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DIPARTIMENTO DI ELETTRONICA, INFORMAZIONE E BIOINGEGNERIA

COMSOL Multiphysics
Introduction to CAD exercise

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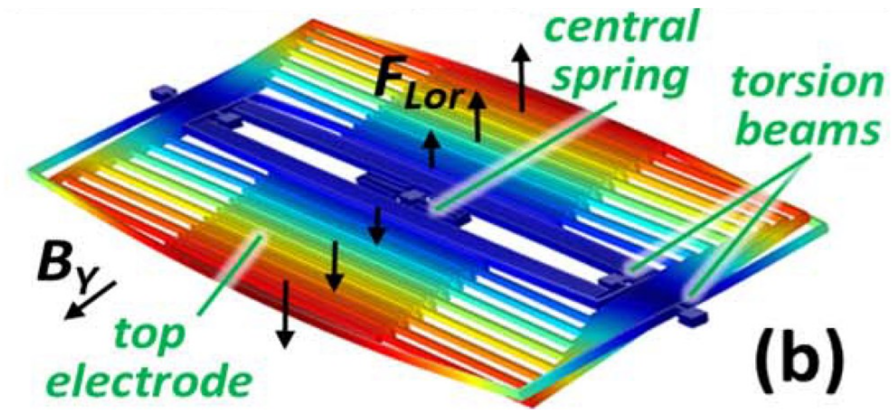
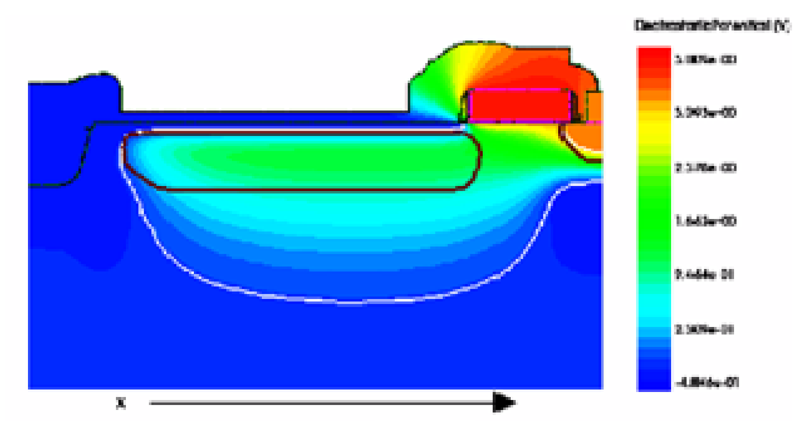
MEMS and Microsensors – M.Sc. in Electronics Engineering

Why Multiphysics?

- Typically, a sensor designer must deal, sometimes simultaneously, with several physical domains. Some examples:
  - **Quasi-static and dynamic mechanics** (for MEMS motion);
  - **Electromagnetism in air** (for MEMS capacitive readout);
  - **Thermodynamics** (for MEMS non-idealities in temperature);
  - **Light/matter interaction** (for CMOS image sensors);
  - **Semiconductor** charge generation and transport (pixel sensors design);
  - **Fluidics** (damping and Q factor simulations)



MEMS Magnetometer



Pinned photodiode

Why simulations?

- Approximated equations seen during lectures could be complicated by some **second-order effects**, neglected in our calculations on paper.

- E.g. the **Hooke's law** in the form below

$$F_{el} = kx$$

- is valid only for small displacements and without electrostatic softening… in some practical cases, the **complete non-linear form** must be considered:

$$F_{el} = kx + k_3 \cdot x^3 + k_{elec}x + k_{elec_3} \cdot x^3$$

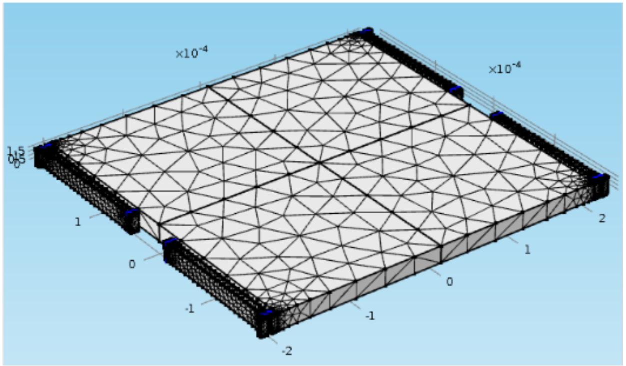
- In general, 1-D studies are only an approximations of a **3D problem , whose solution** is not so easy just relying on equations…

- Moreover, **different physical domains cannot be solved as standalone domains**. (e.g. the pull-in effect that you studied in lectures: here mechanical and electrostatic domains interact → **second order nonlinear differential equation**).

- A simulator helps the designer to solve similar issues in a fast way.

Why Finite Elements Method (FEM) simulations?

- **FEM simulations**:
  - the **device is approximated with a finite grid of point** (mesh): the **solver will solve the equations in these points** and, using specific **convergence iterative algorithms**, will find the **problem solution**.



- In **classes and exercises** we considered our **seismic mass** as a **point-like mass**. This approximation can be **not accurate in sensors with complex geometries** or with **nested frames** (as gyroscope, see next classes).

- In other cases, is **simply impossible to use point-like approximations**, like the case study we will see today: the capacitance variation in a tilting capacitance with a perforated plate.

Typical simulation steps: phase 1 – model definition

- **Choice of the physical domain(s) and problem definition**, some examples:
  - Solid Mechanics Domain:
    - Eigenfrequency
    - Stationary;
  - Semiconductor Domain;
  - And many more…

- **Geometry definition**:
  - 2D geometry: save computational cost;
  - 3D geometry only when needed!

- **Mesh definition**:
  - Non-uniform spatial sampling: more **points** where it is expected a **significant variation of the solution** (e.g. on the deflecting springs of an accelerometer, or at the edges of a capacitance);

- **Boundary conditions definition**:
  - force the solution in some points of the mesh (e.g. anchor points or DC bias);
    - **Dirichlet** contour conditions (the value of the variable is fixed);
    - **Neumann** contour conditions (the value of the derivative is fixed);
  - In modern solvers you define contour conditions in a more '*qualitative*' way.

Typical simulation steps: phase 2 – problem solution

- **Solve the problem:**
  - The solutor start to compute equations;
  - If the solution doesn't converge, you can act on some parameter: mesh, contour conditions, solution tolerance…

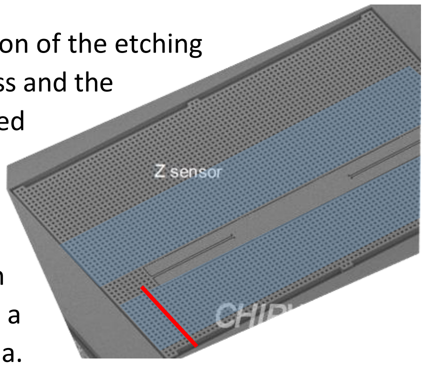
- **Analyze the results:**
  - ALWAYS check the simulations results and compare them to your expected theoretical predictions!
  - Simulators can be themselves wrong sometimes (in the end their codes are written by human beings)…

COMSOL Multiphysics: perforated capacitor in an out-of-plane structure

Giacomo Langfelder e Luca Pileri

07/10/2024

The purpose of this exercise is to estimate the value of the capacitance (and its variation under displacements, dC/dz) in a common situation for out-of-plane (OOP) MEMS devices: one plate of the variable capacitor is perforated and suspended over a buried interconnection forming the second, fixed plate.



