Boundary Conditions in SIMION

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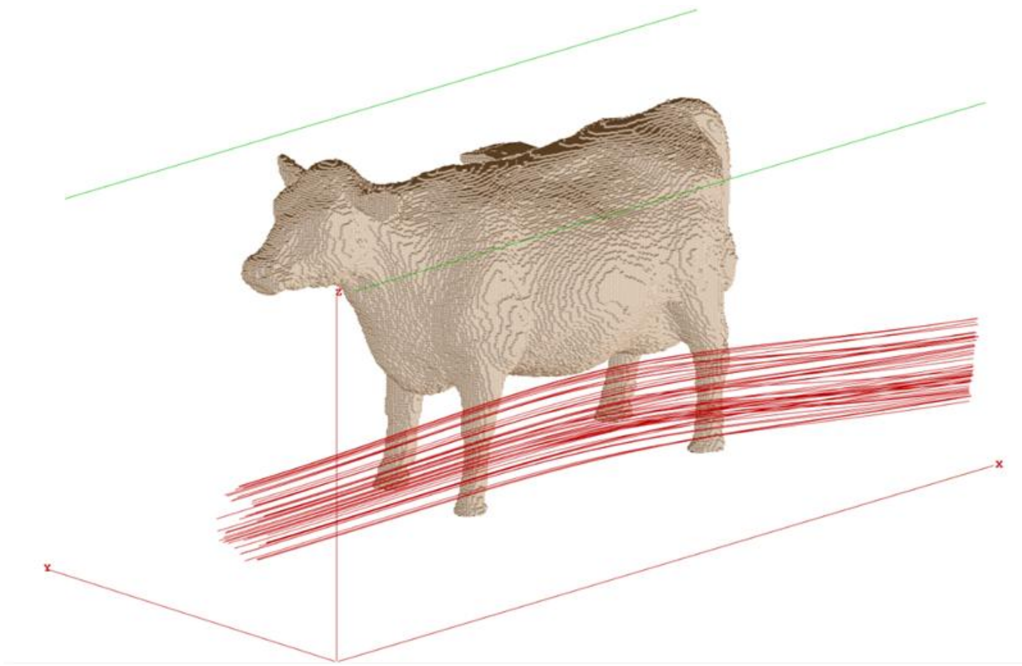
SIMION Users Meeting



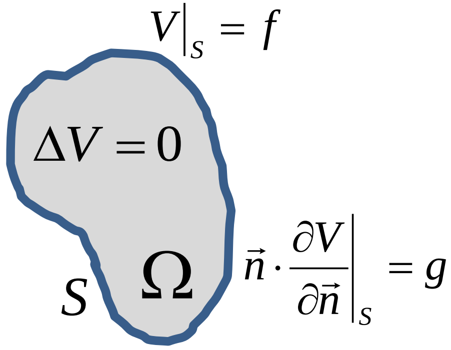
Boundary Conditions in SIMION

MOTIVATION

- By doing a *refine*, SIMION calculates the electric potential *V* all over the space inside a given box, by solving the Laplace equation: $\Delta V=0$

- To obtain the accurate electric potential, proper attention must be paid to *boundary conditions*. "Boundary conditions are what constrain the solution to the Laplace equation, which otherwise have an infinite number of solutions." *SIMION 8.1 Supplemental Documentation*

Solution to a Boundary Value Problem

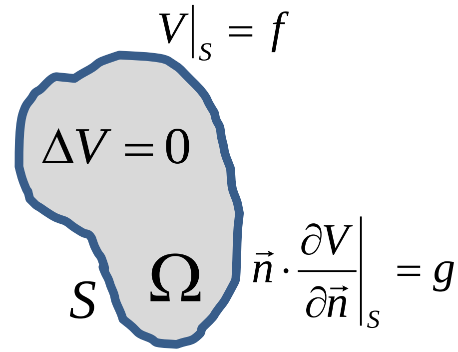


The solution to the Laplace equation in some volume ***Ω*** is uniquely determined if the potential **xor** its normal derivative is specified on the boundary ***S***

