



1. Surface Charge Density on an Arbitrary Surface/Normal Boundary Conditions

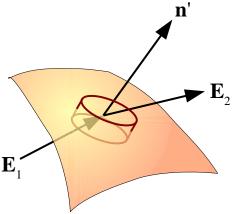
- Take Gauss's Law in Integral Form

$$\oint \mathbf{E} \cdot \mathbf{n} \, da = \frac{1}{\epsilon_0} \int \rho(\mathbf{x}) \, d^3 \mathbf{x}$$

- Where **n** is the vector normal to the bounding surface, and **n**' is the vector normal to the charged surface.

- Choose a small volume that just barely bounds a small patch on the surface so that the only charge in the volume is the surface charge: $\rho(\mathbf{x}) = \sigma \delta(n' - n'_0)$ where *n'* is the component of the position vector in the direction normal to the charged surface and n'_0 is the position of the surface in that dimension.

$$\oint \mathbf{E} \cdot \mathbf{n} d^2 \mathbf{x} = \frac{1}{\epsilon_0} \int \sigma \,\delta(n' - n'_0) d^3 \mathbf{x}$$



- The surface bounding the volume has three sides: the top, the bottom, and the curved side. - The curved side can be chosen parallel to the electric fields so that their contribution cancels. - All that remains is the top and bottom. If the volume is sufficiently small, the patch of charged surface in the volume can be assumed to be flat so that $\mathbf{n} = \mathbf{n}'$ over the top side and $\mathbf{n} = -\mathbf{n}'$ over the bottom side.

$$\int_{\text{top}} \mathbf{E}_2 \cdot \mathbf{n}' d^2 \mathbf{x} - \int_{\text{bottom}} \mathbf{E}_1 \cdot \mathbf{n}' d^2 \mathbf{x} = \frac{1}{\epsilon_0} \int \sigma \,\delta(n' - n'_0) d^3 \mathbf{x}$$

- Also, if the bounding volume is taken small enough, all of the variables can be assumed to be constant and can be taken out of the integrals:

$$\mathbf{E}_{2} \cdot \mathbf{n}' \Big[\int_{\text{top}} d^{2} \mathbf{x} \Big] - \mathbf{E}_{1} \cdot \mathbf{n}' \Big[\int_{\text{bottom}} d^{2} \mathbf{x} \Big] = \frac{1}{\epsilon_{0}} \sigma \Big[\int d^{2} \mathbf{x} \Big] \int \delta (n' - n'_{0}) d\mathbf{n}'$$

- All three surfaces are identical and have identical area integrals that cancel out:

$$\mathbf{E}_{2} \cdot \mathbf{n}' - \mathbf{E}_{1} \cdot \mathbf{n}' = \frac{1}{\epsilon_{0}} \sigma \int \delta(n' - n'_{0}) d\mathbf{n}'$$

- Take the integral of the delta function and drop the primes to simplify notation:

$$\left[\left(\mathbf{E}_2 - \mathbf{E}_1 \right) \cdot \mathbf{n} = \frac{1}{\epsilon_0} \sigma \right]_{n=n_0}$$

- This does not specify the electric field completely and everywhere. It only specifies the normal component, and only on the surface. It is very useful however and will be used again and again. It is essential that you master this derivation.

- This is the first general boundary condition of Maxwell's equations.

- This equation can be used for the following:

1. To find the surface charge density if we know the fields

2. To connect two regions at their boundary if we know the fields in both regions up to a constant

3. To find the fields everywhere if we know the surface charge density and the geometry is especially simple.

2. Tangential Boundary Conditions

- The surface charge density equation above can be used as a boundary condition linking two regions, but it only specifies the normal components of the fields. What about the tangential components?

- As mentioned earlier, electrostatic fields are experimentally observed to be irrotational:

 $\nabla \times \mathbf{E} = 0$

- Integrate over some arbitrary open surface the component of this equation that is normal to the surface:

$$\int (\nabla \times \mathbf{E}) \cdot \mathbf{n} \, da = 0$$

- Use Stokes's theorem to convert this to a closed line integral around the edge of the surface:

$$\oint \mathbf{E} \cdot d\mathbf{l} = 0$$

- This is a useful equation in itself; it is just the integral form of the statement that electrostatic fields are irrotational.