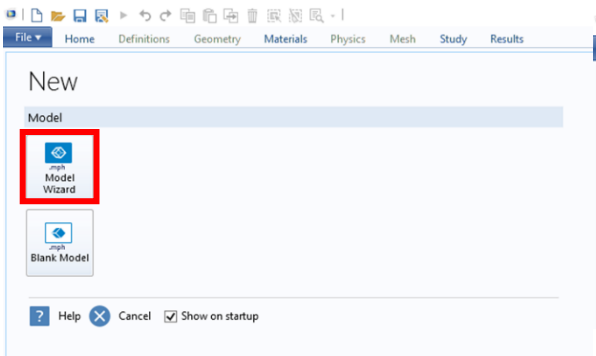
As discussed in lectures, holes are mandatory for a correct releasing action of the etching acids: but what about the capacitance formed between a perforated mass and the electrodes underneath (as in the example aside)? Can this be approximated to an ideal parallel-plate (infinitely long) capacitance or not? One can think that the calculation is readily done: it is simply a capacitor with less facing area (in other words, the perforated area can be subtracted). This statement is not correct, and we can find a more accurate expression of the capacitance exploiting FEM simulations: the goal is thus to extract a correction factor α_{Cap} to be used in the accelerometer sensitivity formula.

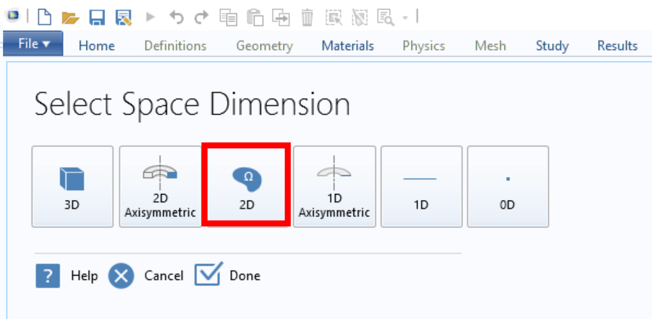
In order to solve this problem with a low computational cost, we can simplify it to a 2D geometry: we can assume that this kind of geometry is a slice of our tilting device (e.g. along the cross section indicated in red in the figure above).

We can begin the problem by simulating the value of an *ideal* MEMS variable parallel-plate capacitance (and the corresponding $\frac{dC}{dz}$), by comparing it to theoretical predictions (to check the validity of simulations), and then we can design a perforated structure, repeating the same elaboration to find the correction factor α_{Cap}.

1. Design of the structure

We now start the design of the 2D geometry that we want to analyze. Open Comsol Multiphysics → choose "Model Wizard" → in Select Space Dimension choose "2D"

