Electric Currents, Dielectrophoresis and Impedance Computations

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Introduction

This example illustrates modeling using the Electric Currents application mode of the COMSOL Multiphysics Electomagnetics Module and its applications for dielectrophoresis (DEP), impedance sensors within BioMEMS, as well as general capacitance-resistance computations where inductive effects can be neglected. The model was inspired by the COMSOL based papers of Ref. 1 and Ref. 2 below.

Model Definition

The modeling domain consists of a cube of side 30 μm. The cube is filled with a buffer (see Ref. 1) with σ=0.56 S/m and ε_r=78. The five upper boundaries of the cube represents an artificial truncation of the buffer volume. The lower boundary of the cube is partitioned into five segments representing four gold electrodes and a non-conducting boundary. Two of the electrodes are grounded and the other two have a peak potential of 10 V at 1 MHz. The electrodes are modeled as perfect conductors and are considered to be equipotential surfaces with no finite thickness. The advantage of modeling the electrodes as infinitely thin is that much fewer elements are needed to accurately capture the most important aspects. Fewer elements means lower memory requirements and faster computation times.
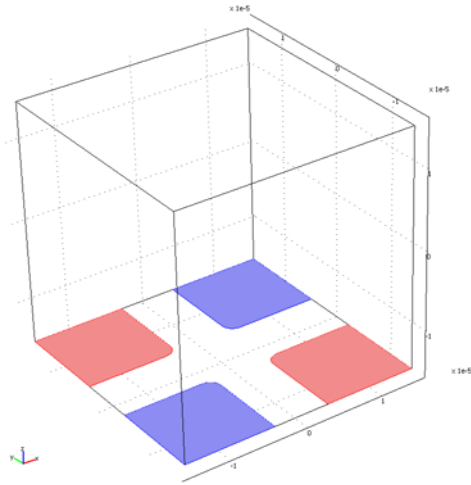
The modeled domain. The red electrodes are set to 10 V (AC) and the blue electrodes are set to ground (0 V).

This example uses the Electric Currents application mode and the unknown field quantity is the voltage *V=V(x,y,z)*, a complex-valued quantity. The Electric Currents application mode is used to model devices with alternating currents (AC) where magnetic-inductive effects can be neglected and only resistive-conductive and electric-capacitive effects are accounted for. Generally speaking, this approximation gets better the lower the frequency and the smaller the device. When this approximation cannot be applied, you instead need to use the Electric and Induction Currents application mode.

For more information on the various approximations used, see the below section on *Model Approximation*s.

The geometry is meshed using the automatic tet-mesher and the default "nodal-based" second order elements are used.
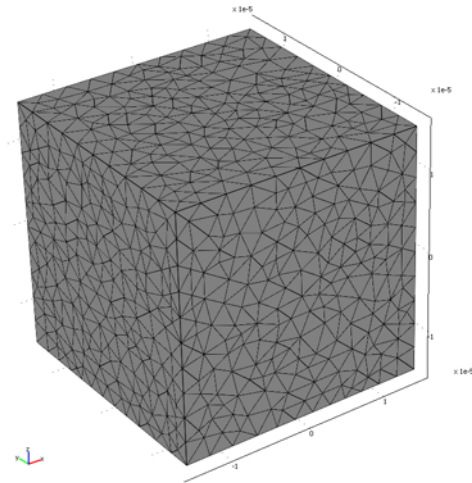
The finite element mesh. Second order tetrahedral elements are used for discretizing the complex valued electric potential V.

Please note that this simulation can be made with just 1/4 of the geometry due to symmetry.

## Modeling Using the Graphical User Interface

MODEL NAVIGATOR

1 Start **COMSOL Multiphysics**.

2 In the **Model Navigator**, select **3D** in the **Space Dimension** list and then **Electromagnetics Module>Quasi-statics, Electric>Electric Currents>Time-harmonic analysis** in the list of application modes.

3 Click **OK**.

GEOMETRY MODELING

Firstly, create the box containing the buffer (a truncated portion of the real-world volume).

**1** From the **Draw** menu, select **Work Plane Settings**.

2 Click **OK** to create a default work plane located at *z=0*.

3 Shift-Click the second **Rectangle/Square** button. A **Square** dialog box opens.

4 Type 30e-6 in the **Width** text field.

5 Change the **Base** to **Center**.

6 Click **OK** to create the square.

7 Click the **Zoom Extents** button to adjust the axis settings down to the micron scale.

8 From the **Draw** menu, select **Extrude**.

9 For **Distance**, type 30e-6. The dimensions are SI by default - so the distance entered is 30 micrometers. If needed, this can be changed form the **Physics** menu>**Model Settings**.

