EM & Optics - Lab Session: Numerical Solution of 3D Laplace Equation

The target of the simulation is explained first. Then, the numerical method is described. Its implementation (using any language you desire - FORTRAN, C, Python, Matlab....) is described in detail. Some programming work is required from you to complete it. Once answers have been found for all questions, upload it to the appropriate link in Aula Global. For any other questions, e-mail me at **raul.sanchez@uc3m.es**

Target of this Numerical Lab Session.-

Your main objective will be to write a code able to **calculate the electric potential created by a charged, parallel-plate finite capacitor (see Figs. 1 and 2) both inside and around it**. The capacitor will be enclosed by a much larger and perfectly conducting square box, being located at its geometrical center.

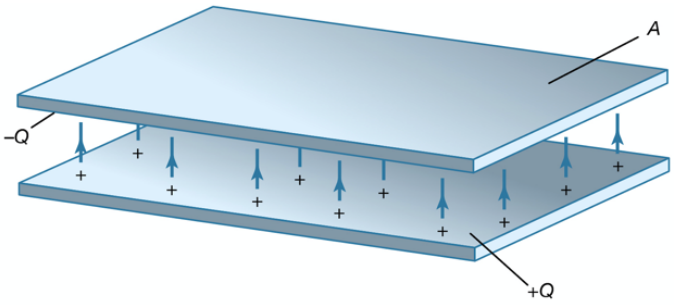

Figure 1: Sketch of a parallel-plate capacitor. Each plate contains the same amount of charge of opposite signs and is at a unique potential value.

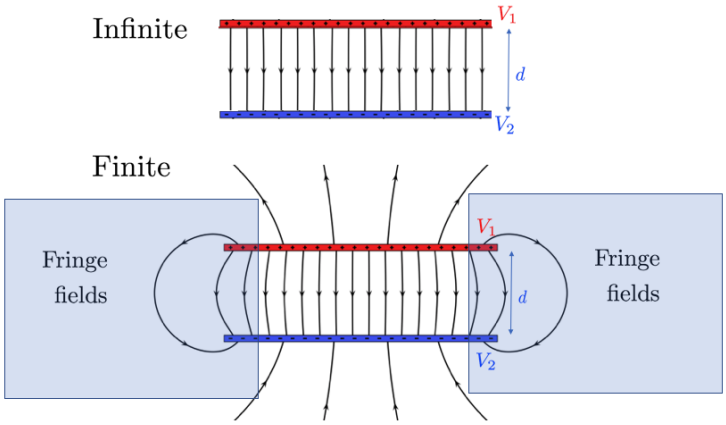

Figure 2: The difference between the potential value of each plate determines the electric field inside the plates in the case seen in class of infinitely extended plates, being zero outside. A capacitor with finite plates has an electric field outside as well as non-straight field lines as we approach the plate edges. This increases its capacity with respect to the infinite case for the same potential difference, what is known as the **fringing effect.**

Description of the problem.-

In Electrostatics, the electric field that occupies any area of space, $\mathbf{E}(\mathbf{r})$, must satisfy Gauss's law that, in differential form, is given by:

$$\nabla \cdot \mathbf{E} = \frac{\partial E_x}{\partial x} + \frac{\partial E_y}{\partial y} + \frac{\partial E_z}{\partial z} = \frac{\rho}{\epsilon_0} \tag{1}$$

where $\rho(\mathbf{r})$ is the electric charge density that tells how charge is distributed throughout the region. In the absence of any electric charge, this equation reduces to,

$$\frac{\partial E_x}{\partial x} + \frac{\partial E_y}{\partial y} + \frac{\partial E_z}{\partial z} = 0. \tag{2}$$

Either way, these three-dimensional PDEs must be solved in the region of space of interest, once the charge distribution is known, with the addition of adequate boundary conditions (for instance, the value of the electric field at the boundary of the domain) to find out the electric field. This type of calculation is the bread-and-butter of many engineering applications.