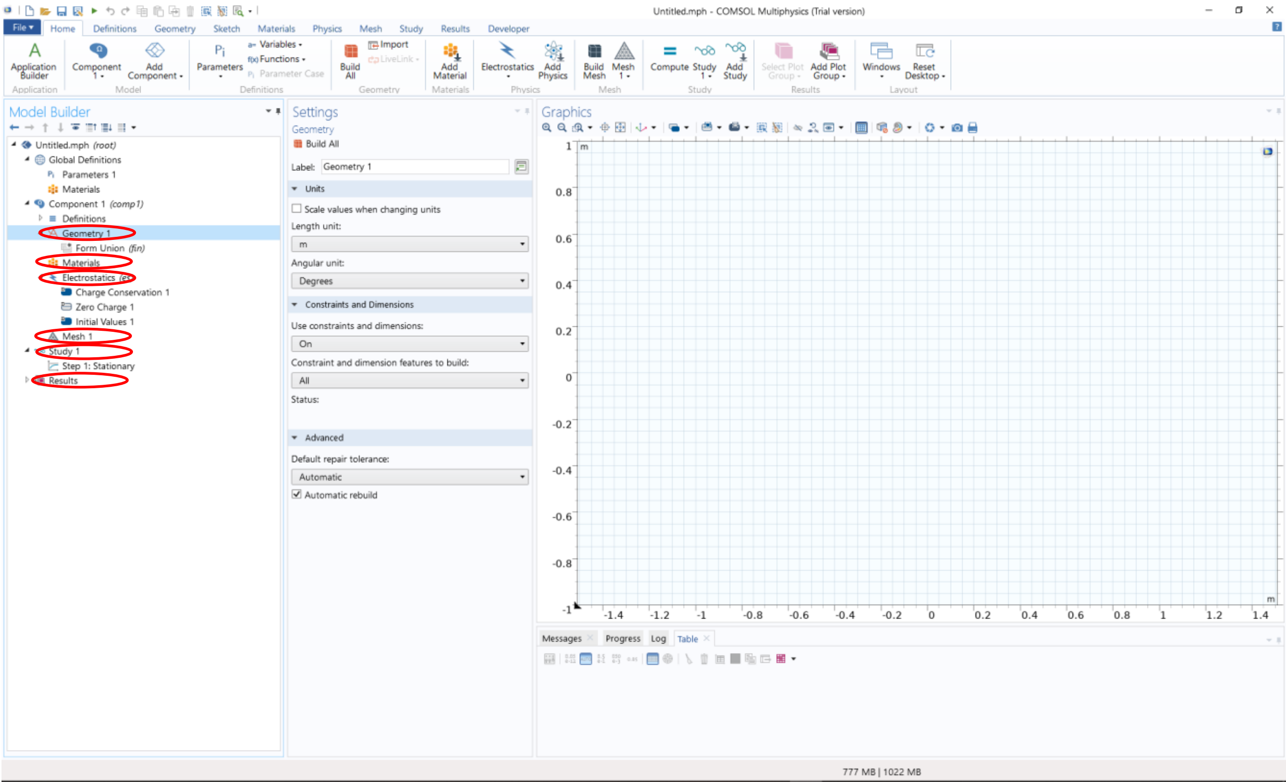




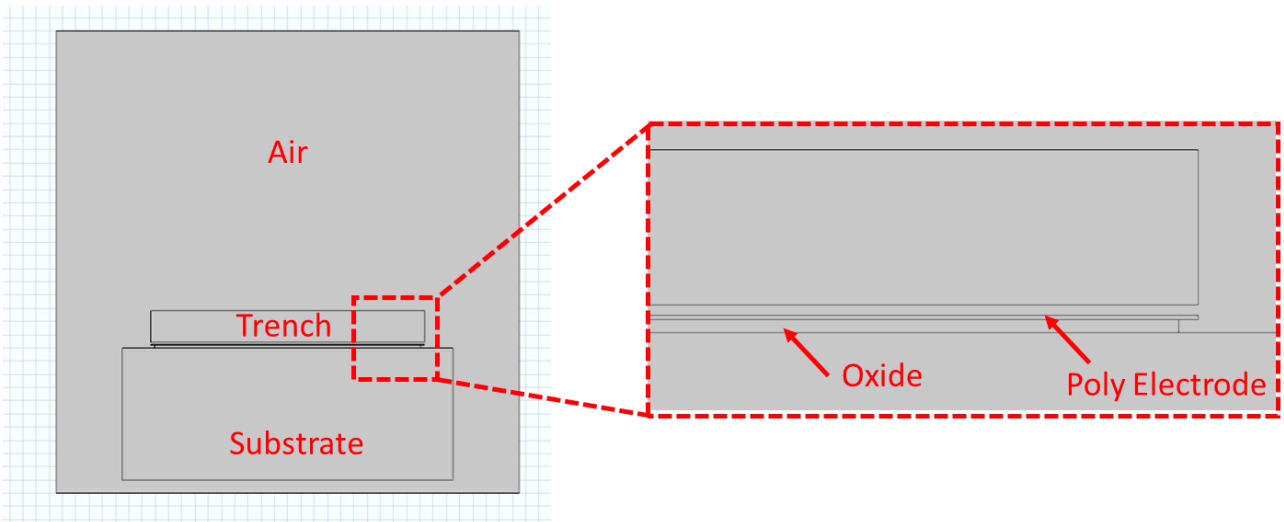
We want to evaluate an electrical capacitance: let us thus select the appropriate physical domain for this type of simulation. In Select Physics: 1) open the selection window “AC/DC” → 2) choose “Electric Fields and Currents” → “Electrostatics” → 3) click “Add”, the selected physic appears inside the box “Added physics interfaces” → 4) click “Study”

In “Select Study”, click on “Stationary” (we will study a quasi-stationary problem) → click on “Done”

The main COMSOL interface is now open. Highlighted in red you see the main simulation steps: geometry and materials design, definition of equations and boundary conditions, mesh, solution and results.



We can model the geometry of our problem as represented in the figure below. **Trench** is another way to call the epitaxial structural layer that forms the moving part of a MEMS sensor. Note the relatively large air volume left on top of the sensor: this is needed to correctly model the field streamlines, as we will see.



Let us now understand how to create such a geometry in COMSOL.

A clever choice is to define a set of **parameters**: indeed, designing parametrized geometries allows you to quickly change your settings if you want then to simulate a different geometry.

In the "Model Builder" window, under "Global Definition" you find the sub-window "Parameters". We add all the dimensions of our geometry (the column "Description" is facultative).

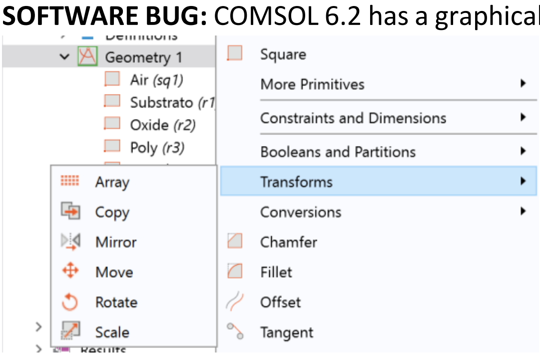
Parameters

Parameters

Name	Expression	Value	Description
Lair	350e-6 [m]	3.5000E-4 m	
Wsub	250e-6 [m]	2.5000E-4 m	
Hsub	100e-6 [m]	1.0000E-4 m	
space	10e-6 [m]	1.0000E-5 m	
gap	1.6e-6 [m]	1.6000E-6 m	
Htrench	24e-6 [m]	2.4000E-5 m	
Wtrench	207e-6 [m]	2.0700E-4 m	
Wpoly	Wtrench	2.0700E-4 m	
Hpoly	700e-9 [m]	7.0000E-7 m	
Wox	Wpoly-6e-6[m]	2.0100E-4 m	
Hox	2e-6 [m]	2.0000E-6 m	

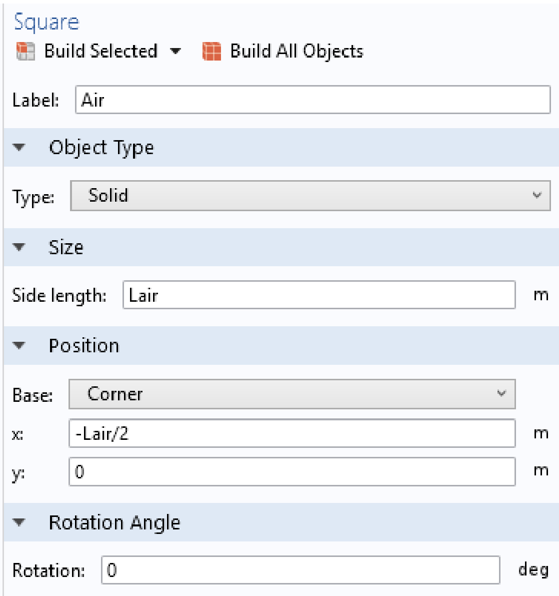
Now we start the design, using consecutive insertion of geometrical items which will form the structure.

SOFTWARE BUG: COMSOL 6.2 has a graphical bug in 2D geometry for which only the perimeter of the design parts is visible. To correct it, I suggest to right click on "Geometry" and in pop-up window select one of the transformation functions shown in figure.

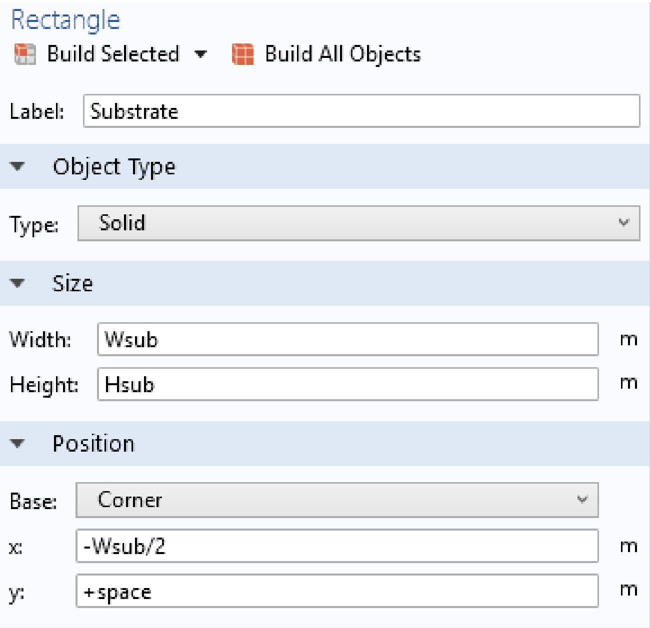


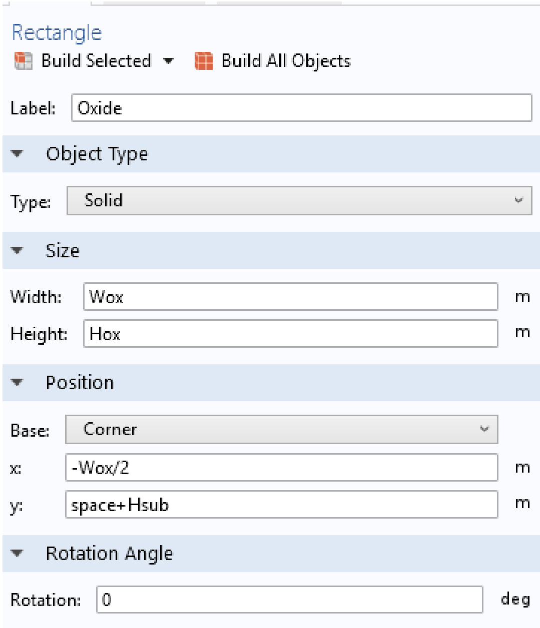
Then, you can remove this part because it is not necessary for this CAD laboratory (maybe).