10 Click **OK**.
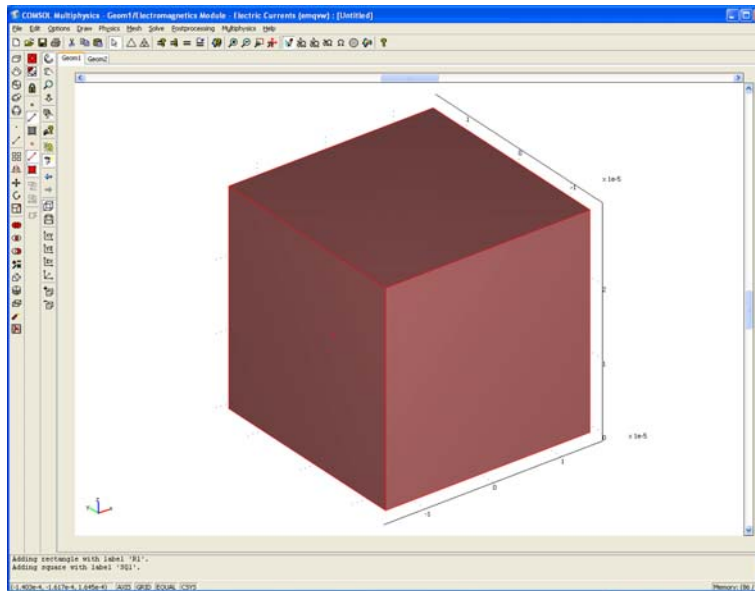
Secondly, create the four electrodes.

1 Click the **Geom2** tab to get back into the work plane.

2 Create a rectangle covering the upper left quarter of the already drawn square.

3 Double-click the rectangle, a **Rectangle** dialog box opens.

4 Adjust the settings to **Width:** 1.15E-5, **Height:** 1.15E-5, **Base: Corner**, **x:** -1.5E-5, **y:** 3.5E-6.

5 Continue in the same way to create rectangles covering the other three corners of the square.
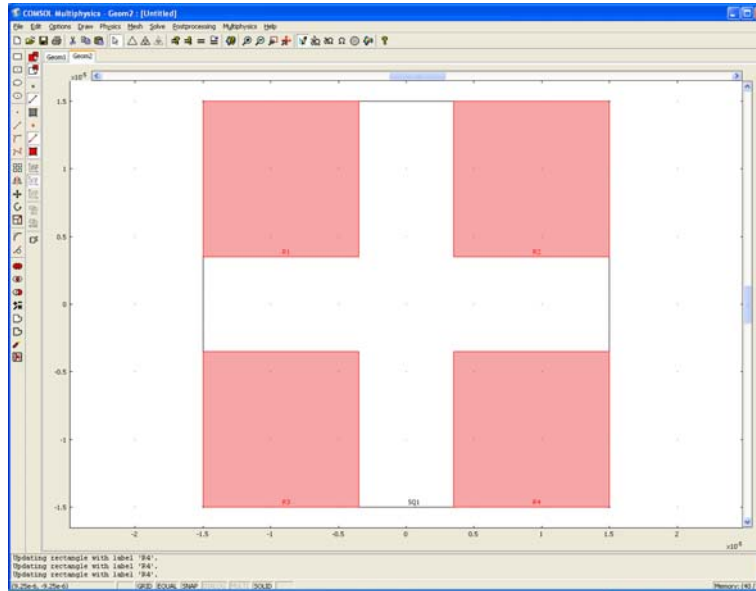
6 Click the **Chamfer/Fillet** toolbar button to open the corresponding dialog box.

7 Click the inner corners of the four smaller squares (use Ctrl-Click for multiple selection).
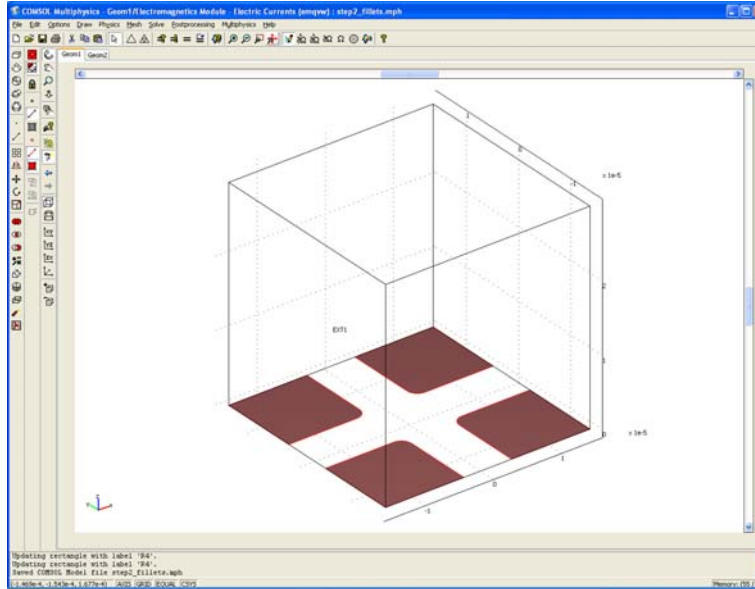
8 Use a fillet-radius of 0.15e-5.