DEMONSTRATION

Solution to a Boundary Value Problem

The solution to the Laplace equation in some volume $\boldsymbol{\Omega}$ is uniquely determined if the potential **xor** its normal derivative is specified on the boundary $\boldsymbol{S}$



DEMONSTRATION

- We introduce the particular Green function: $G_0 = \dfrac{1}{4\pi|\vec{x} - \vec{x}'|}$, $\Delta' G_0 = -\delta(\vec{x} - \vec{x}')$

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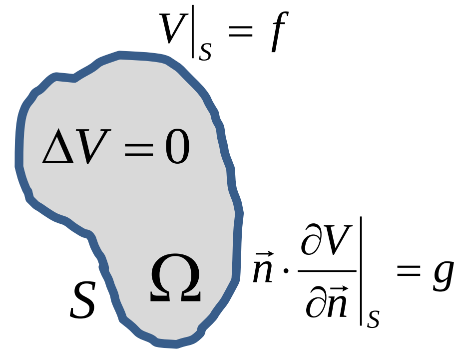

DEMONSTRATION

- We introduce the particular Green function: $G_0 = \dfrac{1}{4\pi|\vec{x} - \vec{x}'|}$, $\Delta' G_0 = -\delta(\vec{x} - \vec{x}')$
- We introduce the Green theorem: $\int_\Omega \left(G_0 \Delta V - V \Delta G_0\right) d^3x = \oint_S \left(G_0 \dfrac{\partial V}{\partial \vec{n}} - V \dfrac{\partial G_0}{\partial \vec{n}} \right) d\vec{s}$

Solution to a Boundary Value Problem

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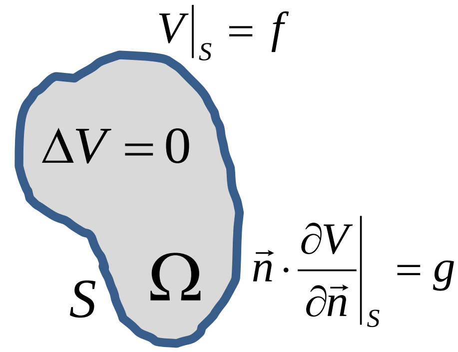

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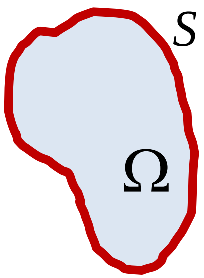
- We transform the differential equation of Laplace into an integral equation :

$$V(\vec{x}) = \oint_S G_0(\vec{x} - \vec{x}') \boxed{\frac{\partial V(\vec{x}')}{\partial n'}} ds' - \oint_S \boxed{V(\vec{x}')} \frac{\partial G_0(\vec{x} - \vec{x}')}{\partial n'} ds', \quad \forall \vec{x} \in \Omega / S$$

Integral formulation of Laplace equation

DEMONSTRATION (end)



- The potential inside the volume *Ω/S*

$$V(\vec{x}) = \oint_S G_0(\vec{x}-\vec{x}')\frac{\partial V(\vec{x}')}{\partial \vec{n}'}d\vec{s}' - \oint_S V(\vec{x}')\frac{\partial G_0(\vec{x}-\vec{x}')}{\partial \vec{n}'}d\vec{s}', \quad \forall \vec{x} \in \Omega / S$$

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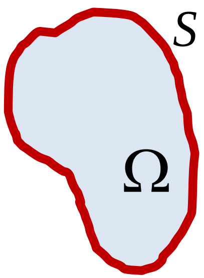

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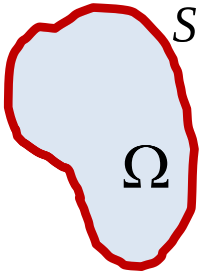
- The potential on the boundary S

$$\frac{1}{2}V(\vec{x}) = \oint_S G_0(\vec{x}-\vec{x}')\frac{\partial V(\vec{x}')}{\partial \vec{n}'}d\vec{s}' - \oint_S V(\vec{x}')\frac{\partial G_0(\vec{x}-\vec{x}')}{\partial \vec{n}'}d\vec{s}', \quad \forall \vec{x} \in S$$