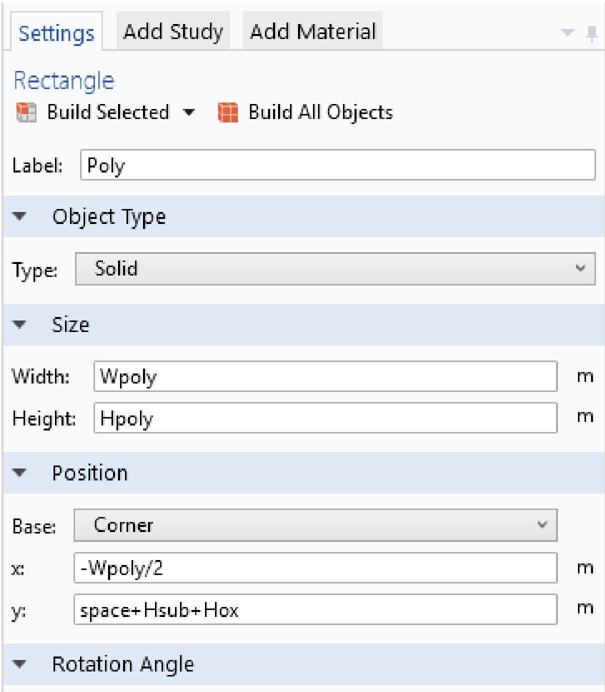
In "Model Builder" window, press *right click* on "Geometry" → in the pop-up window select "Square". We can write on the label "Air" in order to remember what this geometrical element represents, and we can set the parameters as in the figure (we have to insert the side length and the position of the bottom left corner of the square).

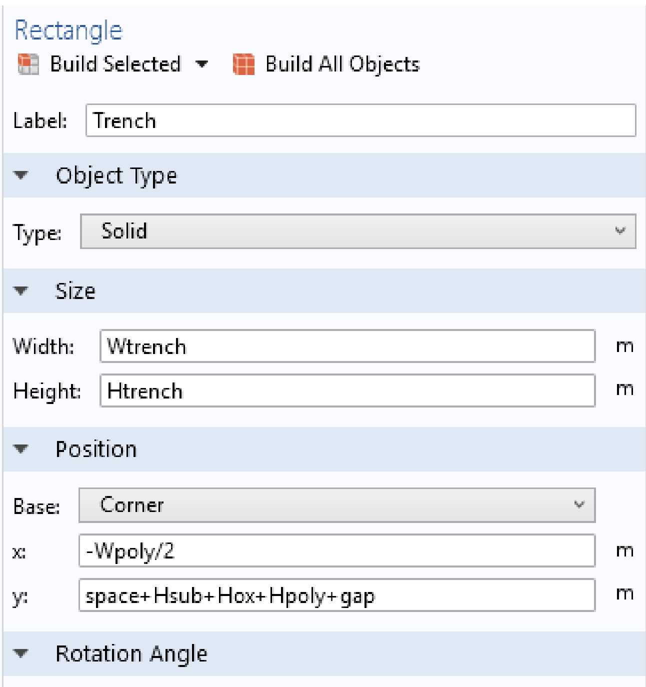


In “Model Builder” window, press *right click* on “Geometry” → in the pop-up window select “Rectangle”. This is our “Substrate” (top left figure). In the same way, we define the following layers: oxide, poly and trench. It should be noted that poly and trench are separated by an air gap of 1.6μm.





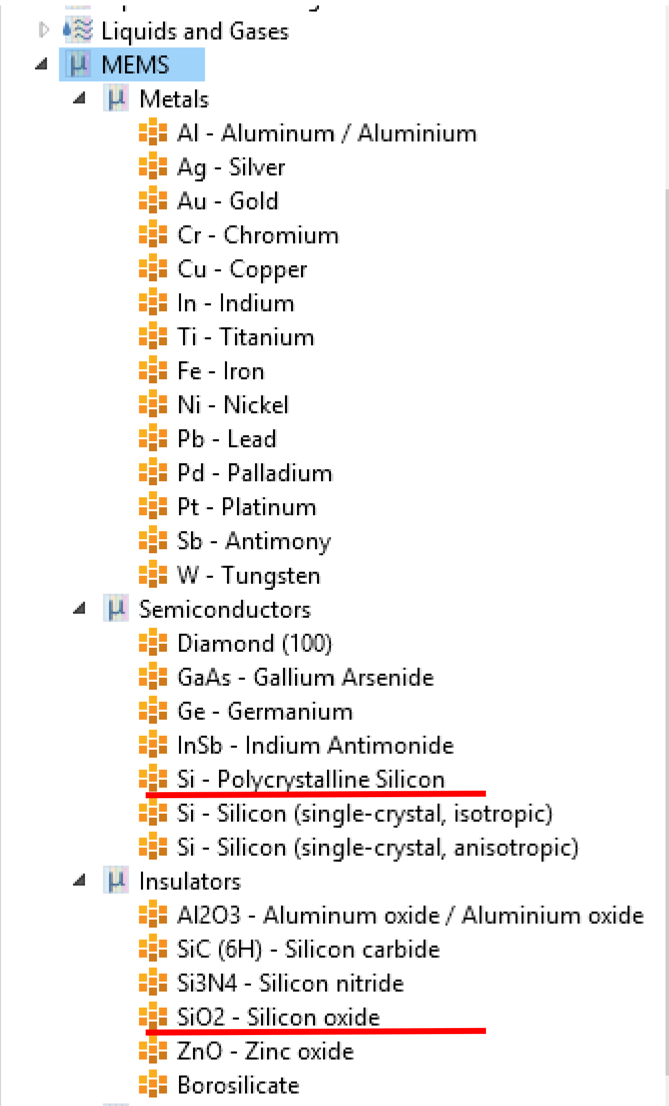


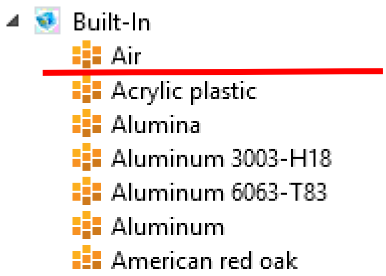


Our geometry is complete. Left click on “Geometry”, click on “Build All” and verify that the visualized geometry is the desired one.