9 Click **OK** to create the fillets.
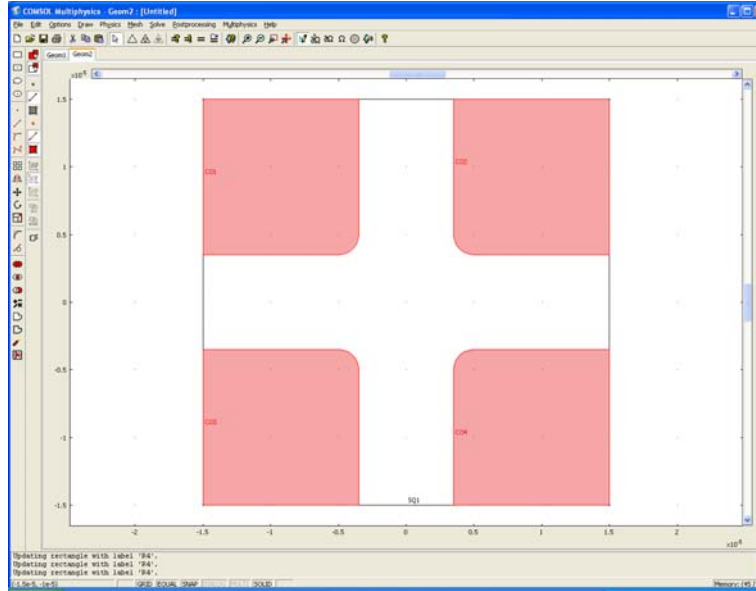
10 From the **Draw** menu, select **Embed.**

11 Select all four filleted-squares (do not select the larger square!).

I2 Click **OK** to embed the objects in 3D.

PHYSICS SETTINGS

Subdomain Settings
The following steps will set the material properties for the buffer.

1 From the **Physics** menu, open **Subdomain Settings**.

2 For the **Electric conductivity**, type 0.56.

3 For the **Relative permittivity,** type 78.

4 Click **OK**.

Boundary Conditions

1 From the **Physics** menu, open **Boundary Settings**.

2 Press **Ctrl+A** to select all boundaries and change the **Boundary condition** to **Electric insulation**.

3 Select boundaries **3** and **9** (two of the gold electrodes) and change the **Boundary condition** to **Ground**.

4 Select boundaries **6** and **8** (the other two of the gold electrodes) and change the **Boundary condition** to **Electric potential** and type 10 for the **Electric potential**. This will define a time-varying potential *V(t)=10cos(2πft)* for these two electrodes.

5 Click **OK**.

Scalar Variables (Setting the Frequency)

For the first part of the simulation, the frequency will be fixed.

1 From the **Physics** menu, select **Scalar Variables**.

2 Change the **Frequency** to 1MHz by typing 1e6 in the corresponding text field.

3 Click **OK**.

MESH GENERATION

For this model, the default mesh will do.

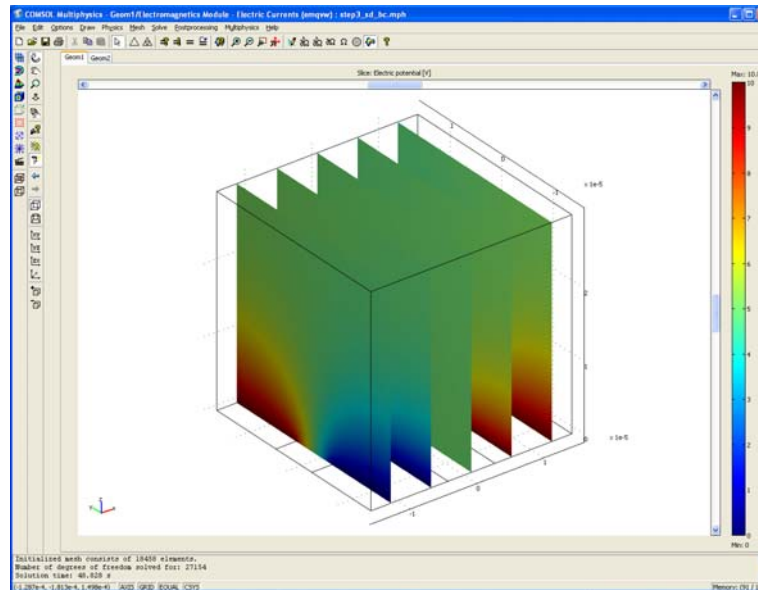**1** Click the **Initialize Mesh** button.

COMPUTING THE SOLUTION

For this model, the default solver settings will do.