$V(\vec{x}')\big|_S$ and $\left.\dfrac{\partial V(\vec{x}')}{\partial \vec{n}'}\right|_S$ are linked at the boundary. One is deduced from the other ➡ (BEM)

Integral formulation of Laplace equation



DEMONSTRATION (end)

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$V(\vec{x}')\big|_S$ and $\left.\frac{\partial V(\vec{x}')}{\partial \vec{n}'}\right|_S$ are linked at the boundary. One is deduced from the other ⇒ (BEM)

⇒ It is sufficient to specify an **arbitrary** value for potential or its normal derivative at the boundary, but not both simultaneously

Solution to a Boundary Value Problem

$$\boxed{\Delta V(\vec{x}) = 0 \quad \vec{x} \in \Omega}$$

Dirichlet Boundary conditions

Neumann Boundary conditions

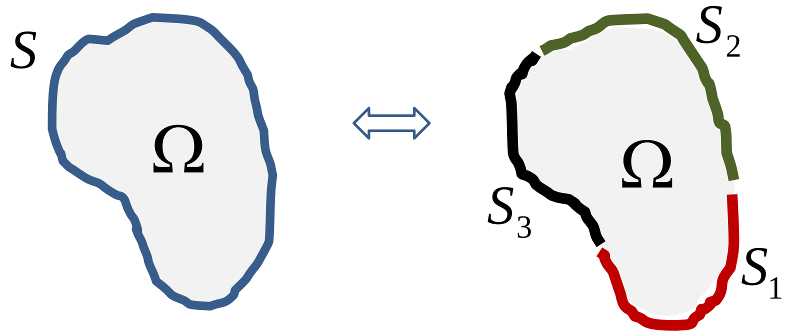
$$\boxed{V(\vec{x}) = f(\vec{x}) \quad \vec{x} \in S}$$

$$\boxed{\vec{n} \cdot \frac{\partial V(\vec{x})}{\partial \vec{n}} = k(\vec{x}) \quad \vec{x} \in S}$$

SIMION

- Dirichlet boundary conditions are typically voltages on the surfaces of electrodes
- Neumann boundary conditions are generally (k=0) , corresponding to planes of mirror symmetry or by By default, non-electrode PA edges are taken as zero Neumann boundary conditions

