

Lab 3: COMSOL models

Introduction

This lab introduces the use of COMSOL software for creating electrostatic models of the brain. COMSOL is a powerful finite element analysis tool that's very useful for simulations of electrophysiological recordings in different physical scenarios. We first go through a short tutorial of COMSOL, then replicate results from a 2005 paper. We finish by creating our own head model and implementing a state-of-the-art electrostatic modeling tool. This lab will introduce COMSOL software and some of its cutting-edge applications in neural engineering.

Software

This lab must be completed using COMSOL, and MATLAB or Python. Both Research and Student versions should work. I used the student instructional license in COMSOL 5.5

Part 1) COMSOL tutorial

We'll start by walking through a short tutorial on building a simple electrostatic field model of a point current at the center of a sphere.

The first several steps set up the type of model we're trying to create.

1. Open COMSOL and select to create a new model (default startup option).
2. Use the *Model Wizard* to create your new model.
3. Select *3D* space dimension.
4. Add *Electric Currents (ec)* physics (under *AC/DC*) and click on *Study*.
5. Select *Stationary* study and click *Done*. This means we're going to simulate everything at steady state at a single point in time.

COMSOL now knows what kind of model we're planning to build, so we can begin building and assembling the parts to our model.

6. To create our sphere, right click on *Geometry* in the *Model Builder* tab and select *Sphere*. Note that you can name it, resize it, position it, etc, in the *Settings* tab just to the right. Leave it with its default parameters for now (1m radius at origin). However, make sure that the sphere is selectable by checking "Resulting objects selection". This should be checked for all new objects you create in this lab.
7. To build the sphere in your model, click on *Build Selected* in the *Settings* tab. You should see the sphere appear in the *Graphics* tab.

This is a good time to play with some of the settings in the *Graphics* tab. Note that you can reorient your view of the model, change rendering options, etc. Turn on *Transparency* to make the sphere transparent.

8. To set the material properties of the sphere, we'll need to define a new material. Right click on *Materials* (below the *Geometry* section) in the *Model Builder* tab and select *Blank Material*. With the new material selected in the *Model Builder* tab, set *Electrical conductivity* to 0.33 S/m. Leave *Relative permittivity* blank.
9. To set the sphere to take on the material properties of our new material, stay in the *Settings* tab of the material. Select *Domain* for *Geometric entity level* and select your sphere object from the *Selection* dropdown menu.
10. To create a point current source at the origin, right click on *Geometry* and select *More Primitives* → *Point*. Click on *Build Selected* to make sure it appears where you expect it. If you turned transparency on in *Graphics* you should see it at the center of the sphere. In the *Settings* tab, make sure *Resulting objects selection* is checked and select *All levels* in the *Show in physics* dropdown menu. We'll want to be able to select it later to give it a current.
11. To create a current at the point we created, right click on *Electric Currents (ec)* and select *Points* → *Point Current Source*. Note that there are no points selected in the *Point Selection* section. With *Selection* set to *Manual*, click on the point you just created. A number should appear in the *Point Selection* list, indicating the reference number of the selected point. (Note that these numbers are not assigned in any obvious order.)
12. In the *Settings* tab for the point current source, set the current to 1 A.
13. We'll also need an electric ground for our model. Right click *Electric Currents (ec)* and select *Ground*. In the *Settings* tab, select *Manual* for *Boundary Selection*. Click each of the sphere's surfaces (there are eight) to set them to ground.

We've build our model and are now ready to run it!

14. In the *Model Builder* tab, right click on *Study 1* and select *Compute*. After a bit of computation, the *Graphics* window should show a heat map representation of the electric potential in your model.

Part 2) Replicate Moffit and McIntyre (2005) head model

Moffit and McIntyre published a 2005 paper that used a computational head model to investigate factors that affect neural recordings from intracranial sites. Here, you will replicate a scaled version of their head model and export the resulting K matrix to observe an important high-level phenomenon of electric field recordings.

We'll start by creating the scalp to introduce the *Difference* geometry.

1. Start a new COMSOL model and create a sphere with a 10 cm radius at the origin. Name it 'scalp+'.
2. Create a sphere with a 9 cm radius at the origin and name it 'skull+'. Build both spheres so that they are visible in the *Graphics* tab. Make sure *Transparency* is turned on in the *Graphics* tab so that you can see both spheres.
3. Right click on *Geometry* and select *Booleans and Partitions* → *Difference*. Call this new object 'scalp'.