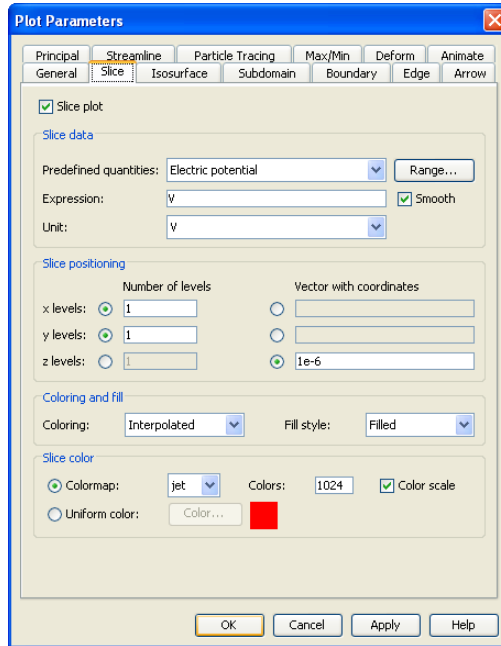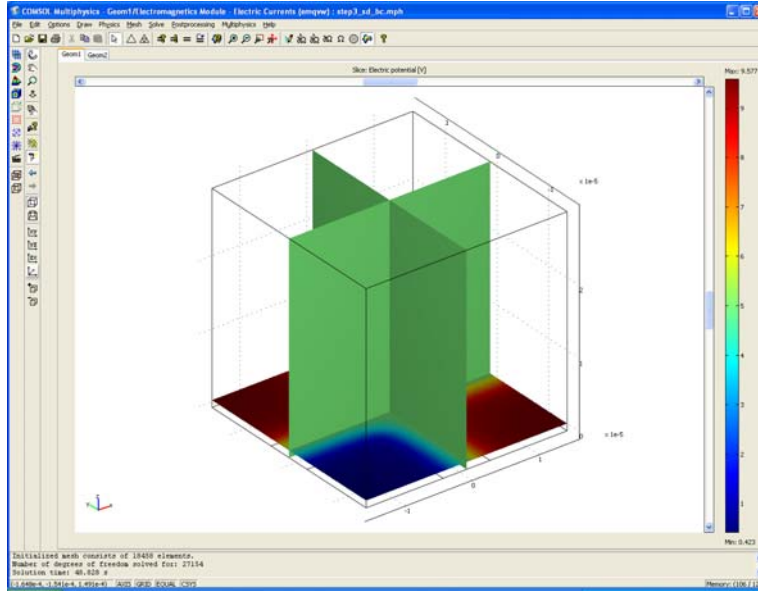**1** Click the **Solve** button.

VISUALIZATION

The default plot shows a slice plot of the electric potential:

1 From the **Postprocessing** menu, open the **Plot Parameters** dialog box.

2 On the **Slice** page, change the **Number of levels** to be 1 in the x-direction, 1 in the y-direction, and **Vector of coordinates** set to 1e-6 for the z-direction:

DEP Force Field Visualization

This section covers DEP force field visualization. If you are interested in frequency dependent impedance (resistance+capacitance) computations, please skip to the next section *Impedance Computation*.

A quantity that is of interest for dielectrophoresis (DEP) simulations is the magnitude of the square of the gradient of the electric field:

$$F_{DEP} = k\sqrt{\nabla(\mathbf{E} \cdot \mathbf{E}^*) \cdot \nabla(\mathbf{E} \cdot \mathbf{E}^*)}$$

where the * denotes complex-conjugation and *k* is a coefficient that depends on the shape of the particle. This so called DEP-force acts on a small dielectric particle in a nonuniform field. For more information see Ref. 1 and Ref. 3, page 10-8.

The force vector on the particle is:

$$\mathbf{F}_{DEP} = k\nabla(\mathbf{E} \cdot \mathbf{E}^*)$$

The DEP force expression is not a built-in expression for the Electric Currents application mode, but can be formed as a composite expression of the already defined components of the electric field: `Ex_emqvw`, `Ey_emqvw`, and `Ez_emqvw` (or equivalently the already defined components of the gradient of the electric potential `Vx`, `Vy`, and `Vz`).

The expression is a bit lengthy, but a minimum of computations is needed if the built-in `diff()` operator is used. As an example of the use of the `diff`-operator, consider the expression `diff(V,x)` that means the partial derivative of the electric field *V* with respect to *x* (also available as the built-in `Vx`).

To make it easier, we can first use the fact that the quantity:

$$\sqrt{\mathbf{E} \cdot \mathbf{E^*}} = |\mathbf{E}|$$

is already a named variable `normE_emqvw` - the magnitude, or norm, of the electric field. We can then get the square of the electric field as `normE_emqvw^2`.

The gradient components can then be computed as: `diff(normE_emqvw^2,x)`, `diff(normE_emqvw^2,y)`, and `diff(normE_emqvw^2,z)`.

Finally, the DEP force can be computed as the expression:

```
k*sqrt(diff(normE_emqvw^2,x)^2+diff(normE_emqvw^2,y)^2+
  diff(normE_emqvw^2,z)^2)
```

Now, let's create a user-defined expression for this force:

1 From the **Options** menu, select **Expressions>Scalar Expressions**.

2 Create an **Expression** variable with the name `k` and expression equal to `1` (we do not pay attention to the particle shape at this stage).

3 Create an **Expression** variable with the name `FDEP` and expression as above.

4 Click **OK**.

To visualize the force-field, we first need to evaluate the expression:

1 From the **Solve** menu, select **Update Model**.

This will evaluate the expression for `FDEP` throughout the mesh and make it available for visualization and postprocessing.