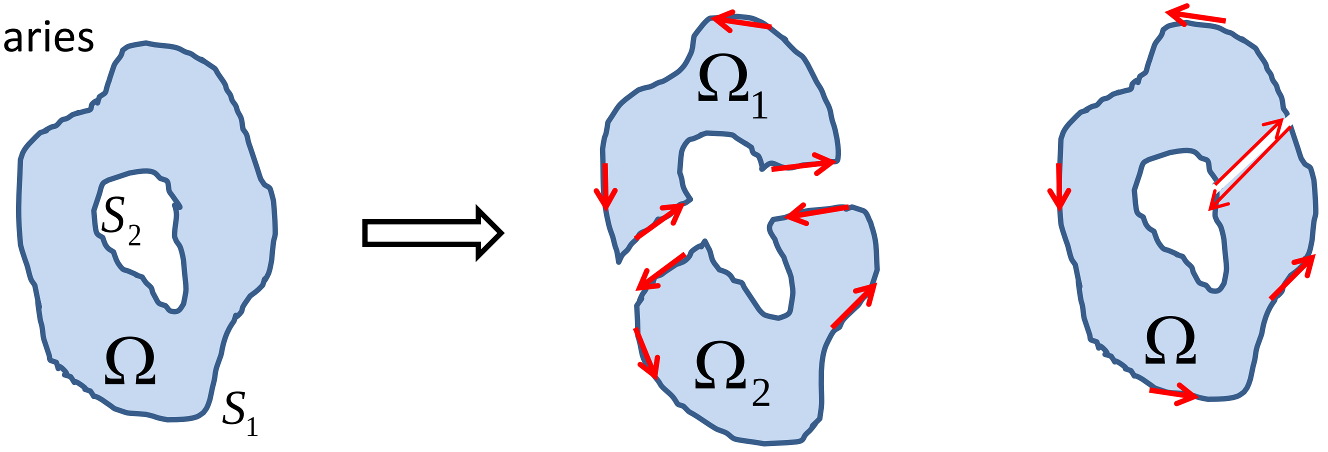
Mixed Boundary Conditions



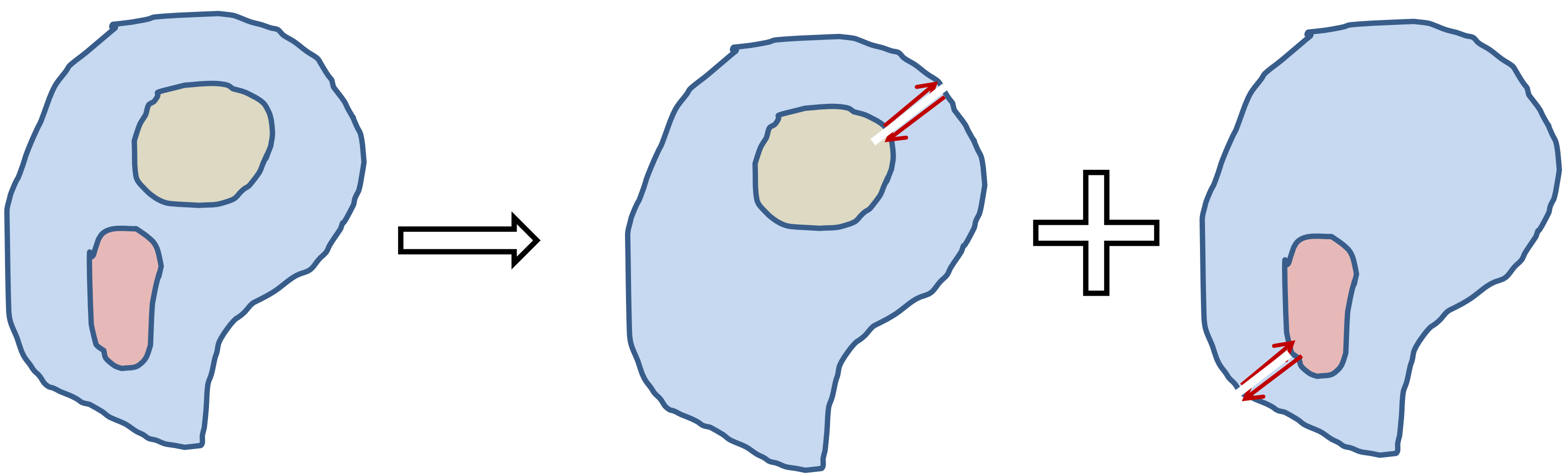
$$\Delta V(\vec{x}) = 0 \quad \vec{x} \in \Omega \quad \text{with} \quad \left| \begin{array}{ll} V(\vec{x}) = f_1(\vec{x}) & \vec{x} \in S_1 \\ V(\vec{x}) = f_2(\vec{x}) & \vec{x} \in S_2 \\ \vec{n} \cdot \dfrac{\partial V(\vec{x})}{\partial \vec{n}} = k(\vec{x}) & \vec{x} \in S_3 \end{array} \right.$$

Special Boundaries

- Disjoint Boundaries



- Multiple Disjoint Boundaries

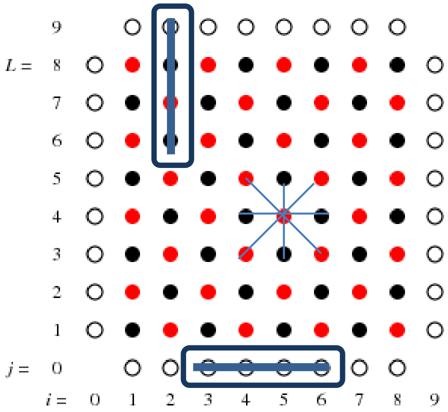


Technical approaches

- Boundary Element Method (BEM)

  -> Charged Particle Optics (CPO) http://www.electronoptics.com/:

