Boundary Conditions in SIMION

Giglio Eric
Centre de Recherche sur les Ions, les Matériaux et la Photonique (CIMAP), F-14000, Caen

giglio@ganil.fr

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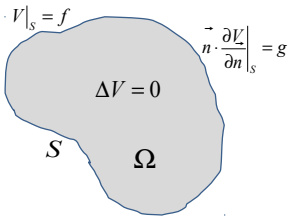
Introduction

By pressing the *refine* button, SIMION calculates the electric potential all over the empty space inside a given box, which may contain electrodes at a given voltage, by solving the Laplace equation

$$\nabla^2 V(\vec{r}) = 0 \quad . \tag{1}$$

For the solution to exist and to be unique, the potential must fulfil certain conditions on the boundaries enclosing that space. Indeed, boundary conditions are what constrain the solution to the Laplace equation, which otherwise has an infinite number of solutions [1]. The boundary conditions on the Laplace equation typically take the form of specifying the values of potential or its derivative over the enclosing surface. Theorems, that tell us what types of boundary conditions give unique solutions to such equations are called uniqueness theorems.

Uniqueness Theorems



Let us imagine that we have discovered a solution to the Laplace equation subject to certain boundary conditions on S by following some procedure. Having found one solution, we would like to know whether this solution is unique. If yes, then the problem is completely solved.

First uniqueness theorem: The solution to the Laplace Equation in some volume is uniquely determined if the potential voltage is specified on the boundary surface. This is the so-called **Dirichlet Boundary Conditions** . Mathematically, this writes:

$$\nabla^2 V(\vec{r}) = 0 \qquad \vec{r} \in \Omega \tag{2}$$
$$V(\vec{r}) = f(\vec{r}) \qquad \vec{r} \in S \tag{3}$$

[1] extracted from SIMION 8.1 Supplemental Documentation, http://simion.com/info/

where V stands for the electric potential in the volume Ω and f for the specified potential on the boundary S.

Second uniqueness theorem The Laplace equation still has a unique solution if part of this boundary is instead defined by a **Neumann Boundary Condition**, in which the normal derivative of the potential (not the potential itself) on the boundary is specified. Let the boundary S be divided into two pieces S_1 and S_2, such that $S = S_1 + S_2$. The second uniqueness theorem allows then to write:

$$\nabla^2 V(\vec{r}) = 0 \qquad \vec{r} \in \Omega \tag{4}$$
$$V(\vec{r}) = f(\vec{r}) \qquad \vec{r} \in S_1 \tag{5}$$
$$\frac{\partial V}{\partial n}(\vec{r}) = g(\vec{r}) \qquad \vec{r} \in S_2 \tag{6}$$

where $\frac{\partial V}{\partial n}$ stands for the normal derivative of the potential pointing outside. Thus on S_1, the boundary condition (BC) is given by Dirichlet boundary condition, while on S_2 it is given by the Neumann one. It is important to understand here that at a given boundary, let us say S_1, one cannot use at the same time both Dirichlet and Neumann BC. They are mutually exclusive. An exception are Robin BC for which the boundaries are instead defined by a linear combination of the Neumann and Dirichlet BC. This case however does not occur in electrostatics and will no longer be discussed here.

Integral Formulation of the Laplace Equation

In order to understand why the solution is uniquely defined by Dirichlet or Neumann BC, we can look at the integral formulation of the Laplace equation. To do so, we first introduce the Green function defined as

$$G(\vec{r},\vec{r}') = \frac{1}{|\vec{r}-\vec{r}'|}, \quad \nabla^2_{r'} G(\vec{r},\vec{r}') = -4\pi\delta(\vec{r},\vec{r}') \tag{7}$$

It represents the Coulomb potential of a discrete particle at the position $\vec{r}'$. Then we introduce the Green theorem which links a volume integral containing the Laplace operator to a surface integral over the boundaries of the volume, namely

$$\int_\Omega (G\nabla^2 V - V\nabla^2 G) d^3r = \int_S (G\vec{\nabla}V - V\vec{\nabla}G)\cdot\vec{n}\, ds \tag{8}$$