2. Material Definition

Several physical parameters depend upon the specific material (permittivity, Young's modulus, ecc…), and thus we have to choose them accordingly. Right click on "Materials", click on "Add Material from Library". In the MEMS group, within Semiconductors find Si- Polycristalline Silicon and within Insulators find SiO2 – Silicon oxide. Select each of the two materials and click on Add to Component. Do the same thing with the Air in the Built-in group.

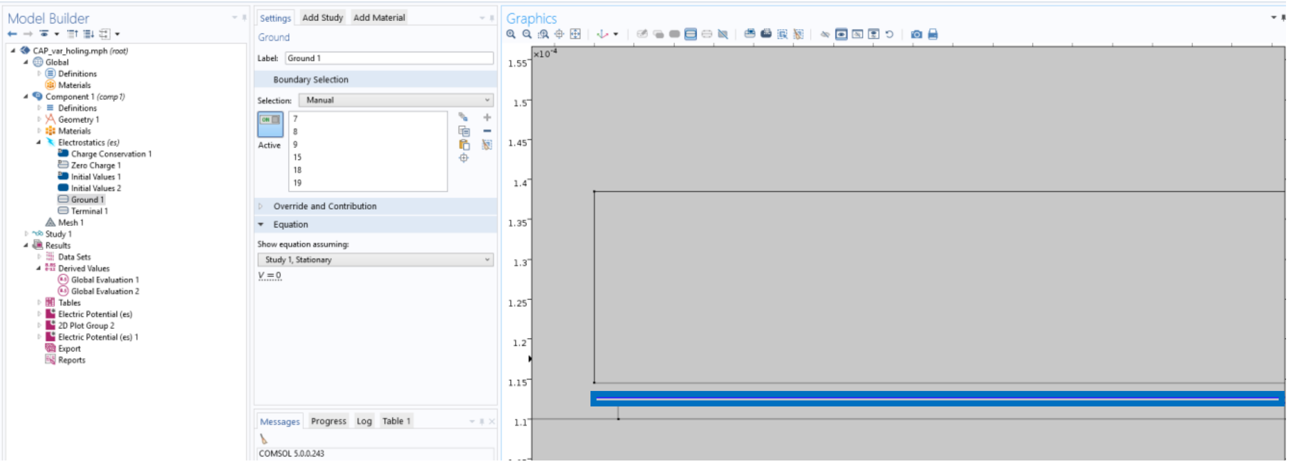


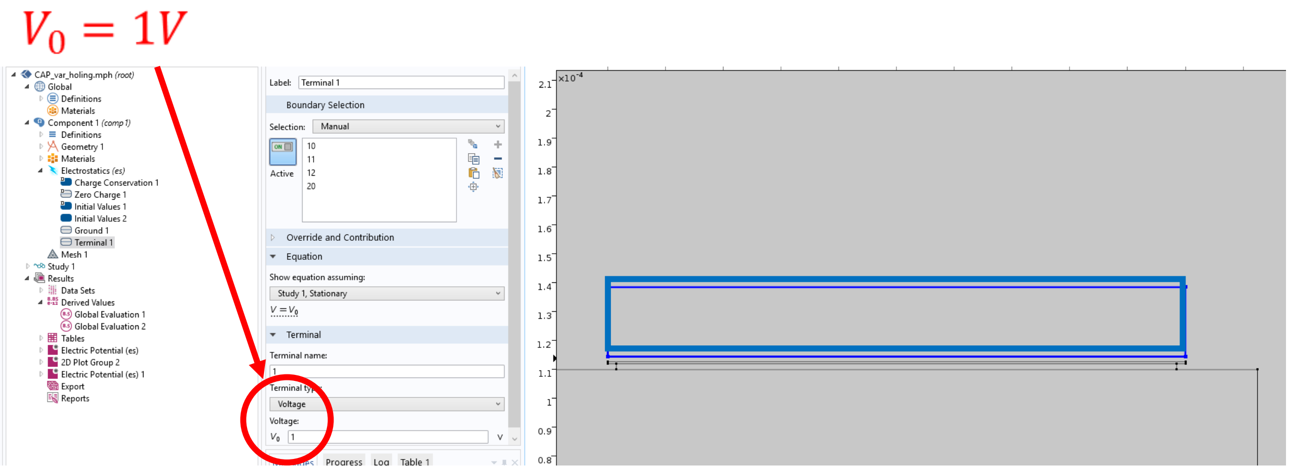


Expand "Materials" and, for each added material, left-click on it and select on the geometry the correct domain (the "Air" external square, the "Polycrystalline" Trench, Poly Electrode and Substrate and the "SiO2" oxide layer). When a domain is selected, it becomes blue. You can clean your selection clicking again on each selected domain or clicking on the little broom on the right.

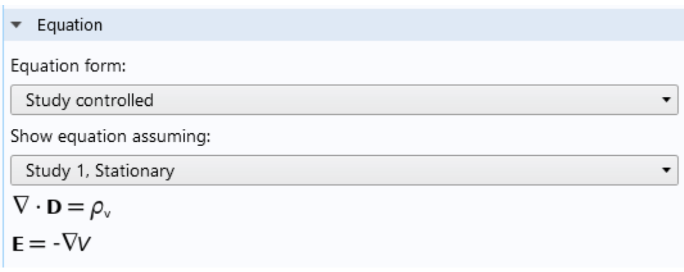
3. Boundary Settings

As discussed, every problem based on a PDE set needs its boundary conditions. Right click on "Electrostatics" and click on "Ground" and "Terminal" conditions. Assign these boundary conditions, respectively, to the poly electrode and to the trench (as depicted in figure). **Pay attention** to set the "Terminal Type" as "Voltage". Later, we are going to evaluate the capacitance between ''Terminal'' and ''Ground''. Do not modify the other default boundary conditions.





Note: if you expand the “Equation” section in the “Electrostatic” window, you are shown the equations that later the solver will compute, point by point and iteratively in your geometry. In this case we find the Gauss theorem equation (the divergence of the electric displacement field equals the free electric charge density) and the relationship between potential and electric field.



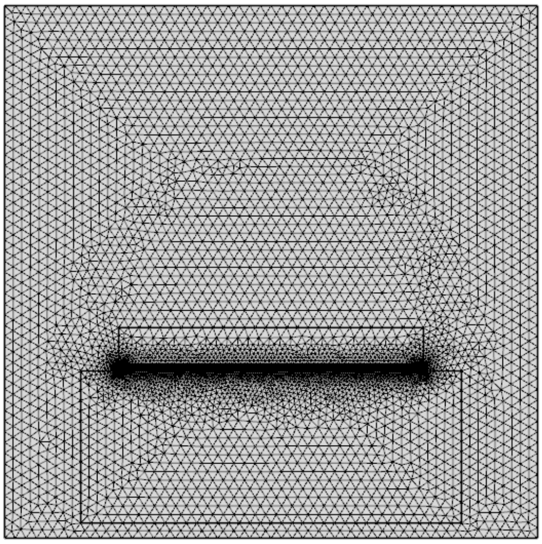
Note: at the end of the class you can try to put the substrate to a third terminal and set it to 0V. Check whether the capacitance between rotor and stators changes.

