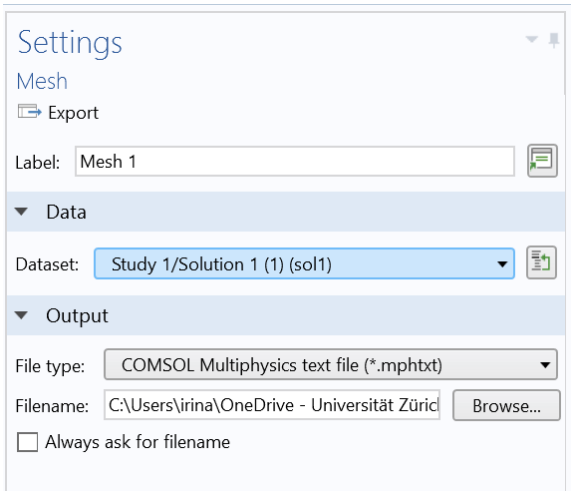

Fig. 1.13: Screenshot of COMSOL V5.5: Settings for mesh export.

2. IMPORT A COMSOL MODEL TO GARFIELD++

After the creation of your model in COMSOL and exporting the electric potential and mesh, the next step is to import the COMSOL model to Garfield. The code in regard to COMSOL imports can be found in ComponentComsol.cc.

To create a new COMSOL component use the following code:

```
ComponentComsol* fm = new ComponentComsol();
fm->Initialise(INPUT_PATH_MESH,          //mesh
               INPUT_PATH_MAT_MAPPING,   //mplist
               INPUT_PATH_FIELD,         //field
               "cm");                    //unit
```

where `INPUT_PATH_MESH` would be the path to your mesh file (.../dataset/mesh.mphtxt), `INPUT_PATH_FIELD` the path to your electric potential file (.../dataset/field.txt) and `"cm"` is the unit used in your COMSOL model as a string. The parameter `INPUT_PATH_MAT_MAPPING` is the path to a mat mapping file (.../dataset/mplist.txt), which needs to be manually created by the user. This will be explained in more detail now.

The mat mapping file is used by Garfield to connect the COMSOL domains to their respective material regions in Garfield. This assignment must be performed and checked by the user. Let us first look at how such a file looks like and how the syntax works, and then explain how it can be obtained.

The `mplist.txt` file contains two rows of numbers, for example like this:

```
2 1 2
4 3 1 8 1 9 1 10 1
```

The first row specifies which materials are available and the second row assigns domains from COMSOL to these materials.

- The first number in the first row specifies the number of materials (in this case: 2).
- The second number in the first row specifies the permittivity of the first material.
- The third number specifies the permittivity of the second material and so on.
- The first material has index ”0”, the second material has index ”1”.

- The material with index "1" is the drift medium, in our case propane gas.

In order to get an overview over the different materials and their permittivity you can execute the code:

```
//Create gas medium
MediumMagboltz* gas = new MediumMagboltz();
gas->SetComposition(GAS_CHEMICAL_COMPOSITION, 100.);
gas->Initialise();
gas->SetMaxElectronEnergy(300);
gas->LoadGasFile("propane-2torr-293.15k-extended.gas");
gas->SetTemperature(GAS_TEMPERATURE);
gas->SetPressure(GAS_PRESSURE);

//Assign gas medium
const unsigned int nMaterials = fm->GetNumberOfMaterials();
for (unsigned int i = 0; i < nMaterials; ++i) {
  const double eps = fm->GetPermittivity(i);
  if (i == 1) { // i=1 ->is gas
    fm->SetMedium(i, gas); //Assign medium
    std::cout << "Medium " << i << " (eps = " << eps << " ) set to
   Magboltz gas." << std::endl;
  }
}
fm->PrintMaterials();
```