Since the electrostatic field is conservative, one can always introduce the **electrostatic potential**, $V(\mathbf{r})$, that is related to the electric field vector as,

$$\mathbf{E} = -\nabla V(\mathbf{r}). \tag{3}$$

Calculating the potential is almost always simpler, since it is a scalar quantity instead of a full vector. The potential satisfies its own PDEs, that naturally emerge from the previous ones for the electric field. Namely,

$$\nabla^2 V = \frac{\partial^2 V}{\partial x^2} + \frac{\partial^2 V}{\partial y^2} + \frac{\partial^2 V}{\partial z^2} = -\frac{\rho}{\epsilon_0} \tag{4}$$

known as the **Poisson equation**, or, in the absence of any electric charges,

$$\frac{\partial^2 V}{\partial x^2} + \frac{\partial^2 V}{\partial y^2} + \frac{\partial^2 V}{\partial z^2} = 0. \tag{5}$$

The latter is known as the **Laplace equation**. As before, the solution of the equation requires to impose proper boundary conditions for the potential.

In this lab session, you will solve Laplace's equation to find out the electrostatic potential for a **three-dimensional, parallel-plate finite capacitor** (see Fig. 1). In this case, the only place where electric charge exists is inside of the capacitor plates. However, we can ignore them and still use Laplace's equation simply by *imposing that the solution takes the value of the potential at each of the plates prescribed by the capacitor*. To complete the required boundary conditions, we will also assume that the capacitor is enclosed in a *much bigger, perfectly-conducting parallepipedon where we can set the potential to zero.*

Objective: Integrate Laplace's equation numerically in the case of a three-dimensional, parallel plate charged capacitor for a prescribed potential difference between the plates.

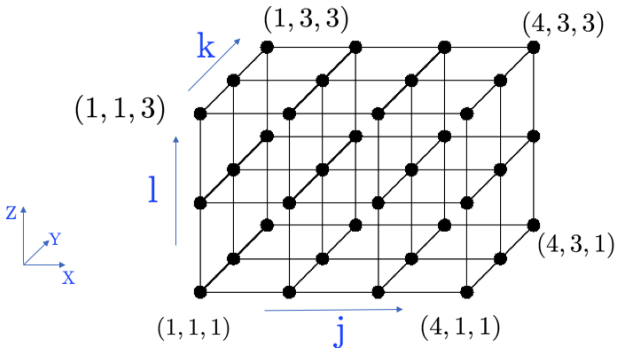

Figure 3: Illustration of the 3-dimensional discrete mesh considered in the text. The value of the indices is shown for some selected points.

Discretization of the problem.-

Spatial mesh:

To solve any PDE numerically in a computer, one must consider both time and space as discrete variables that form a **mesh**. Since Laplace's equation does not contain time, a three-dimensional spatial mesh will be sufficient (see Fig. 3). The process of constructing a mesh basically goes like this:

Each spatial dimension is replaced by a discrete variable that runs between a minimum and a maximum value.

For instance, in the case of the x coordinate, it would run between ($-\mathrm{x_{min}}$) and maximum value ($\mathrm{x_{max}}$) in Δx increments,

$$x = \{-x_{\mathrm{min}}, -x_{\mathrm{xmin}} + \Delta x, -x_{\mathrm{xmin}} + 2\Delta x, \cdots, x_{\mathrm{xmax}} - \Delta x, x_{\mathrm{xmax}}\}\,. \tag{6}$$

The number of points (M_x) in set by the value of Δx. The points in the mesh are:

$$x_j = -x_{\mathrm{min}} + (j-1)\cdot\Delta x, \quad j = 1, 2, \cdots, M_x, \quad \text{with} \quad \Delta x = \frac{x_{\mathrm{max}} + x_{\mathrm{xmin}}}{M_x - 1}, \tag{7}$$

Similarly, for y we will have,

$$y_k = -y_{\mathrm{min}} + (k-1)\cdot\Delta y, \quad k = 1, 2, \cdots, M_y, \quad \text{with} \quad \Delta y = \frac{y_{\mathrm{max}} + y_{\mathrm{xmin}}}{M_y - 1}, \tag{8}$$

and for z,

$$z_l = -z_{\mathrm{min}} + (l-1)\cdot\Delta l, \quad l = 1, 2, \cdots, M_z, \quad \text{with} \quad \Delta z = \frac{z_{\mathrm{max}} + z_{\mathrm{xmin}}}{M_z - 1}. \tag{9}$$

By combining these 1D meshes, we end up with a numerical 3D mesh that consists of $M_x \cdot M_y \cdot M_z$ points (or nodes). We can locate any point in our numerical mesh by means of its values for the three indices, j, k and l, that locate the point at the position vector:

$$\mathbf{r}_{jkl} = (x_j, y_k, z_l). \tag{10}$$

Finally, the mesh is called a **regular** mesh if the spacings are all the same in every direction. That is, whenever $\Delta x = \Delta y = \Delta z$. We will always assume a regular mesh in what follows, although that is not strictly necessary. For simplicity, we will use Δs to refer to the spacing, since it is the same in every direction.