Injecting equation (1) and (7) into (8) yields eventually the integral formulation of the Laplace equation

$$4\pi V(\vec{r}) = \int_S (G\frac{\partial V}{\partial n} - V\frac{\partial G}{\partial n}) \cdot \vec{n}\, ds \quad \vec{r} \in \Omega/S \quad . \quad (9)$$

This equation just refers to the potential and its normal derivative on the surface to define the potential inside the volume. This rather surprising result is not a solution to a problem with boundary conditions as given by (2,3) or (4-6), but a simple integral formulation, because an arbitrary specification of V and $\frac{\partial V}{\partial n}$ on the surface (Cauchy boundary condition) would overdetermine the problem and yield no (or only trivial) solutions. For completeness, let me specify that by choosing a different Green function than in (7), namely one that is zero on the surface S,

$$G(\vec{r}, \vec{r}') = 0 \quad \vec{r} \in S, \quad \nabla^2_{r'} G(\vec{r}, \vec{r}') = -4\pi\delta(\vec{r}, \vec{r}') \quad , \quad (10)$$

then equation (10) can be used to solve the Laplace equation with Dirichlet boundary conditions. However, finding G, satisfying the above conditions for an arbitrary boundary shape, is very difficult. This method is mainly used for very simple geometries. The integral formulation however shows that a mutually *exclusive* mix of Dirichlet and Neumann boundary conditions uniquely defines the potential inside a given volume.

Boundary Conditions at the edges of the grid box in SIMION

In SIMION, the grid points on the boundaries (edges) of the volume box need special care. If all those points are well defined electrodes, than the Laplace problem is fully defined and can be uniquely solved by SIMION. However, non-electrode points on box edges are treated by default as zero Neumann BC, regardless if mirroring is defined. A zero Neumann BC imposes the constraint that the directional derivative normal to some boundary surface $\frac{\partial V}{\partial n}$ is zero. There are a number of occasions where zero Neumann BC can occur in a system. Zero Neumann BC commonly occur over a plane of mirror symmetry, which is to say that the potentials at all pairs of points mirrored across a plane are identical. For example, an $x = 0$ mirror plane implies $V(x, y, z) \equiv V(-x, y, z)$ for all points (x, y, z) in space. The derivative might not exist on points on the mirror plane that also happen to have Dirichlet BC because there the potential gradient (negative field) may be discontinuous [2].

In order to illustrate the effect of non-electrode edge points on the Laplace solution, we give several examples which may occur frequently in realistic studies. We start with a finite wire hold at V_0, centred on the symmetry axis of a cylindrical box, for which the left surface disc is an electrode hold at zero potential, as shown in the inset of figure 1. The other edge points are not defined. SIMION replaces then the non-electrode

[2]Extracted from SIMION 8.1 Supplementary Documentation

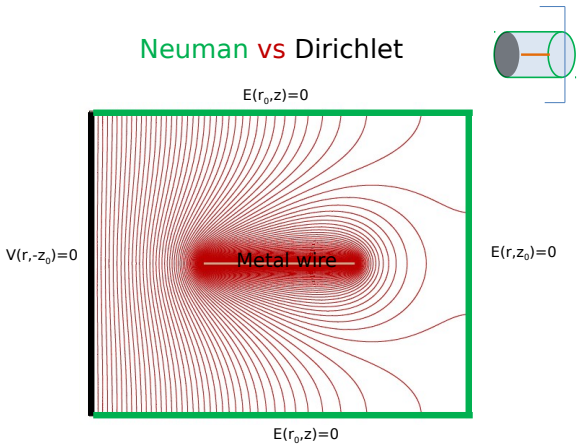


Figure 1: Finite wire at given potential V_0 inside a cylindrical box with mixed Dirichlet (black) and Neumann (green) boundary conditions. Red lines are equipotentials. At the zero Neumann boundary surfaces, the equipotentials run normal to surface, while they are tangent to the Dirichlet boundary surface.