- Iterative Relaxation Method in SIMION



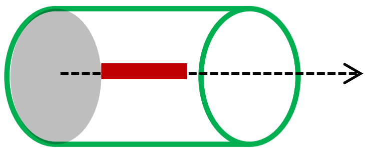
$$V_{i,j}^{n+1} = \frac{4}{5}\left\langle V^n \right\rangle_R + \frac{1}{5}\left\langle V^n \right\rangle_B$$

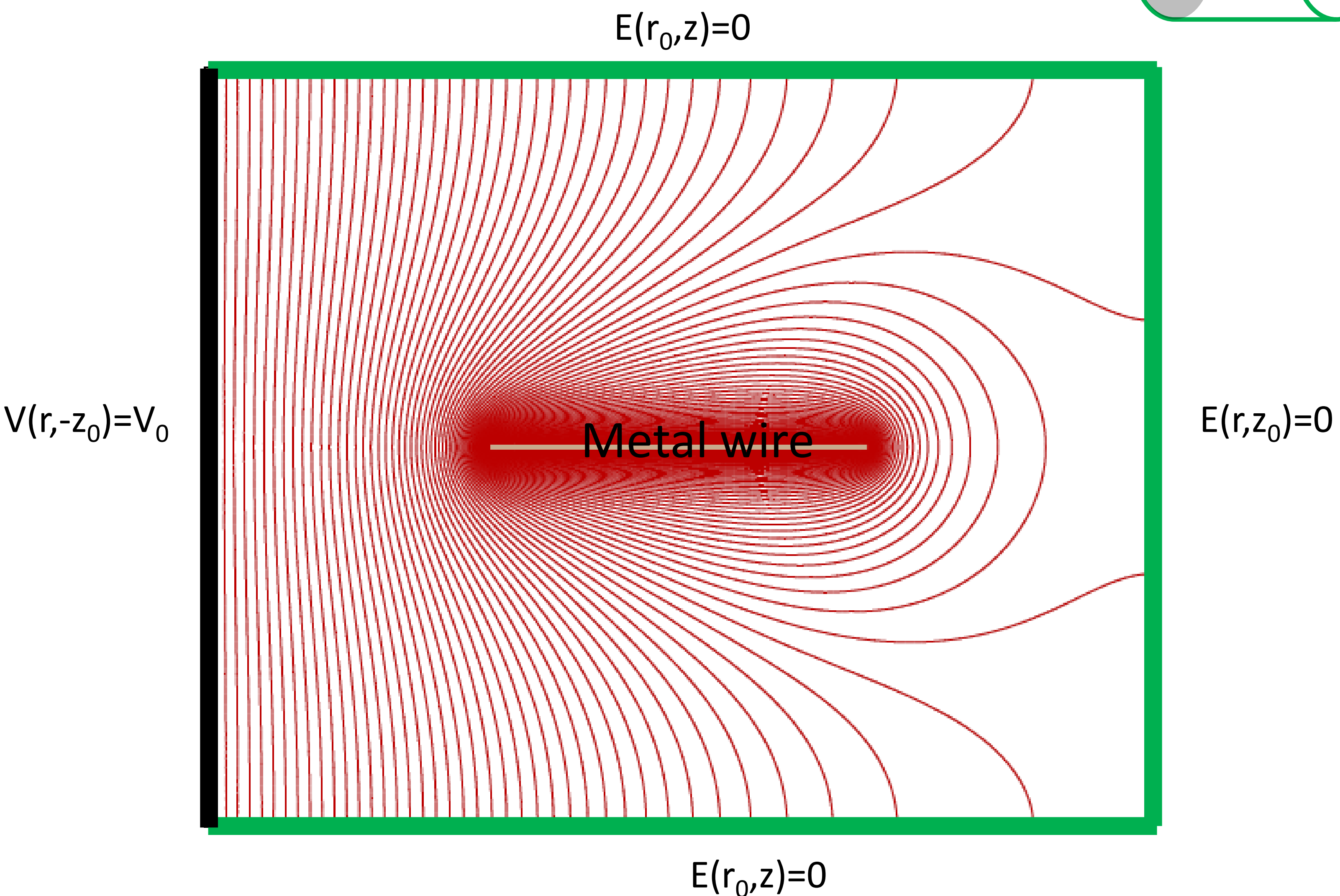
If not specified by a Dirichlet condition, the solution on the border of the volume satisfies the Neumann condition