Electrostatic potential:

The electrostatic potential that will be the solution to Laplace's equation is a **real function** defined on the space-time mesh just introduced as:

$$V_{jkl} \equiv V(x_j, y_k, z_l), \quad j = 1, 2, \cdots, M_x, \quad k = 1, 2, \cdots, M_y, \quad l = 1, 2, \cdots, M_z. \tag{11}$$

As can be seen, the potential carries **three (3) sub-indices** that correspond to the indices of the node where the potential is evaluated.

Discretization of the derivatives.-

There is only one kind of derivative in Laplace's equation, a **spatial second derivative** along one of the coordinates. Here, these derivatives are approximated following an approach known as **finite differences**.

Spatial second derivative of the potential: Starting with the derivative along x, this derivative can be approximated at any point as,

$$\frac{\partial^2 V}{\partial x^2} \simeq \frac{V(x + \Delta x, y, z) - 2V(x, y, z) + V(x - \Delta x, y, z)}{(\Delta x)^2}, \tag{12}$$

for finite, albeit small Δx. On the numerical mesh, this approximation becomes,

$$\left(\frac{\partial^2 V}{\partial x^2}\right)_{jkl} = \frac{V_{j+1,kl} - 2V_{jkl} + V_{j-1,kl}}{(\Delta x)^2} \tag{13}$$

Again, the three subindices represent the node in the numerical mesh where the derivative is evaluated. The same procedure can be followed for the y and z second derivatives, simply by considering the indices k and l instead of j. The result is,

$$\left(\frac{\partial^2 V}{\partial y^2}\right)_{jkl} = \frac{V_{j,k+1,l} - 2V_{jkl} + V_{j,k-1,l}}{(\Delta y)^2} \tag{14}$$

and,

$$\left(\frac{\partial^2 V}{\partial z^2}\right)_{jkl} = \frac{V_{jk,l+1} - 2V_{jkl} + V_{jk,l-1}}{(\Delta z)^2} \tag{15}$$

Discretized Laplace's equation.-

One can now replace the approximations of the derivatives within Laplace's equation (Eq. 5) to get to:

$$\frac{V_{j+1,kl} - 2V_{jkl} + V_{j-1,kl}}{(\Delta x)^2} + \frac{V_{j,k+1,l} - 2V_{jkl} + V_{j,k-1,l}}{(\Delta y)^2} + \frac{V_{jk,l+1} - 2V_{jkl} + V_{jk,l-1}}{(\Delta z)^2} = 0. \tag{16}$$

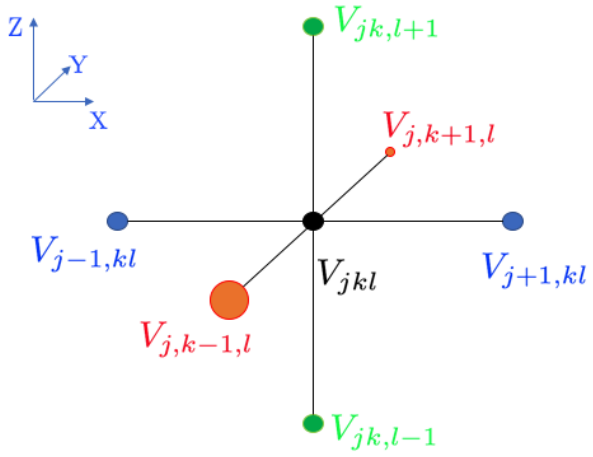

Figure 4: 7-point stencil for Laplace's equation in Cartesian coordinates.