points at the edge by a zero Neumann BC. Figure 1 gives a cut through a symmetry plane containing the symmetry axis. The left black border stands for the zero potential Dirichlet BC, while the green borders are zero Neumann BC. The red curves are equipotentials. Interestingly, for all boundary surfaces defined by zero Neumann BC, the equipotentials run normal to surface, while they are tangent to boundary surfaces defined by Dirichlet BC. *This property allows to recognize immediately what boundary conditions have been used at the boundary surfaces of the grid box for a given solution.*

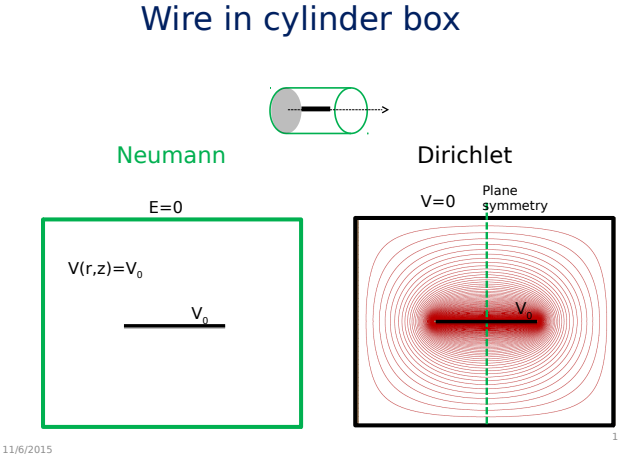


Figure 2: Finite wire at given potential V_0 inside a cylindrical box. *Left*; with zero Neumann boundary conditions (green border). *Right*; with zero Dirichlet boundary condition (black border). Red curves are equipotentials.

In special cases, not defining the potential on the edges, may lead to unexpected (wrong) solutions. This

is illustrate by figure 2, which again represents a wire hold at a given potential. For the left panel, the edge points were not defined. One would expect that the potential decreases like $1/r$. Instead, SIMION replaces the non-electrode edge points by a zero Neumann condition, resulting into a constant potential all over the space. To avoid this, Dirichlet BC must be given by defining explicitly the potential at the boundary of the box (right panel). The $1/r$ behaviour can be recovered approximately by using a very large box with zero potential at the edges.

Another typical example which may occur frequently is a set of parallel plates, with one being grounded and the other hold at a given potential say 1V, as shown in figure 3. One may assume here that the potential at the boundaries of the box do not need to be given, as the electric field in between the plates is largely unaffected by the surroundings. However, this is true only if the distance between the plates is small compared to the dimension of the box. Otherwise, the equipotentials at the entrance of the two plates. are affected by the boundary condition at the edges of the box. This is highlighted by comparing in figure 3 the left panel using Neumann BC to the right one, using Dirichlet BC. The equipotentials at the entrance (and exit) are clearly different and may affect ion trajectories.

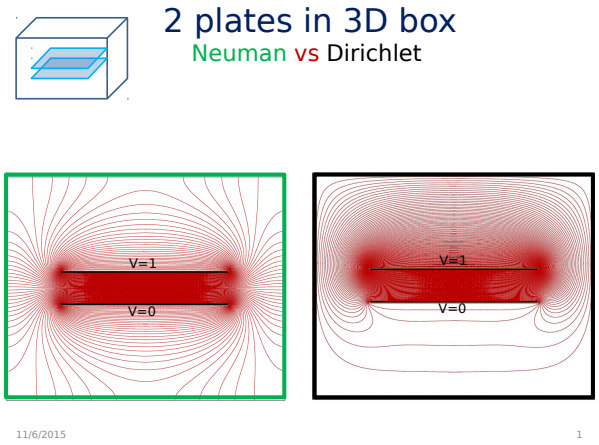


Figure 3: Two plates in a cubic box. *Left*; with zero Neumann boundary conditions (green border). *Right*; with zero Dirichlet boundary condition (black border). Red curves are equipotentials.

Conclusion

The paper tries to illustrate the importance of properly defining the boundaries conditions on the surface enclosing the volume of interest. If parts of the surface are non-electrodes points, then zero Neumann BC are assumed by SIMION for these points. Now, Zero Neumann BC define mirror planes. If this was not the intention of the user, than the solution obtained by SIMION may be not the expected one and lead to inaccurate simulations.