TP2: Poisson’s equation

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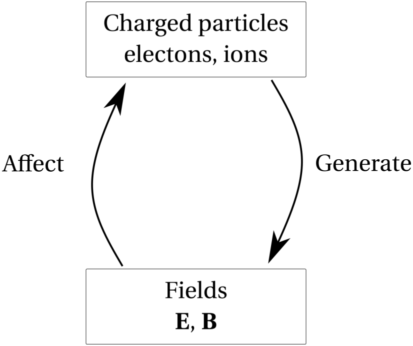
TC5 : TPs sur les méthodes numériques et simulations
Séances du 23 et 26 novembre 2020, En distanciel.

Outline

- For which plasma studies do we need to solve Poisson's equation and not Maxwell equations?
- The Poisson Equation
- Work to be done

For which plasma studies do we need to solve Poisson's equation?

Principle of plasma physics



For which plasma studies do we need to solve Poisson's equation?

The Electrostatic assumtion can be made for low-temperature plasmas:

- Electrostatic Particle-In-Cell (PIC) simulations for low-pressure plasmas
- Fluid simulations of low-temperature plasmas at atmospheric pressure

$\rightarrow$ back-up slides for details

For which plasma studies do we need to solve Poisson's equation?

Maxwell's equations with electrostatic hyothesis:

$$
\begin{aligned}
\text{rot}\ \vec{E} &= -\frac{\partial \vec{B}}{\partial t} = 0 \\
\text{div}\ \vec{B} &= 0 \\
\text{rot}\ \vec{B} &= \mu_0(\epsilon_0 \frac{\partial \vec{E}}{\partial t} + \vec{j}) = 0 \\
\text{div}\ \vec{E} &= \frac{\rho}{\epsilon_0}
\end{aligned}
\tag{1}
$$

$\Rightarrow$ Poisson's equation

$$
\text{div}\ \vec{E} = -\Delta\phi = \frac{\rho}{\epsilon_0} \tag{2}
$$

For which plasma studies do we need to solve Poisson's equation?

Maxwell's equations with electrostatic hyothesis:

$$\begin{aligned}
\text{rot } \vec{E} &= -\frac{\partial \vec{B}}{\partial t} = 0 \\
\text{div } \vec{B} &= 0 \\
\text{rot } \vec{B} &= \mu_0(\epsilon_0 \frac{\partial \vec{E}}{\partial t} + \vec{j}) = 0 \\
\text{div } \vec{E} &= \frac{\rho}{\epsilon_0}
\end{aligned} \tag{1}$$

$\Rightarrow$ Poisson's equation

$$\text{div } \vec{E} = -\Delta \phi = \frac{\rho}{\epsilon_0} \tag{2}$$

Outline

- For which plasma studies do we need to solve Poisson's equation?
- The Poisson Equation
- Work to be done : Solve Poisson's equation in 1D and then in 2D

Poisson Equation $\Delta\phi = f$ is found several times in physics :

- Newtonian Gravity : $\mathrm{div}\,\vec{g} = -\Delta\phi = 4\pi G\rho$
- Incompressible fluid dynamics : $\Delta\vec{p} = -\rho(\nabla\vec{v})$
- Heat equation : $\Delta u = \alpha\frac{\partial u}{\partial t}$
- And so on

Important equation, but **Why so special ?**
$\Rightarrow$ It is *Elliptic*

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Poisson's equation discretization

In a general plasma:

$$\varepsilon_0 \boldsymbol{\nabla} \cdot (\varepsilon_{\rm r} \boldsymbol{\nabla} V) = -q_{\rm e}(n_{\rm p} - n_{\rm n} - n_{\rm e})$$

In this work, the source term will be defined as ρ

$$\varepsilon_0 \boldsymbol{\nabla} \cdot (\varepsilon_{\rm r} \boldsymbol{\nabla} V) = -\rho$$

We propose the following exercices for the TP2 :

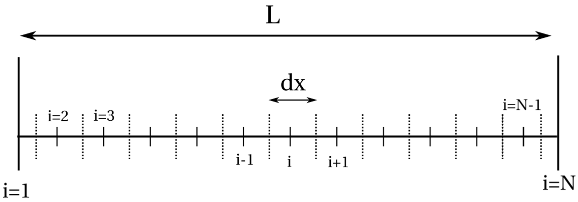
- Exercice 1 : 1D poisson solver for a plasma between metallic walls ($\varepsilon_{\rm r} = 1$)
- Exercice 1bis : 1D poisson solver: performances and nummerical aspects
- Exercice 2 : 2D poisson solver for a plasma between metallic walls
- Exercice 3 (optional) : 1D poisson solver for a plasma between metallic walls covered by dielectric walls