Note that `fm->SetMedium(i,gas)` sets the drift medium, where `gas` is a MediumMagboltz component. The command `fm->PrintMaterials()` prints a table of all materials defined. In this table you can cross check your material definitions for index and permittivity, see figure 2.1.

```
MediumMagboltz::LoadGasFile: Reading gas_files_propane/c3h8-1.5torr-293.15K-emin1-emax1000-setFi
eldGrid6-GenerateGasTable2.gas.
MediumMagboltz::LoadGasFile: Reading header.
    GASOK bits: TFTTFTTTTTTFFFFTFFFF
    Identifier:  C3H8 100%, T=293.15 K, p=0.00197368 atm

    0 excitations, 24 ionisations.
MediumMagboltz::LoadGasFile: Version 12
MediumMagboltz::LoadGasFile:
    Gas composition set to C3H8
MediumMagboltz::LoadGasFile:
    6 electric field(s), 1 magnetic field(s), 1 angle(s).
MediumMagboltz::LoadGasFile: Reading 1D table.
MediumMagboltz::LoadGasFile: Reading footer.
MediumMagboltz::LoadGasFile: Done.
Medium 1 (eps = 2 ) set to Magboltz gas.
-----------------------------------------------
ComponentComsol::PrintMaterials:
    Currently 3 materials are defined.
      Index Permittivity  Resistivity Notes
          0           1          -1 (drift medium)
          1           2          -1 C3H8, drift medium, ionisable (drift medium)
          2          -1          -1
-----------------------------------------------
```

Fig. 2.1: Screenshot of console output for a part of the code snippet above.

In order to create the second row of numbers for the mplist.txt file the user must

assign domains to be gas. For this the meshView is very useful. Set the mesh view to an area of your interest by adjusting `VISUAL_AREA_X` and the other parameters. If the second row is missing from the mapping list file, all domains will be plotted as black. Execute the code to check whether this works. In case some areas remain white despite having not been assigned to gas, this can be explained by a COMSOL mesh which appears to not be compatible with Garfield++ (for example a Swept Mesh). Replacing these mesh components by free tetrahedrals in COMSOL can fix this problem.

```
ViewFEMesh* meshView = new ViewFEMesh();
meshView->SetComponent(fm);
meshView->SetPlane(0,-1,0,0,0,0);
meshView->SetFillMesh(true);
meshView->SetArea(-VISUAL_AREA_X/2,-VISUAL_AREA_Z/2,-VISUAL_AREA_Y
   /2,VISUAL_AREA_X/2,VISUAL_AREA_Z/2,VISUAL_AREA_Y/2);
```

After successfully plotting all components and checking the `SetArea` to display all of the geometry, the next step is the assignment of domains to gas. For this the second row of numbers is used. The syntax is as follows:

- The first number of the second row is equal the number of arguments that follow.
- Every argument consists of two numbers. The first number is the domain number and the second number corresponds to the index of material to be assigned (1 for drift medium).

Start by mapping out which domain corresponds to what by setting mplist.txt to:

```
2 1 2
1 X 1
```

where `X` is the domain number, which varies from 1 to the maximal number of domains used in your COMSOL model. Note which domain corresponds to which element of your model for later reference. In general, the domain numbers should correspond to the domain numbers in COMSOL. Make sure to check them though. After checking which domain corresponds to what part of the model, set all domains that should be filled with gas to index "1", this results in a mesh view as can be seen in figure 2.2.

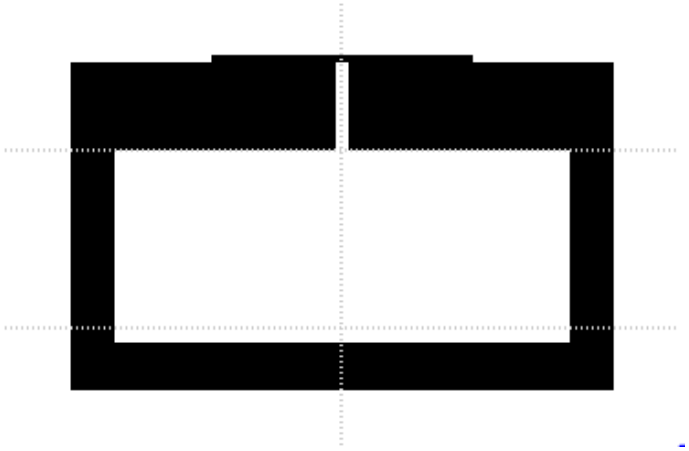

Fig. 2.2: Screenshot of mesh view for correctly assigned domains.

As a resulting general overview the mplist.txt file should be read as follows for the example:

```
2 1 2
4 3 1 8 1 9 1 10 1
```

There are 2 materials. The first material has index 0 and permittivity 1. The second material has index 1 and permittivity 2. There are 4 domains that should be assigned to a special medium: Domains 3, 8, 9 and 10 are assigned to the medium with index 1, hence assigned to drift medium (gas).