To visualize:

1 From the **Postprocessing** menu, open the **Plot Parameter**s dialog box.

2 On the **Slice** page, change the **Expression** to `FDEP`.

3 Click **OK**.
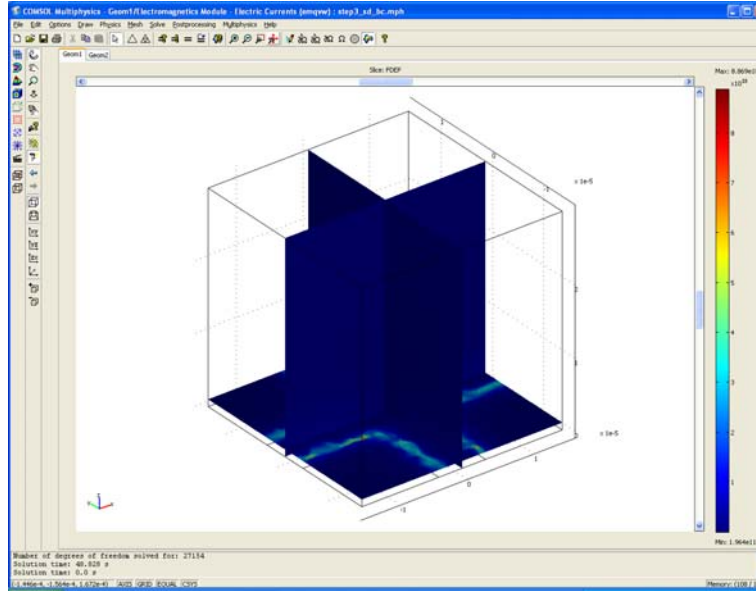
The accuracy of the FDEP computation is quite poor due to the fact that:

1 A very coarse mesh is used that doesn't resolve the fields close to the electrode edges well

2 Second order elements are used. This means that the solution is approximated within each element using second-order polynomials. The DEP force is computed as an expression in the electric field gradients and the electric field, in turn, is computed as the gradient to the electric field. This means that the DEP force is a quantity that is composed of the field variable V differentiated twice. As such, it is represented by a constant value within each element (the second order polynomials differentiated twice).

Remedy for this is to use a finer mesh and/or to increase the element order (from the **Subdomain Settings**, **Element** page). By increasing the element order to cubic elements, the DEP force will be approximated by linear functions within each element.

Let's try refining the mesh and not increasing the element order (to avoid a very memory consuming computation).

1 From the **Mesh** menu, select **Mesh** parameters.

2 On the Edge page, select edges 7,9,13,14,15,17,19, 21,22,23,25, and 26. These are the edges of the electrodes.

3 Change the **Maximum edge size** to 0.1e-6.

4 Click **Remesh**.

Click the **Solve** button to compute the solution for the new mesh.

The force is quickly attenuated as we move away from the electrode edges. To better visualize the force variations we can use a logarithmic plot (with base 10).

1 From the **Postprocessing** menu, open the **Plot Parameter**s dialog box.

2 On the **Slice** page, change the **Expression** to log10(FDEP).

3 To get a slice closer to the electrode, change the **Vector of coordinates** to 1e-7 for the z-direction.

4 Click OK to visualize.
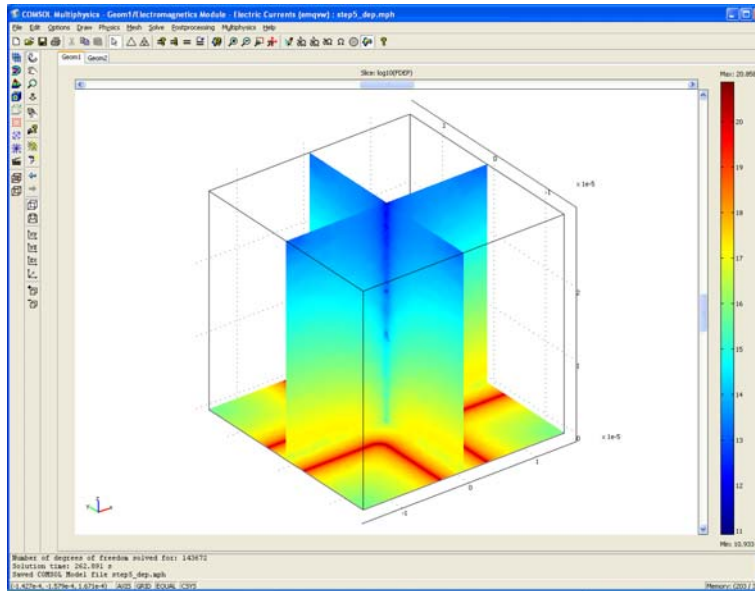
Due to the approximation with infinitely thin gold electrodes, the exact solution would have an infinite DEP force at the edges of the electrodes - the force is singular at the electrode edges. In the finite element simulation this is illustrated by the fact that the maximum value of the force at the edges grows without bound as the mesh

is refined. This is still a very useful simulation since at a small distance from the electrodes, the value of the DEP-force will be very accurate.

The only way to avoid a singular force field would be to model the electrodes with rounded corners and not sharp edges. This is technically possible but would require a finer mesh (to resolve the rounded corners) and be more memory consuming.