4. In *Settings* of 'scalp', click on the toggle switch next to the *Objects to add* list so that the switch is green and says ON. Put your mouse over the spheres in the *Graphics* tab and select the outermost sphere. You can select nested objects by placing your mouse over the objects and using the scroll wheel.
5. Click on the toggle switch next to the *Objects to subtract* list so that the switch is green and says ON. Select the smaller sphere in the *Graphics* tab.
6. Place a check next to *Keep input objects*. Usually, we would want to get rid of the original objects (e.g., scalp+, skull+), because you don't want the model to have different objects overlapping in space. However, we'll want to reuse some of these objects again. We'll delete them at the end.
7. Using the *Difference* geometry object, we just created a model of the scalp by finding the difference of two concentric spheres. Now replicate the rest of the head model detailed in Moffit and McIntyre 2005, with brain, cerebrospinal fluid, skull, and scalp. All necessary parameters can be found in the paper. Note that the paper models a rat head. Since we want to make a human head, scale everything by 10x, so that the head is 10 cm in radius.
8. For the model to run correctly, we'll need to get rid of all the overlapping concentric spheres we used to create the different layers around the brain. Right click on *Geometry* and select *Delete Entities*. Select the appropriate objects to delete.

Note: Make sure this is at the end of the *Geometry* section. COMSOL does everything in order from top to bottom in the *Model Builder* section. That is to say, make sure you call the delete operation after all your objects are built.

9. Create a 1 A point current at the origin and set ground to all external surfaces of the scalp.
10. Certain regions of the simulation will be much more interesting than others. In this particular case, we know that most of the action will be going on near the current source, due to $1/r$ behavior. COMSOL can refine the mesh size to increase density where it matters, using *Adaptive Mesh Refinement*. Right click on *Stationary Solver* under *Study 1* → *Solution 1*. Find *Adaptation and error estimates*. Change it from *None* to *Adaptation and error estimates* to reveal more options. Set *Maximum number of adaptations* to 3 and *Adaptation method* to *Rebuild Mesh*.
11. Run the simulation.
12. To export data, right click *Export* in the *Results* section (in the *Model Builder* tab) and select *Data*.
13. For *Data Set*, select *Study 1/Adaptive Mesh Refinement 1*.
14. In the *Expression* section, click on the + symbol to see the different variables that can be exported. Find and select electric potential under *Component 1*.
15. In the *Output* section, click on *Browse...* and select a filename for the export file.
16. In the *Advanced* section in *Settings*, uncheck *Include header*. This will make it easier to read into MATLAB or Python.
17. Click on the *Export* button at the top of the *Settings* tab to export data to a text file. This will create a text file with X, Y, Z, and V as columns (all in SI units).

18. In Matlab or Python, import the data and create a plot of voltage versus distance from the stimulus. Describe (qualitatively and quantitatively) the relationship between voltage and distance.

Part 3) Create a simple deep brain stimulation model

Deep brain stimulation (DBS) is a real-world application of a head model like the one you just created. Here, we will create a simple model of DBS using the model from Part 2 and use the outputs to make predictions about the effects of DBS.

Conventional deep brain stimulation probes have multiple contacts along its length that can be activated separately. In this model, we will have one active contact with two adjacent contacts acting as current sinks.

1. Copy the model you created for Part 2 to a new file.
2. Change the current to 5 mA. This is much closer to what real DBS amplitudes would be.
3. Add new point objects 3 mm above and below the original point current source.
4. Make the superior point a 1.25 mA current sink and the inferior point a 3.75 mA current sink. You should now have three point currents: a current source near the origin and two current sinks above and below it. Make sure that the scalp is still set as ground.
5. Run the simulation and export data to MATLAB or Python.
6. Calculate the second spatial derivative of the voltage in the direction going away from the active contact and perpendicular to the probe (for example, in the x-direction). You will need to implement a basic interpolation scheme to find the voltage at specific locations. Plot your results and comment on what this means for DBS.

Guidelines for Lab Report (on Labs 3 and 4 together)

Introduction: The introduction should be one paragraph long summarizing the motivation for electrostatic models, what data they draw upon from past experiments, and a brief summary of everything you will show in this lab report.

Methods: From Lab 3, there should be three methods paragraphs (and diagrams if you like) on:

1. Assumptions of the models used
2. How the models were designed
3. The different levels of model complexity

Include the code as an Appendix to your report. Cite sources for any values used in your models.

Results: You should include the following in your Results:

1. Include the plot of voltage vs. distance from part 2.
2. Describe the effects of increasing model complexity (include screenshots of the COMSOL electric potential plots from the Part 3).
3. Include your plot of the second derivative from part 3

Include any other figures produced by COMSOL and MATLAB/Python that could help explain and illustrate your findings.

Discussion: Should be ~2 paragraphs long describing what you could use these techniques for in the future.

The report (not including Appendix) should be no longer than 4 pages. Use 12 pt. font and 1.15-1.5 line spacing. If your text is over the 4-page limit with figures, you can move your figures to an appendix section that goes beyond the 4-page limit.

Please upload your report to Canvas. Be sure different lines on your plots are distinguishable (using color or different line styles).