$$\vec{n} \cdot \frac{\partial V(\vec{x})}{\partial \vec{n}} = 0$$

Wire in cylinder box

Neuman vs Dirichlet





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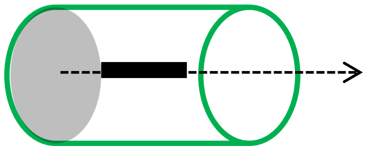
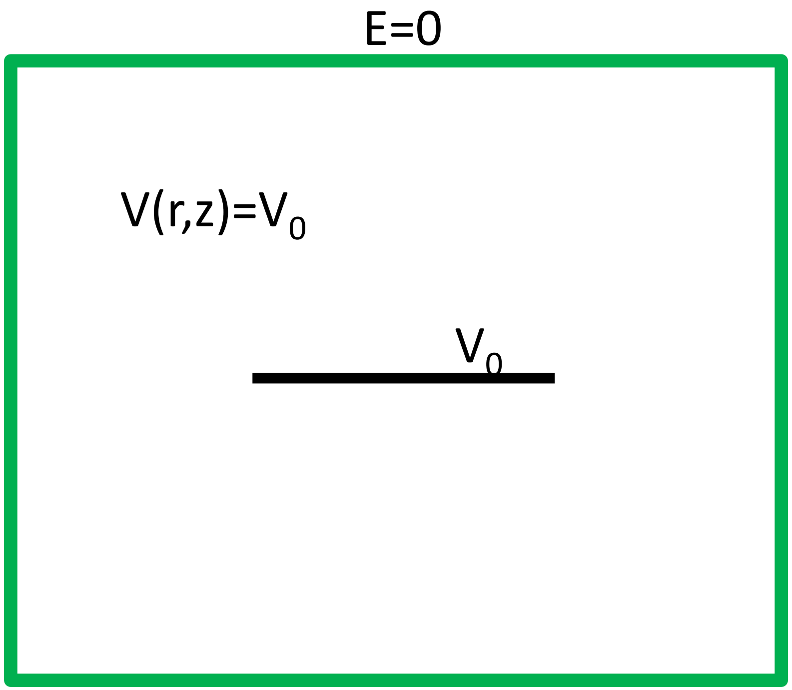
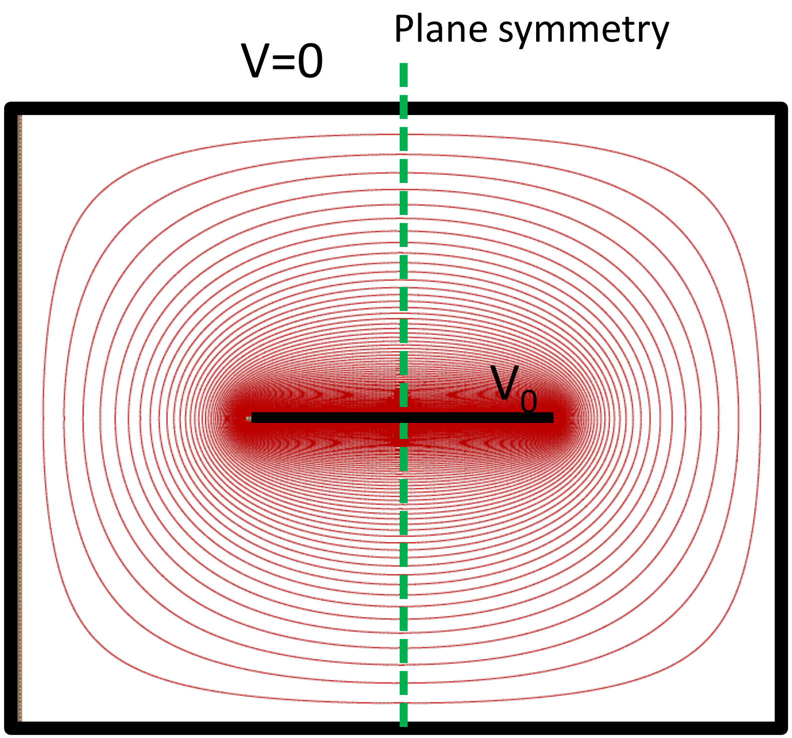
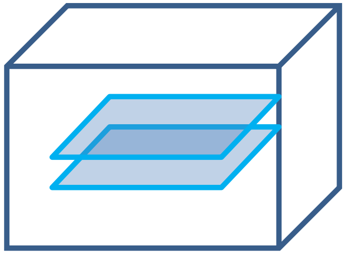