Assuming now that we are using a regular mesh, this equation reduces to:

$$\frac{V_{j+1,kl} + V_{j-1,kl} + V_{j,k+1,l} + V_{j,k-1,l} + V_{jk,l+1} + V_{jk,l-1}}{6} = V_{jkl}. \tag{17}$$

This has a nice geometrical interpretation (see Fig. 4). It tells us that any solution of Laplace's equation must satisfy that, at any point in the mesh, *the value of the potential must be equal to the average of the potential over its six closest neighbours*: one at its left, another on the right, one from above and one from below and one from the front and the last one at the back of the original node. These seven points form the **local stencil**. The location of the stencil in the mesh is specified by giving the location of its central node.

Integration method: successive relaxation

How does one find numerically a solution that satisfies Eq. 17 for a problem like ours?

We will describe an easy method that belongs to the family of **successive relaxation methods**. It starts by assigning an initial value of the electrostatic potential to each node in the 3D mesh, each labeled by the indices (j, k, l). These values should be as close as possible to the final solution. The better the approximation, the faster the convergence to the final result. Once the initial values have been loaded, one just needs to go around the mesh, one node at a time, and: i) *compute the arithmetic average over the six non-central nodes of the local stencil* and ii) *replace the value at the central node by this average.*

This update procedure is carried out at every node of the mesh, one after the other. Once every node has been visited and updated, one must return to the first node and start again. As many of these cycles will be completed as needed for the **error** to fall below a certain prescribed tolerance, $r_{\rm tol}$. And what is a good measure of the error here? We will use the **maximum value of the local residual**, defined as *the (absolute value of the) difference between the potential value at the central node and the arithmetic average of the other values in the stencil.* As a extra safeguard, we will also compare the errors of any two successive cycles and stop the relaxation if they become equal. A better solution is no longer possible.

Integration method: boundary conditions

What about boundary conditions? One needs to consider two sets of them.

First, the ones that have to do with the **capacitor plates** themselves. Since each plate is at a constant potential that is known from the start, one just needs to *identify the nodes of the spatial mesh where the plates are located* and to *keep the values of the potential at those nodes unchanged through the procedure and equal to the nominal capacitor values.*

Secondly, one has to deal with the surrounding **conducting box**. The nodes for this box are the most exterior nodes in each direction. That is, all nodes that have $j = 1$ or $j = M_x$, $k = 1$ or $k = M_y$ and $l = 1$ or $l = M_z$. One just needs to *keep the potential at every one of these nodes at zero* during the relaxation, since the potential is always constant throughout a conductor and we will choose the potential zero to be here.

Parameter values to be used in your computer code:

The capacitor we are going to use has two parallel plates of linear sizes[1] $l_y = 5$cm and $l_z = 10$ cm separated by a distance $d = 1$cm inside a conducting box of linear sizes $L_x = 10$cm, $L_y = 15$cm and $L_z = 30$cm. The electrostatic potential of the capacitor plates are, respectively, $V_1 = 10$V and $V_2 = -5$V. These values are relative to the potential of the outer box, that is at $V = 0$.

We will use a regular numerical mesh with $\Delta s = 0.1$cm. That means that the number of points in each direction is $M_x = 101$, $M_y = 151$ and $M_z = 301$. The total number of points in our simulation is, thus, $M = M_x * M_y * M_z = 4,590,551$.

Parameter	value
Δs	0.1
$x_{\min}$	-5
$x_{\max}$	5
$y_{\min}$	-7.5
$y_{\max}$	7.5
$z_{\min}$	-15
$z_{\max}$	15
V_1	10
V_2	-5
r_{tol}	10^{-2}

Table 1: Parameters values to be used for the simulation.

[1] We will choose, for simplicity, the X, Y and Z axis so that the capacitor is parallel to the YZ plane. The sub-indices signal along which directions the lengths provided should be measured.