4. Mesh

Now, we have to define the points where the software calculates the solutions of the electrostatic problem.

There are a lot of different possibility to create a “Mesh”. The easiest one is the “Free triangular”: right click on “Mesh” → click on “Free Triangular”. Click on “Build All”.

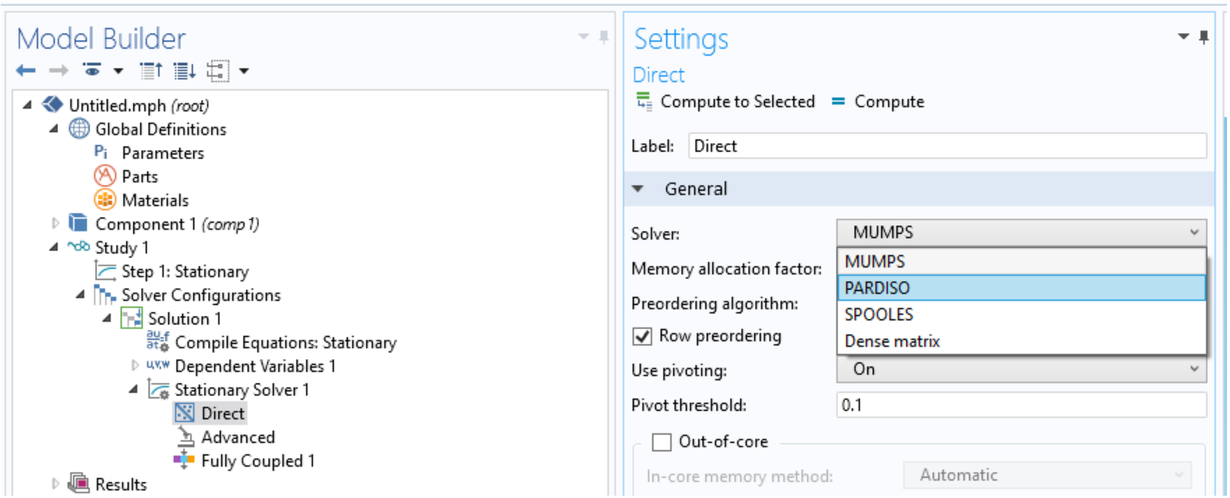
You will obtain a grid similar to the one represented in figure. (N.B. You can set the grid size right clicking on “Free Triangular” and clicking on “Size”, but the default mesh size is sufficient for this exercise).



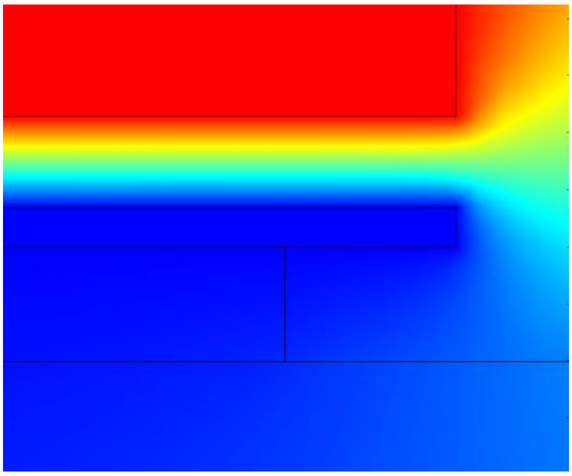
Different grid types are more or less suitable for different types of problems… this point will not be deepened however within this CAD classes.

5. Study and results

To begin your solution, you have to choose a solver, i.e. a mathematical iterative procedure that solves your problem on the mesh points. Right click on "Study" → click on "Show Default Solver" → expand "Solution 1" → expand "Stationary Solver 1" → click on "Direct" → in "Setting" window → change the "Solver" into PARDISO. This solver uses the symmetry of the problem to decrease the computational time. Click on "Compute".

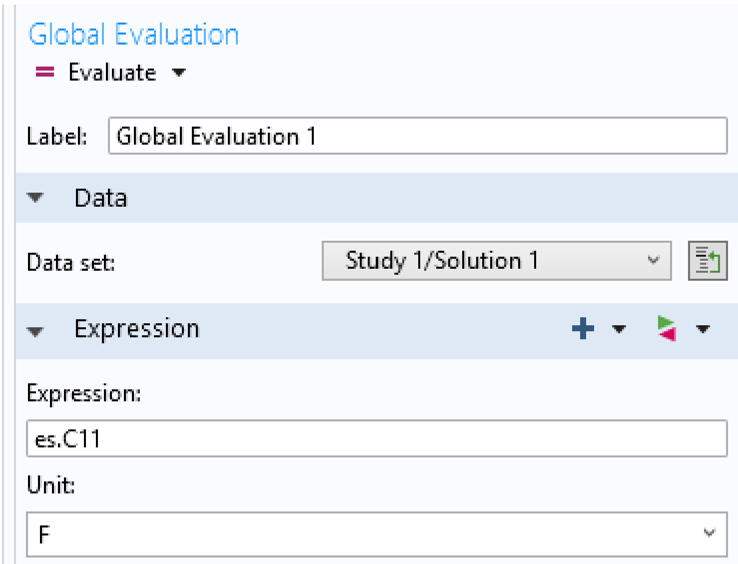


Comsol starts with the simulation and then the result appears in the "Graphic window". By default, the plot of the Electrostatic Potential is shown. As we expect, within the gap between two parallel plates, this changes linearly – though some fringe effects are visible at the edges.



We are however interested in the capacitance value, so we can right-click on "Derived Value" → "Global Evaluation" → write in the expression field: "es.C11" (stays for electrostatic Capacitance). This is a shortcut: otherwise, you can click on the red/ green arrows and choose the physical quantity to evaluate.

NOTE: COMSOL evaluates the capacitance through the Maxwell capacitance matrix calculation. Hence, the software simulates for each capacitance C_{ij} the charges on the terminal $'i'$ when a voltage is applied on the terminal $'j'$. We are interested on the capacitance value on the bottom plate, the one at ground.



Click on "Evaluate". Are the shown results coherent with theoretical predictions? (**N.B., we are in a 2D geometry, the resulting capacitance is per unit of depth.**) So, the theoretical formula is:

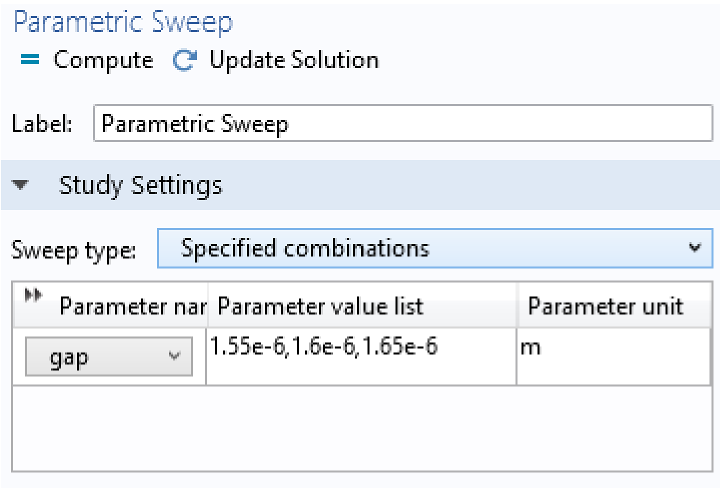
$$C'_0 = \frac{\epsilon_0 W_{trench}}{g} = 1.14\ nF/m$$

The simulated value is found to be 1.17 nF/m, quite close to the predicted one.