Neumann



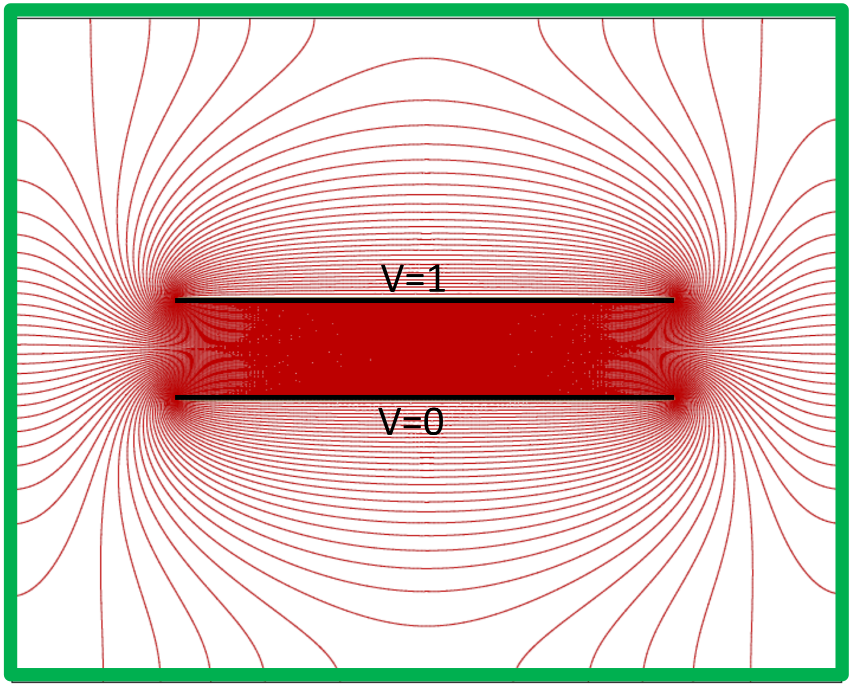
Dirichlet

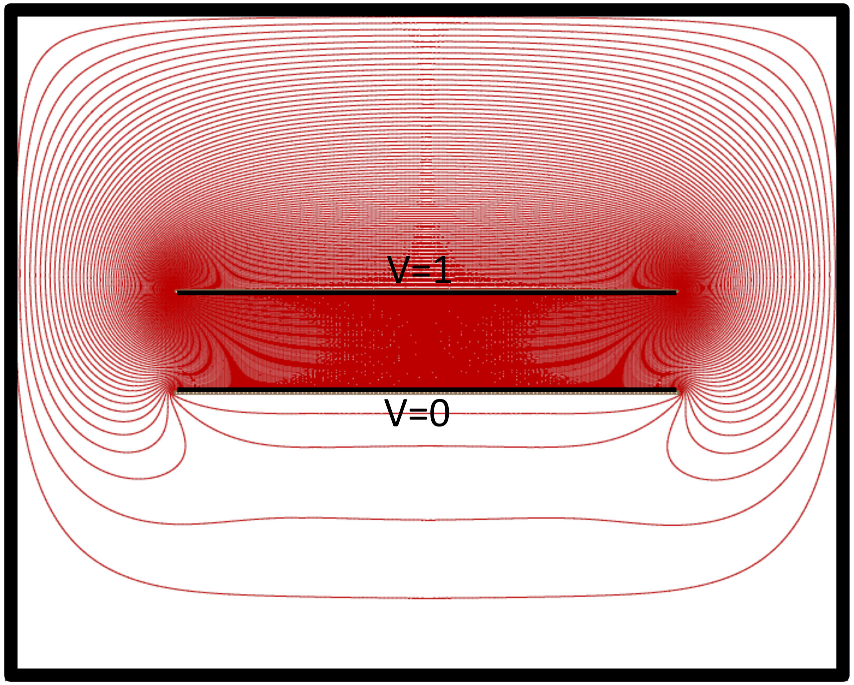




2 plates in 3D box

Neuman vs Dirichlet





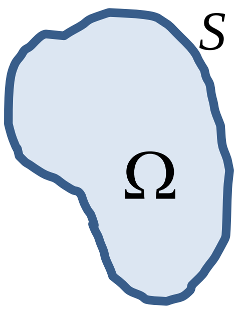
CONCLUSION

Never forget to specify all the boundary conditions on the boundary of the box

Thank You for your attention

Integral formulation of Laplace equation

DEMONSTRATION (suite)



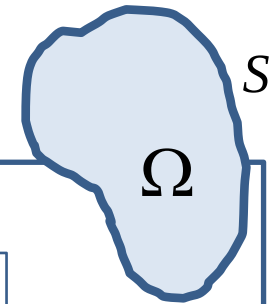
$$V(\vec{x}) = \oint_S G_0(\vec{x}-\vec{x}')\boxed{\frac{\partial V(\vec{x}')}{\partial \vec{n}'}}d\vec{s}' - \oint_S \boxed{V(\vec{x}')}\frac{\partial G_0(\vec{x}-\vec{x}')}{\partial \vec{n}'}d\vec{s}', \quad \forall \vec{x} \in \Omega / S$$

The potential inside the volume Ω only depends on the potential **and** its normal derivative at the boundary

! One cannot specify for the same boundary element simultaneously an **arbitrary** value for the potential and for its normal derivative (*Cauchy conditions*), which over determines the problem and the equation has then no non-trivial solution.

- Indeed, $V(\vec{x}')\big|_S$ and $\left.\frac{\partial V(\vec{x}')}{\partial \vec{n}'}\right|_S$ are linked at the boundary, and one is deduced from the other