- Take the line integral over a rectangular loop that straddles the boundary surface and shrink it such that the contributions from the sides disappear and the contributions from the top and bottom become constant and can come out of the integral:

$$\int_{a}^{b} \mathbf{E}_{1} \cdot d\mathbf{l} + \int_{b}^{a} \mathbf{E}_{2} \cdot d\mathbf{l} = 0$$
$$\mathbf{E}_{1} \cdot \int_{a}^{b} d\mathbf{l} - \mathbf{E}_{2} \cdot \int_{a}^{b} d\mathbf{l} = 0$$
$$E_{1,T} = E_{2,T}$$

- The components of the electric field that are tangential to a surface are continuous across the

surface even if a surface charge density is present.

- This is the second general boundary condition of Maxwell's equations.

- Note that every surface has two orthogonal directions that are both tangential to it at a point.

- This equation applies to both tangential directions and is therefore really two boundary conditions.

- To make this fact clear, this boundary condition is better expressed in vector form as the total field that is perpendicular to the surface normal vector **n**:

$$\mathbf{E}_1 \times \mathbf{n} = \mathbf{E}_2 \times \mathbf{n}$$

<u>3. Green Functions</u>

- Coulomb's Law can be transformed to include boundary conditions instead of an integral over the whole universe through the use of mathematical tools called Green functions which are applications of the divergence theorem: $\oint \mathbf{A} \cdot \mathbf{n} \, da' = \int \nabla \cdot \mathbf{A} \, d^3 \mathbf{x}'$

- Define the vector field **A** in terms of some arbitrary scalars $\mathbf{A} = \phi \nabla' \psi$ where the prime denotes that the gradient is taken with respect to **x**'. Plug this into the divergence theorem:

$$\oint [\phi \nabla' \psi] \cdot \mathbf{n}' da' = \int \nabla' \cdot [\phi \nabla' \psi] d^3 \mathbf{x}'$$
$$\oint \phi \frac{d\psi}{dn'} da' = \int [\nabla' \phi \cdot \nabla' \psi + \phi \nabla'^2 \psi] d^3 \mathbf{x}'$$

- Write this down again with the scalars interchanged and subtract the two equations:

$$\int (\Phi \nabla'^2 \psi - \psi \nabla'^2 \Phi) d^3 \mathbf{x}' = \oint \left(\Phi \frac{d \psi}{d n'} - \psi \frac{d \Phi}{d n'} \right) da'$$

- Now assign $\phi = \Phi$ and $\psi = G(\mathbf{x}, \mathbf{x'}) = \frac{1}{|\mathbf{x} - \mathbf{x'}|} + F(\mathbf{x}, \mathbf{x'})$ where G is called a Green function.

- If we require *F* to satisfy $\nabla'^2 F(\mathbf{x}, \mathbf{x'}) = 0$ and use the identity $\nabla'^2 \left(\frac{1}{|\mathbf{x} - \mathbf{x'}|}\right) = -4\pi \,\delta(\mathbf{x} - \mathbf{x'})$, it becomes apparent that $\nabla'^2 G(\mathbf{x}, \mathbf{x'}) = -4\pi \,\delta(\mathbf{x} - \mathbf{x'})$ so that:

$$\int \left(\Phi \left(-4\pi \delta \left(\mathbf{x} - \mathbf{x}' \right) \right) - G \nabla'^2 \Phi \right) d^3 \mathbf{x}' = \oint \left(\Phi \frac{d G}{d n'} - G \frac{d \Phi}{d n'} \right) da'$$

- Use the Poisson Equation and evaluate the integral:

$$-4\pi\Phi(\mathbf{x}) + \frac{1}{\epsilon_0}\int\rho(\mathbf{x}')G\,d^3\mathbf{x}' = \oint \left(\Phi\frac{d\,G}{d\,n'} - G\frac{d\,\Phi}{d\,n'}\right)da'$$

- Solve for the scalar potential:

$$\Phi(\mathbf{x}) = \frac{1}{4\pi\epsilon_0} \int \rho(\mathbf{x}') G d^3 \mathbf{x}' + \frac{1}{4\pi} \oint \left(G \frac{d\Phi}{dn'} - \Phi \frac{dG}{dn'} \right) da'$$

- This is the Green function solution to the electrostatic equations.