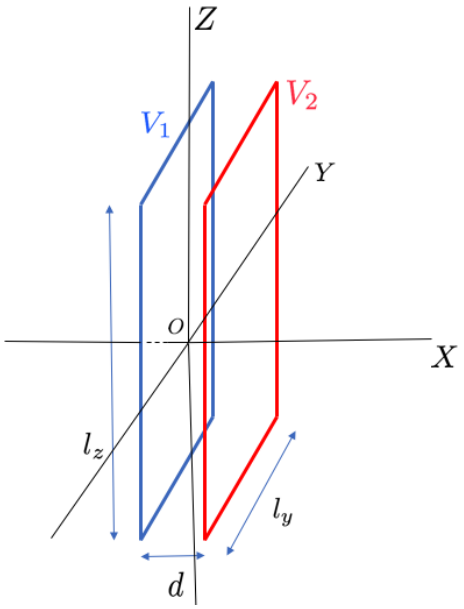

Figure 5: Location of the capacitor with respect to coordinate axes.

Location of the capacitor plates:

The location of the plates on the numerical mesh is rather straightforward to find. First, the plates are parallel to the OYZ plane that contains the origin of the coordinate system (see Fig. 5). Secondly, we will locate the plates symmetrically with respect to the origin, with the $V_1(= 10\text{V})$ plate at $x = -0.5\text{cm}$ and the $V_2(= -5\text{V})$ at $x = 0.5\text{cm}$, so that the distance between them is the required $d = 1\text{cm}$. Since the origin corresponds to the central numerical node $(j, k, l) = 51, 76, 151$ and $\Delta s = 0.1$ cm, all nodes of the left plate will then have an index $j = 46$ and all nodes on the right plated will have $j = 56$. Third, the linear size of the plate in the Z direction is $l_z = 10$. Thus, the values of the l index go from $l = 101$ to $l = 201$ for both plates. Similarly, the linear size of the plate in the Y direction is $l_z = 5$, meaning that the k index runs from $k = 51$ to $k = 101$.

Boundary conditions:

The boundary condition at the capacitor plates thus reduces to keeping:

$$V(46, 51 : 101, 101 : 201) = V_1(= 10\text{V}) \tag{18}$$

for the left plate and,

$$V(56, 51 : 101, 101 : 201) = V_2(= -5\text{V}) \tag{19}$$

for the right one throughout the procedure[2]. The notation $A : B$ naturally stands for all index valules between A and B. Similarly, the boundary conditions for the outer conducting box trivially reduce to:

$$V(1, :, :) = V(101, :, :) = V(:, 1, :) = V(:, 201, :) = V(:, :, 1) = V(:, :, 301) = 0 \tag{20}$$

where the (:) symbol represents the whole range of that index.

[2]Here, we have replaced the notation $V_{jkl} = V(j, k, l)$ in the sake of clarity.

Algorithm YOU MUST implement:

Using any software of your preference (i.e., FORTRAN90, C, Python, Matlab,....) write a code by yourself to simulate the process just described. You should follow these steps:

1. Define the parameters of the problem. Use all parameter values collected in Table 1.

2. Define a three-index matrix to contain the potential.- You will need to define and keep in memory at least a matrix POTENTIAL$(1{:}M_x, 1{:}M_y, 1{:}M_z)$ that contains the electrostatic potential at every node of the mesh. This matrix will be updated as the relaxation procedure advances.

3. Construct initial potential guess.- At the beginning of the run you will have to start by filling with values the matrix POTENTIAL. A possible choice [3] is to set everything to zero except for the values at the nodes where each of the capacitor plates are, that should be respectively given V_1 and V_2.

4. Iterate the relaxation cycle for as many iterations as required.- Remember that the boundary conditions require that all nodes corresponding to the exterior conducting box or the plates must keep their potential value unchanged. For all other nodes, replace the local value by the arithmetic value of the potential over the rest of nodes in the local stencil.

5. Keep track of relaxation error.- Keep record of the maximum of the local residual (i.e., the difference between the local potential and the arithmetic average over the rest of the nodes in the local stencil) over the whole domain for each cycle. Once the cycle is completed, check whether the residual exceeds or not the maximum allowed tolerance. If it turns out to be below that tolerance, you are done! Also, check that the residual is not identical to the previous value. In that case, even if above tolerance, you must abandon the relaxation since the solution will not improve.

6. Produce required output.- It is convenient to store in a text file the value of the potential matrix at the end of the calculation. This file will be key in order to be able produce to graphs requested and to perform the various calculations required. You should also include appropriate additional lines to calculate the quantities needed to complete the "**Results and Data Analysis**" section.