- It is sufficient to specify the potential xor its normal derivative at the boundary

Solution to a Boundary Value Problem



DEMONSTRATION (end)

- General Green function:

$$G(\vec{x},\vec{x}') = \frac{1}{4\pi|\vec{x}-\vec{x}'|} + h(\vec{x},\vec{x}') \quad \text{with} \quad \boxed{\Delta' h(\vec{x},\vec{x}') = 0} \;\Rightarrow\; \boxed{\Delta' G(\vec{x},\vec{x}') = -\delta(\vec{x}-\vec{x}')}$$

$$\boxed{V(\vec{x}) = \oint_S G(\vec{x},\vec{x}')\frac{\partial V(\vec{x}')}{\partial \vec{n}'}d\vec{s}' - \oint_S V(\vec{x}')\frac{\partial G(\vec{x},\vec{x}')}{\partial \vec{n}'}d\vec{s}'}$$

- If we choose h(x,x') such as

$$\boxed{G(\vec{x},\vec{x}') = 0 \quad \vec{x}' \in S} \;\Rightarrow\; \boxed{V(\vec{x}) = -\oint_S V(\vec{x}')\frac{\partial G(\vec{x},\vec{x}')}{\partial \vec{n}'}d\vec{s}'}$$

Dirichlet

$$\boxed{\vec{n}\cdot\frac{\partial G(\vec{x},\vec{x}')}{\partial \vec{n}'} = 0 \quad \vec{x}' \in S} \;\Rightarrow\; \boxed{V(\vec{x}) = \oint_S G(\vec{x},\vec{x}')\frac{\partial V(\vec{x}')}{\partial \vec{n}'}d\vec{s}'}$$

Neumann

h(x,x') depends on the geometry of the problem!