- We have, in a sense, converted Coulomb's law which contains a volume integral over all space into a corrected integral over a limited volume plus another correction term. The correction term ends up being an integral of the boundary conditions over the surface enclosing the volume. The Green function G can be thought of as a weighting parameter that makes this approach work.

- To apply the Green function solution in practice, we must first find the appropriate Green function, which is problem dependent.

-We must find the right function F that makes one of the last two terms vanish.

- For Dirichlet boundary conditions ($\Phi(\mathbf{x}')$ is known on the surface of integration) we demand that $G = G_D = 0$ on the surface by use of the proper *F* so that the first term in the surface integral vanishes.

$$\Phi(\mathbf{x}) = \frac{1}{4\pi\epsilon_0} \int \rho(\mathbf{x}') G_D d^3 \mathbf{x}' - \frac{1}{4\pi} \oint \left(\Phi \frac{dG_D}{dn'} \right) da'$$

- For Neumann boundary conditions ($\frac{d \Phi(\mathbf{x}')}{d n'}$ is known on the surface of integration) we

demand that $\frac{d G_N}{d n'} = \frac{-4\pi}{S}$ on the surface where S is the total surface area.

$$\Phi(\mathbf{x}) = \frac{1}{4\pi\epsilon_0} \int \rho(\mathbf{x}') G_N d^3 \mathbf{x}' + \frac{1}{4\pi} \oint \left(G_N \frac{d\Phi}{dn'} \right) da' + \langle \Phi \rangle_S$$

where the last term is the average potential over the whole surface and can be made to vanish with a surface at infinity.

- It is amazing to see that as long as we can find the right Green function G for a particular problem, we can immediately write down the solution to the problem using a straightforward application of the integral equations above. We learn in detail later on how to find the right Green function.

4. Energy Density

- If a test point charge is brought in from infinity and the potential at infinity is set to zero, the total work done (also the total potential energy) is: $W = q_1 \Phi$

$$W = \frac{q_1}{4\pi\epsilon_0} \int \frac{\rho(\mathbf{x}')}{|\mathbf{x} - \mathbf{x}'|} d\mathbf{x}'$$

- If we were to bring multiple charges in from infinity and assemble a charge distribution, their total potential energy would be:

$$W = \frac{1}{8\pi\epsilon_0} \int \int \frac{\rho(\mathbf{x})\rho(\mathbf{x'})}{|\mathbf{x}-\mathbf{x'}|} d\mathbf{x'} d\mathbf{x}$$

- The extra ½ factor arises from the fact that the only work done is that by the charge distribution on itself while being assembled. For instance, halfway through the assembling process, the next bit of charge being brought is affected by the electric field of only half of the final total charge distribution.

- The potential energy can also be thought of as held in the electric field instead of in the charge distribution.

- Using Coulomb's Law and the Poisson Equation:

$$W = -\frac{\epsilon_0}{2} \int \Phi \nabla^2 \Phi \, d \mathbf{x}$$

- Integration by parts yields:

$$W = \frac{\epsilon_0}{2} \int |\nabla \Phi|^2 d\mathbf{x}$$
$$W = \frac{\epsilon_0}{2} \int |\mathbf{E}|^2 d\mathbf{x}$$

- The integrand can be identified as the energy density:

$$w = \frac{\epsilon_0}{2} |\mathbf{E}|^2$$

5. Computational Approaches

At UMass Lowell, research is currently being done on Quantum Cascade Lasers (QCL)
In order to predict QCL phenomena, the one-dimensional Poisson equation must be solved computationally, where the initial conditions are known:

$$\frac{d^2\Phi(z)}{dz^2} = -\frac{1}{\epsilon_0}\rho(z)$$

- Define a new variable $\Phi_2(z) = \frac{d \Phi(z)}{d z}$ so that the problem reduces down to two coupled first-order differential equations:

$$\frac{d \Phi_2(z)}{dz} = -\frac{1}{\epsilon_0} \rho(z)$$
$$\frac{d \Phi(z)}{d z} = \Phi_2(z)$$