NOTE: if you want to simulate a capacitance assuming a certain depth in the third direction, you can specify it in the “Electrostatic” window. E.g. if you put a realistic value of 200 µm, and solve your problem again, you will find a realistic value of 235.7 fF (the theoretical calculation yields 229 fF).

Now, we want to derivate the value of the dC/dz, the capacitance variation per unit of out-of-plane displacement. A simple way to do this is to repeat our stationary simulation for different values of the gap. For simplicity, we can do a parametric simulation with three values of the gap.

Right click on “Study” → select “Parametric Sweep” → Right click on the parameter table and select “Add” → select our “gap” parameter and fill the Parameter value list as follows (note that 50 nm is a small displacement for the gap we are simulating):



Click on compute and repeat the Global evaluation as in the previous Study, selecting this time ‘’Study 1, parameteric sweep’’ as Data Set. Now you will obtain different capacitance values for every value of the gap. We can approximate the dC/dz as follows:

$$\frac{\Delta C}{\Delta z} \approx \frac{\mathrm{C}_{\mathrm{gap\ min}} - C_{gap\ max}}{g_{max} - g_{min}} = \frac{243.2\ fF - 228.8 fF}{0.1\ \mu m} = 144 \frac{fF}{\mu m}$$

Is this value consistent with the theoretical prediction? **Note that a factor 2 is missing with respect to the formula seen in lectures, because this is not a differential configuration but a single-ended one.**

$$\frac{\mathrm{d}C}{\mathrm{dz}} = \frac{C_0}{g} = \frac{235\ fF}{1.6\ \mu m} = 146 \frac{fF}{\mu m}$$

The results are quite coherent with theoretical predictions. Small deviations can be ascribed to fringe effects. We can conclude that our simulation works properly, and thus pass to simulate the more complicated geometry.

By clicking on “Table Graph” in the Table tab you can visualize the graph of the capacitance vs gap.

Note: you can do yourselves additional tests, e.g. by investigating nonlinearities at large displacements, or the influence of grounding the substrate instead of leaving it floating.

6. Perforated Structure

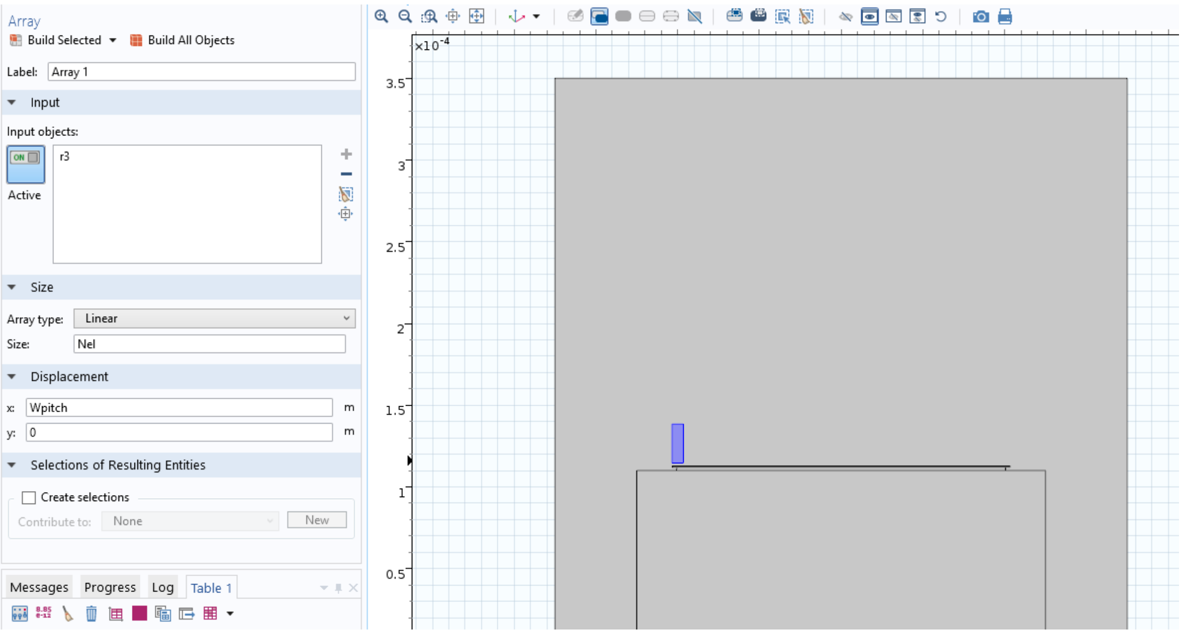
We can now repeat the same study for a perforated trench. Let us add some parameters to our list:

Name	Expression	Value	Description
Lair	350e-6 [m]	3.5000E-4 m	
Wsub	250e-6 [m]	2.5000E-4 m	
Hsub	100e-6 [m]	1.0000E-4 m	
space	10e-6 [m]	1.0000E-5 m	
gap	1.8e-6 [m]	1.8000E-6 m	
Htrench	24e-6 [m]	2.4000E-5 m	
Wtrench	207e-6 [m]	2.0700E-4 m	
Wpoly	Wtrench	2.0700E-4 m	
Hpoly	700e-9 [m]	7.0000E-7 m	
Wox	Wpoly-6e-6[m]	2.0100E-4 m	
Hox	2e-6 [m]	2.0000E-6 m	
Wpitch	10e-6[m]	1.0000E-5 m	
Wfull	7e-6 [m]	7.0000E-6 m	
Nel	21	21	

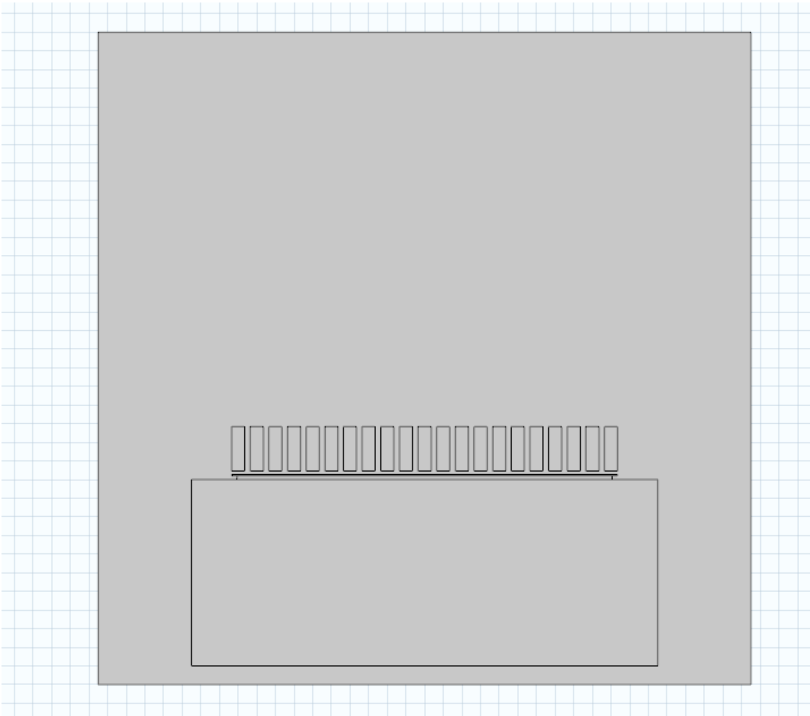
Wfull is the dimension of the full portion of the rotor, while Wpitch is the void+full length (repeated Nel times over the electrode).