Impedance Computation

In order to demonstrate how to perform impedance (or admittance) computations (complex valued) we will assume, for simplicity, that we have a one-port structure where three of the electrodes are grounded and one is an input port. More information on lumped parameter computations for single and multiport structures can be found in the *COMSOL Multiphysics 3.2 Electromagnetics Module User's Guide* pages 96-103, in the section called *Lumped Parameters*.

- From the **Physics** menu, select **Boundary Settings**.
- Set the **Boundary condition** of boundaries 3, 6, and 9 to **Ground**.
- Select boundary 8 and change the **Boundary condition** to **Port**. This enables the **Port** page.
- Click the **Port** page.
- Make sure the **Port number** is **1** and select the checkbox **Use port as input**.
- Change the **Input property** to **Forced voltage**.
- Click **OK** to close the dialog box.
- Click the **Solve Problem (=)** menu item or button to re-solve the problem.
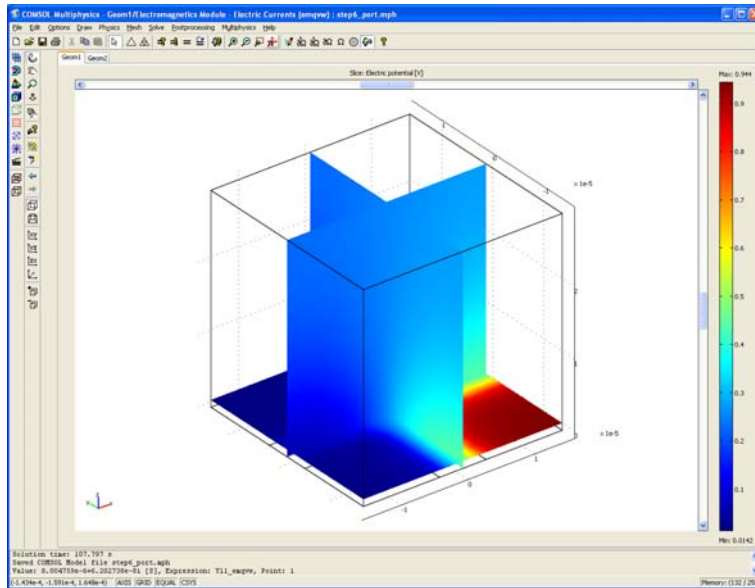
The visualization above shows the voltage distribution for the automatically computed load cases where the voltage of the input port is set to 1 V. If you have a multiport structure, a unit load will be applied in a cyclic manner as to create an impedance matrix **Z** or admittance matrix **Y**, depending on the type of load.

To see the value of the, in this case, complex valued admittance:

• From the **Postprocessing** menu, select **Point evaluation**.

• Click on an arbitrary point (the admittance variable(s) is(are) made available globally, say point **1**.

• Change the **Predefined quantities** to **Admittance matrix, element 11**.

• Click **Apply** to evaluate the value of the variable Y11_emqvw.

A value of about `8.0e-6+6.2e-8i` is printed at the bottom of the main GUI window, in the so called history log. This corresponds to $Y=G+Bi$, where G is the conductance and B is the susceptance. You get the impedance Z from the admittance as $Z=1/Y=R+Xi$, where R is the resistance and X the reactance. This model assumes that there is no inductive effect, only resistive and capacitive, so that $X=-1/(2\pi fC)$, where f is the frequency and C is the capacitance. The following relationships will give us the capacitance C starting from the admittance:

$$Y = G + Bi$$

$$Z = \frac{1}{Y} = \frac{G - Bi}{G^2 + B^2} = \frac{G}{G^2 + B^2} + \frac{(-B)}{G^2 + B^2}i = R + Xi$$

$$C = -\frac{1}{2\pi fX} = -\frac{1}{2\pi f\dfrac{(-B)}{G^2 + B^2}} = \frac{G^2 + B^2}{2\pi fB}$$

With values inserted we get that the capacitance equals
`((8.0e-6)^2+(6.2e-8)^2)/(2*pi*fq*6.2e-8)` and this can be calculated for
instance by using the **Constants** dialog box as a pocket calculator.
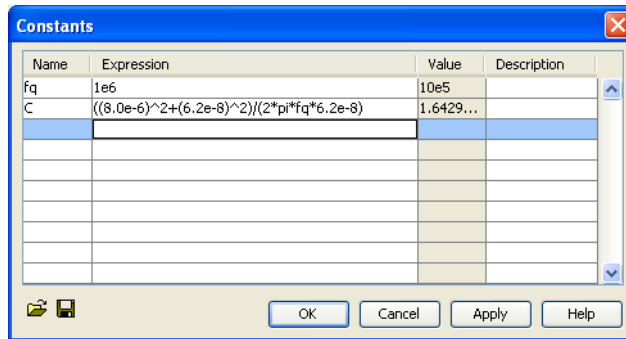
The computed value of the capacitance is approximately 160 pF.

One can also define a scalar expression for the capacitance and then sweep over a
range of frequencies to see the frequency dependent capacitance. We will use the
`real()` and `imag()` operators to extract the value of G and B automatically from
the computed lumped parameter variable `Y11_emqvw`:

• From the **Options** menu, select **Expressions>Scalar Expressions**.