- Use the finite difference expansion of the derivative:

$$\begin{split} & \frac{\Phi_{2}(z_{i+1}) - \Phi_{2}(z_{i})}{z_{i+1} - z_{i}} = -\frac{1}{\epsilon_{0}} \rho(z_{i}) \\ & \frac{\Phi(z_{i+1}) - \Phi(z_{i})}{z_{i+1} - z_{i}} = \Phi_{2}(z_{i}) \end{split}$$

-Solve for the next terms as functions of the previous terms to get the iteration equations:

$$\Phi_{2}(z_{i+1}) = \Phi_{2}(z_{i}) + (z_{i+1} - z_{i}) \left(-\frac{1}{\epsilon_{0}} \rho(z_{i}) \right)$$
$$\Phi(z_{i+1}) = \Phi(z_{i}) + (z_{i+1} - z_{i}) \left(\Phi_{2}(z_{i}) \right)$$

- The algorithm starts with the known initial conditions:

$$\Phi(z_0) = A$$
 and $\Phi_2(z_0) = \left[\frac{d \Phi}{dz}\right]_{z_0} = B$

and then uses the iteration equations to get the values at the point z_i and so on until the functions are solved for all points desired.

- It should be noted that if the boundary conditions are known instead of the initial conditions, then initial conditions must be guessed and then the guess refined until the boundary conditions are met.

- Typically, more accurate expansions of the derivative are used then the one shown here, but the same general approach is used.

6. Relaxation Method

- What if instead of the one-dimensional Poisson equation, we need to solve the twodimensional Poisson equation:

$$\frac{\partial^2 \Phi(x, y)}{\partial x^2} + \frac{\partial^2 \Phi(x, y)}{\partial y^2} = -\frac{1}{\epsilon_0} \rho(x, y)$$

- Again expand each derivative using finite differences.

$$\begin{split} \frac{\partial}{\partial x} & \left(\frac{\Phi(x_{i+1}, y_i) - \Phi(x_i, y_i)}{x_{i+1} - x_i} \right) + \frac{\partial}{\partial y} \left(\frac{\Phi(x_i, y_{i+1}) - \Phi(x_i, y_i)}{y_{i+1} - y_i} \right) = -\frac{1}{\epsilon_0} \rho(x_i, y_i) \\ & \left(\frac{\Phi(x_{i+1}, y_i) - \Phi(x_i, y_i)}{(x_{i+1} - x_i)(x_i - x_{i-1})} \right) - \left(\frac{\Phi(x_i, y_i) - \Phi(x_{i-1}, y_i)}{(x_{i+1} - x_i)(x_i - x_{i-1})} \right) \\ & + \left(\frac{\Phi(x_i, y_{i+1}) - \Phi(x_i, y_i)}{(y_{i+1} - y_i)(y_i - y_{i-1})} \right) - \left(\frac{\Phi(x_i, y_i) - \Phi(x_i, y_{i-1})}{(y_{i+1} - y_i)(y_i - y_{i-1})} \right) = -\frac{1}{\epsilon_0} \rho(x_i, y_i) \end{split}$$

- Make a uniform grid of (x, y) points so that the distance between them is always the same. Call this distance the step size *h*.

$$\Phi(x_{i+1}, y_i) + \Phi(x_{i-1}, y_i) + \Phi(x_i, y_{i+1}) + \Phi(x_i, y_{i-1}) - 4\Phi(x_i, y_i) = -\frac{1}{\epsilon_0}h^2\rho(x_i, y_i)$$

- Solve for the central point (x_i, y_i) :

$$\Phi(x_{i}, y_{i}) = \frac{1}{4} \left(\Phi(x_{i+1}, y_{i}) + \Phi(x_{i-1}, y_{i}) + \Phi(x_{i}, y_{i+1}) + \Phi(x_{i}, y_{i-1}) + \frac{1}{\epsilon_{0}} h^{2} \rho(x_{i}, y_{i}) \right)$$

- If the charge is zero at a point, we see that the potential at any point is just the average of its neighboring points (the point above it, the point below it, the point to its left, and the point to its right). The potential is said to relax to the average value.

- This is very easy to implement computationally. We just permanently fix the potential along the boundary of the region at the boundary values inputted in, then continually find the potential at all points as the average of its neighbors plus the charge term.