[3] A better choice for the potential would be to give zero everywhere except **at the plates and across the inner space between them**; for those inner nodes between plates you could give the expression of potential obtained for an infinite parallel plate capacitor!

Results and Data analysis.-

Once your code is ready and running, you should have easily converged to a final solution for the electrostatic potential at any point of the mesh, $V(j,k,l)$. Using that solution, carry out the following tasks:

1. Produce a plot (or sequence of plots) showing **the variation of the electrostatic potential along the straight lines, parallel to the X direction, that cross through**[4]: i) **the center of the plates** O; ii) **the mid-point of the left side of the plates** A and iii) the **mid-point of the top side of the plates** B.

   Compare the resulting graphs with the theoretical value of the electrostatic potential for a parallel plate capacitor with infinite plates separated by a distance d and with respective potentials V_1 and V_2, that is given by,

$$V(x) = \begin{cases} V_2 + (V_1 - V_2) \cdot \left(\dfrac{d - 2x}{2d} \right), & -d/2 \leq x \leq d/2 \\ 0, & |x| > d/2 \end{cases} \tag{21}$$

   Your results should look like those shown in Fig. 6.

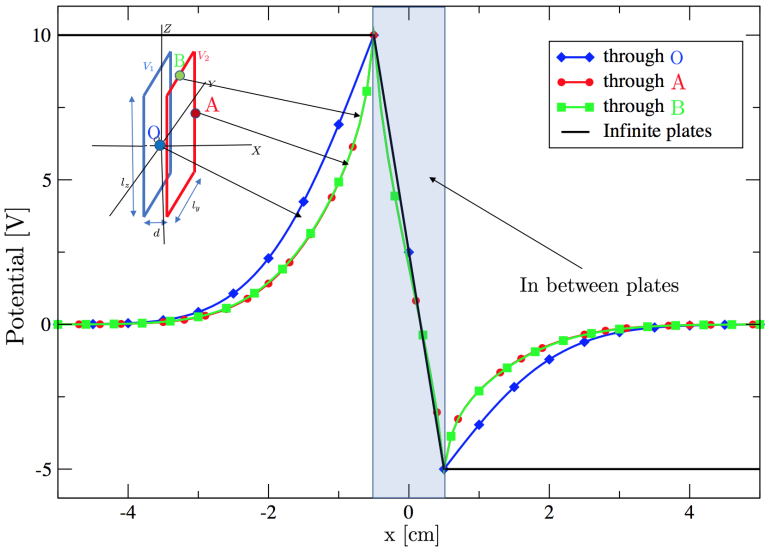

Figure 6: Variation of the electrostatic potential along the lines (parallel to X) crossing points O (in blue), A (in red) and B (in green) as shown in the upper-left sketch of the capacitor. The electrostatic potential for a parallel plate infinite capacitor along the X axis is shown in black.

2. **Produce a plot showing the percentage difference between the values of electrostatic potential along the OY axis for the finite and infinite capacitors**. The percentage difference will be defined here by the ratio of the difference between the two potential values and the value of the potential for the infinite capacitor. Determine from the resulting plot:

[4] The actual location of these points is shown in Fig.6.

i) **the distance from the origin along the Y axis beyond which the difference is larger than** 10%;
ii) **the percentage difference at the left edge of the finite capacitor.**

Your plots should look similar to those shown in Fig. 7.