- Type in names and expressions according to the below picture:
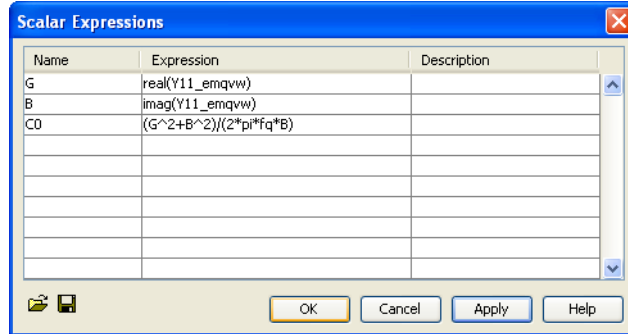
We will sweep for the parameter `fq`, frequency. In this case the fact that we have already defined it as a constant is OK due to the fact that the parametric sweep variable will have precedence in the computation over any constant or expression. We renamed the capacitance `C0` for not conflicting with the constant `C` calculated earlier.

- Click **OK** to close the dialog box.
- From the **Physics** menu, select **Scalar Variables**.
- Replace the value `1e6` for the frequency with the variable `fq`.
- Click **OK** to close the dialog box.
- From the **Solve** menu, select **Solver Parameters**.
- Set the **Solver** to **Parametric linear**.
- In the **Parameter** pane, type `fq` for the **Name of parameter** and `linspace(1e6,5e6,10)` for the **List of parameter values**. The `linspace` command creates 10 frequency cases linearly distributed between `1e6` and `5e6`.
- Click **OK** to close the dialog box.
- Click the **Solve Problem** (**=**) menu item or button.

  To plot the frequency dependent capacitance:

- From the **Postprocessing** menu, select **Domain Plot Parameters**.
- On the **General** page, make sure all parameters are highlighted (blue color).
- Click the **Point** tab.
- Highlight point number 1 (arbitrary).
- For the **Expression**, type C0.
- For the **x-axis data**, click the **Expression** button.

- For the **Expression** type fq (for frequency).
- Click OK in the opened dialog boxes to get the following plot:
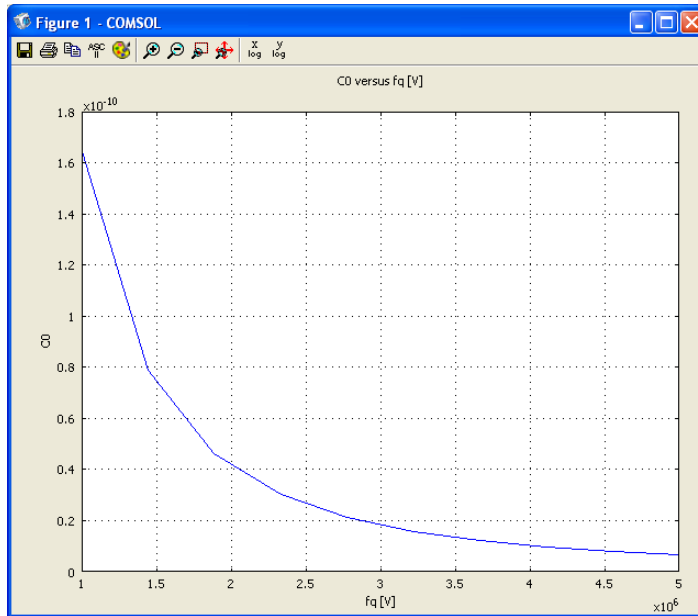
The capacitance decreases with increased frequency. This is typical for a capacitive device; it will have the characteristics of a high-pass filter.

Model Approximations

ELECTRODE APPROXIMATION

The perfect conductor approximation of the electrodes is justified by the fact that the real electrodes have a thickness of about $0.1 \mu m$ and is made of gold and that no significant field dilatation will occur across the surfaces of the electrodes; all points at the gold surface will essentially have the same phase angle. In addition, the approximation with zero thickness means that edge effects from the vertical sides of the electrodes are neglected.

The perfect conductor approximation is also motivated by the contrast in conductivity between the buffer, 0.56 S/m, and the gold electrodes, $45.2 \cdot 10^6$ S/m that would be prohibitively large to resolve within the machine precision. For a finite element simulation $45.2 \cdot 10^6$ S/m is a virtually unlimited conductivity in

comparison with 0.56 S/m. Explicitly simulating such a large material property contrast might render an ill-conditioned finite element model and deteriorate accuracy since it would correspond to linear algebra system matrix entries with scale differences on the order of 10^8 ($45.2 \cdot 10^6 / 0.56$).

THE ELECTRIC CURRENTS APPROXIMATION

The Electric Currents application mode is used to model devices with alternating currents (AC) where magnetic-inductive effects can be neglected and only resistive-conductive and electric-capacitive effects are accounted for. Generally speaking, this approximation gets better the lower the frequency and the smaller the device. When this approximation cannot be applied, you instead need to use the Electric and Induction Currents application mode.