Expand “Geometry” → click on “Trench” and set as width “Wfull”

Right click on “Geometry” → click on “Transforms” → click on “Array”. Select the piece of trench as the input object and fill the settings as follows:



You will obtain the following geometry:



That represent a slice of our tilting holed mass. Now you can repeat the same parametric study of the "full mass" case. What about the value of C_0? What about $\frac{\Delta C}{\Delta z}$?

$$\frac{\Delta \mathrm{C}}{\Delta z} = \frac{\mathrm{C}_{\mathrm{gap\ min}} - C_{gap\ max}}{g_{max} - g_{min}} = \frac{226.1\ fF - 213.6 fF}{0.1\ \mu m} = 126 \frac{fF}{\mu m}$$

This behavior cannot be predicted with scratch-paper calculations. Indeed, if you simply take the area ratio between the perforated and full plate, you obtain a factor 0.71. Instead, from simulations we obtain a ratio between the two values of capacitance variation:

$$\alpha_{cap,7-3} = \frac{126}{146} = 0.87$$

The penalty given by the presence of the holes is thus much less than expected! It is also important to note that this value changes with a different full/void ratio in the mass. Try yourselves to solve again the problem with different hole sizes and pitches! For example, with holes of $5\mu m$ and full parts of $5\mu m$ we have, despite an area ratio of roughly 0.5, a capacitive variation coefficient:

$$\alpha_{cap,5-5} = 0.68$$

In conclusions, in order to evaluate our capacitance variation for a perforated structure like a differential z-axis MEMS torsional accelerometer, we use the formula:

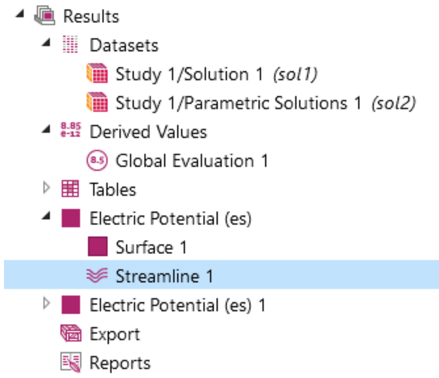
$$\frac{\mathrm{d}C}{\mathrm{d}z} = 2 \cdot \alpha_{cap} \frac{C_0}{g}$$

Where the factor 2 take into accounts the differential readout, and the α_{cap} coefficient is obtained through FEM simulations as we have just done.

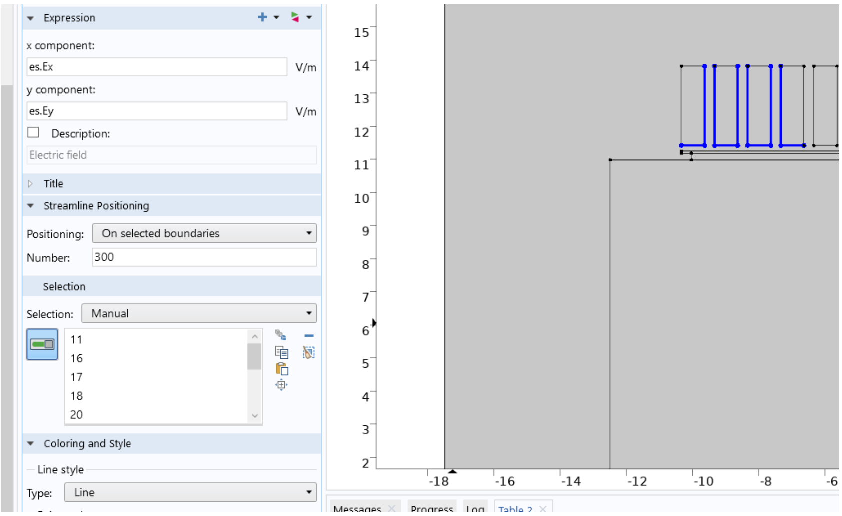
This formula will be readily used in your next numerical exercise!

7. For your curiosity…

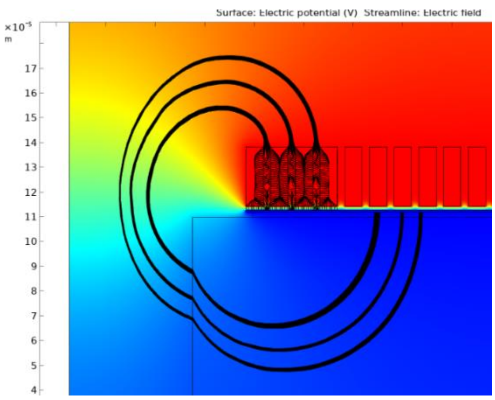
If you want to understand the reason why the actual capacitance and capacitance change are larger (0.87) than for theoretical predictions (0.71), you can have a look at the electric field streamlines. To do this, right click on Electric Potential in the Results tab, and the click on Streamlines.

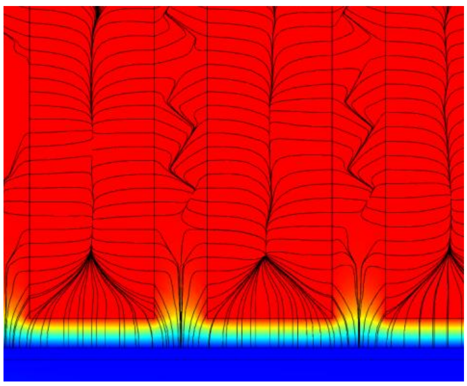


Fill the Streamlines tab as below: in this way we plot only the 2D electric field streamlines starting from the selected boundaries (otherwise the plot becomes hard to understand).



After you plot the result, you will find something like the graph below. We let you note that: (i) the streamlines which begin under the “holed” portion of the trench, close anyway onto the trench, implying that effectively they take part in forming the capacitance; (ii) some streamlines directly connect the trench to the substrate, giving an indication of a parasitic capacitance between these two terminals!





8. Try by yourself now…

Start a new Comsol file from scratch. Consider now a different situation, with an in-plane **comb-finger** capacitor: in classes, we never considered the **parallel plates capacitance** formed by the comb tip and the fixed electrode (depicted in figure and named C_{pp}). How does this unwanted effect modify the dC/dx of the considered geometry with respect to the ideal case? N.B. Calculations on paper are not so straightforward due to fringing field issues… you have to simulate!