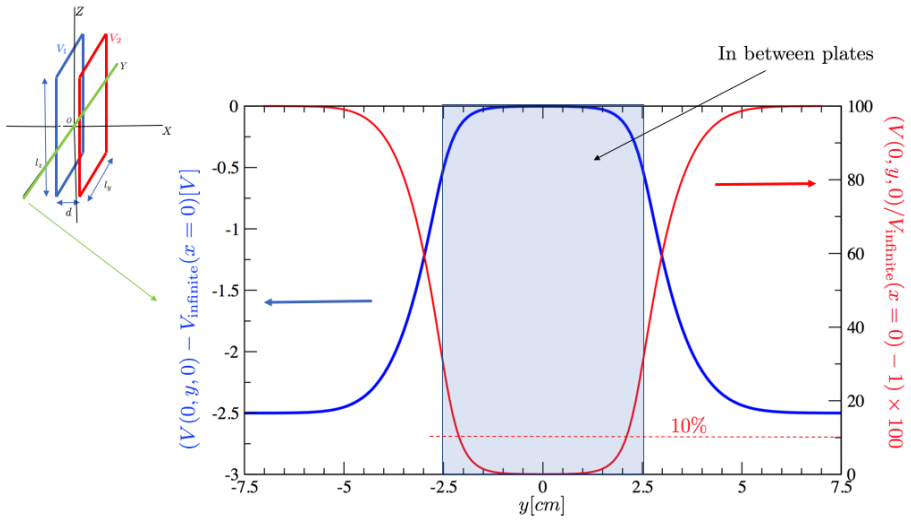

Figure 7: In blue (left axis) difference between potentials for the finite and infinite capacitors along the OY axis (in green); in red (right axis) its percentage difference.

3. **Produce a contour plot (i.e., a plot of the contours of constant value) for the electrostatic potential of the finite capacitor across the** $0XY$ **plane**. An illustration of what you should get is shown in Fig. 8.

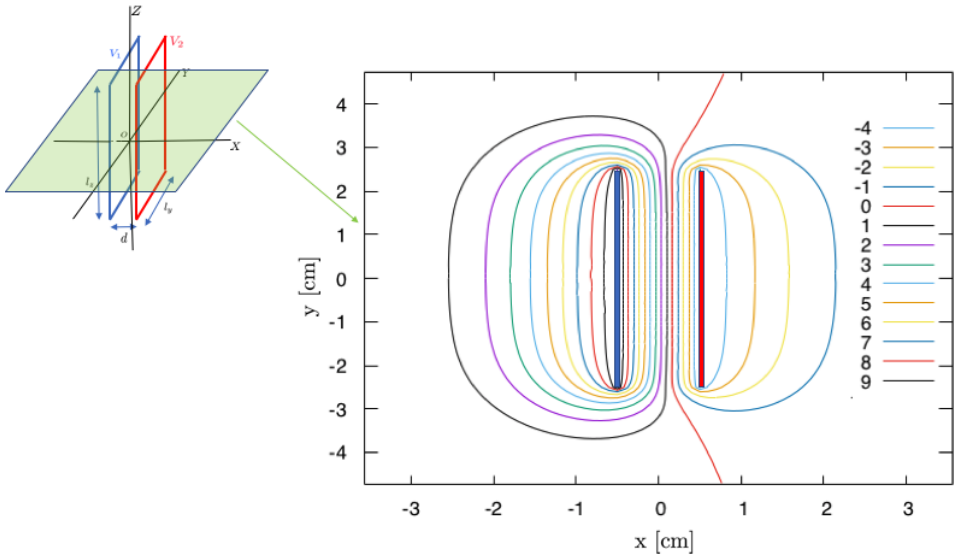

Figure 8: Contour and surface plots of the electrostatic potential on the $0XY$ plane (shown in green) for the finite capacitor. The two plates are shown as two solid rectangles.

With the help of the contour plot for the electrostatic potential you just produced, answer the following questions:

i) **Where is the electric field the strongest across the OXY plane? Why?**

ii) **At which side (outside) of the capacitor is the field stronger on the OXY plane? Why?**

iii) **Draw by your own hand on a printed version of your contour plot a few field lines of the electric field on top of the equipotential contours[5]. How is it different from the field for the infinite parallel plate capacitor? Can you spot the fringe fields?**

iv) **Why does the contour for $V = 0$ leave the capacitor twisting towards positive x's instead of being parallel to the Y axis?**

[5]Once done, please scan the result and add it to your final package for submission! If you can plot the field lines by using a subroutine (PYTHON and MATLAB have some that can do it!), that is also fine!

IMPORTANT:

You need to **write a report** (PDF or Word) in which all the requested tasks and plots are included and discussed, and all proposed questions are answered. You MUST also include a file with the implementation of your code (or script, if using Python or Matlab) so that I can take a look at it. Once all is completed, compress the report, figures and codes into a single zip file and upload it into the **assignment link** that will be ready in Aula Global.

RECOMMENDED DATE FOR UPLOAD: **April 8, 2022**.

FINAL DATE FOR UPLOAD: **April 29, 2022 @12:00AM**.