SKIN DEPTH

The characteristic length scale that determines the accuracy of the electric currents approximation is called the current skin depth δ:

$$\delta = \sqrt{\frac{2}{2\pi f \sigma \mu_0 \mu_r}}$$

where f is the frequency (Hz), s is the electric conductivity, μ_0 is the magnetic permeability of vacuum, and μ_r is the relative permeability. A higher frequency, conductivity, or permeability will give a smaller value of the skin depth.

At a high frequency, currents tend to flow close to the surface of a good conductor, the so called skin effect. This happens since induction currents are generated that flow in a direction opposite to any imposed currents and thereby eliminating the total (vector-sum) current inside the conductor. The skin depth is a characteristic penetration depth of the surface current sheet. If this measure is much larger than the device modeled, then magnetic, or inductive, effects can be neglected. In other words, the device is small enough that no skin effect can be seen.

RLC CIRCUIT EQUIVALENT

Yet another way of viewing the electric current approximation is to say that there are resistance, R, and capacitance, C, contributions to the overall impedance but that the inductance, L, equals zero. Electric circuit theory then tells us that the device we model will act as a high-pass filter. A plot of the magnitude of the impedance vs. frequency will show the magnitude decreasing with higher frequency.

ELECTRIC POTENTIAL

If not for the electric current approximation, we would need to model the full electromagnetic field using the electric potential *V* and the magnetic vector potential *A=(Ax,Ay,Az)*. This is available in the Quasi-Statics, Electric and Induction Currents application mode. However, the electric currents approximation makes use of the electric potential, *V*, alone. This greatly simplifies the modeling process since a smaller set of boundary conditions can be considered and the memory requirements tend to be low - we are solving for one unknown instead of four.

THE TIME-HARMONIC ANALYSIS CASE

This example uses the time-harmonic analysis type of the Electric Currents application mode. This means that the AC voltage and current is assumed to be sinusoidal in shape at one specific frequency. The so called j-omega method is used for this so that the voltage amplitude solved for, *V(x,y,z)*, is a complex time-independent quantity that is related to the real-world voltage, Vhat, by the relationship:

$$\hat{V}(x, y, z, t) = Real\{V(x, y, z)e^{j\omega t}\} = \hat{V}(x, y, z)\cos(\omega t)$$

The complex valued voltage *V* is also referred to as a phasor.

Having the voltage as a complex valued phasor has many advantages. One being that it is very easy to specify or measure phase differences. A phase shift phi at a boundary surface is modeled by multiplying the complex voltage amplitude by `exp(j*w*phi)`. A real value of the voltage phasor means the phase `phi` equals zero. A zero voltage means ground which has no associated phase angle (undefined).

COMSOL Multiphysics lets you operate on any complex variable by the functions `real(), imag(), abs()`, and `angle()`, to retrieve the real part, imaginary part, absolute value (modulus), and phase angle, respectively. These functions are available for boundary, subdomain and material settings, as well as for postprocessing. All variables in COSMOL Multiphysics are allowed to be complex valued.

MATERIAL PROPERTIES

In the Electric Currents application mode, there are two material properties: the electric conductivity s and the relative electric permittivity ε_r. Often, these quantities are frequency dependent and you may use analytical expressions for them in the frequency variable with default name `nu_emqvw`. You can also use look-up table

functions, or user-defined functions from COMSOL Script. The parametric solver will then allow you to sweep for a range of frequencies.

In this example, the skin depth for the buffer at 1 MHz is:

$$\delta = \sqrt{\frac{2}{2\pi f \sigma \mu_0 \mu_r}} = \sqrt{\frac{2}{2\pi 10^6 0.56 \cdot 1.3 \cdot 10^{-6} 1}} \approx 670m$$

This is significantly larger than the 30μm side of the modeled cube-shaped domain.

The skin depth for the gold electrodes is:

$$\delta = \sqrt{\frac{2}{2\pi f \sigma \mu_0 \mu_r}} = \sqrt{\frac{2}{2\pi 10^6 45.2 \cdot 10^6 \cdot 1.3 \cdot 10^{-6} 1}} \approx 75\mu m$$

which is significantly larger than the electrode thickness 0.1 μm. At a higher frequency, the approximation of gold as a perfect conductor might not be valid and another method is needed such as an Electric Shielding boundary condition (surface impedance) or a full volume representation of the electrodes.

ADDITIONAL INFORMATION

You can read more on the Electric Currents application mode in the Electromagnetics User's Guide.

REFERENCES

1. Asokan, S. B., Jawerth L., Carroll R. L., Cheney, R. E., Washburn, S., and Superfine, R., "Two-Dimensional Manipulation and Orientation of Actin-Myosin Systems with Dielectrophoresis", *Nanoletters*, Vol. 3, No. 4 431-437, 2003

2. Hesketh, P. J., Gallivan, M. A., Kumar, S., Erdy, C. J., Zhang, Z., L., "Modeling and Characterization of Dielectrophoretic Assembly Process For Nanobelts", Proceedings of IMECE2005: 2005 ASME International Mechanical Engineering Congress and Exposition

3. Feynman, R. P., Leighton, R. B., Sands, M., *The Feynman Lectures on Physics*, Volume 2, Addison-Wesley, 1977