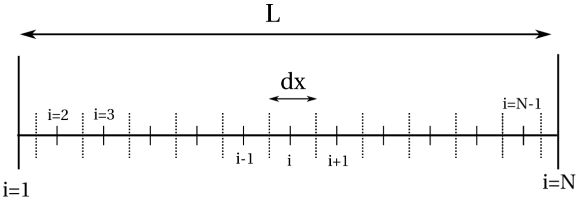
Poisson's equation in 1D

In 1D:

$$\varepsilon_0 \nabla_x \cdot (\varepsilon_{\mathrm{r}} \nabla_x V(x)) = -\rho(x)$$

For the numerical integration : we propose to use a finite volume approach. This approach is conservative
In 1D for a uniform mesh finite volume, and finite difference approaches give the same discretized form.

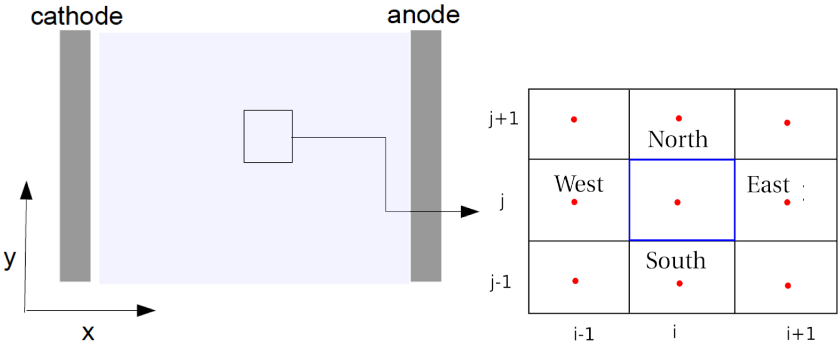




- We discretize the domain $x = [0, Lx]$ in $N - 2$ cells of size dx and 2 half-cells
- The center of each cell is defined by the index i
- The unknown potential $V(x)$ becomes V_i and the source term $\rho(x)$ becomes ρ_i
- The unknowns are mean values at the center of cells
- The center of the cell $i = 1$ correspond to $x = 0$, and $i = N$ corresponds to $x = L_x$

$\rightarrow$ exercices 1 and 2

Discretisation of Poisson's equation in 2D as it is easier to understand
Volume of the domain = $\sum$ elementary cells



Finite volume method in 2D

2/5

$$\varepsilon_0 \boldsymbol{\nabla} \cdot (\varepsilon_\mathrm{r} \boldsymbol{\nabla} V) = -\rho \tag{3}$$

Poisson's equation can be written as :

$$\boldsymbol{\nabla} \cdot \boldsymbol{D} = -\rho \tag{4}$$

with

$$\boldsymbol{D} = -\varepsilon_0 \varepsilon_\mathrm{r} \boldsymbol{\nabla} V = \varepsilon_0 \varepsilon_\mathrm{r} \boldsymbol{E} \tag{5}$$

Finite volume method in 2D

3/5

$$\nabla \cdot \boldsymbol{D} = -\rho \tag{6}$$

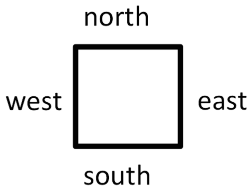
$$\iiint\limits_{V_c} \nabla \cdot \boldsymbol{D} dV = -\iiint\limits_{V_c} \rho dV \tag{7}$$

Using Divergence Theorem (aka Green-Ostrogradsky's, aka Gauss's theorem) :

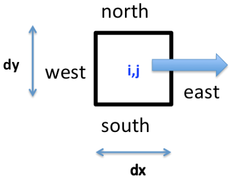
$$\oiint\limits_{S} \boldsymbol{D} \cdot \boldsymbol{dS} = -\bar{\rho} V_c \tag{8}$$

with $\bar{\rho}$ the *mean* charge density in the cell, and V_c the Volume of the cell.

$$\frac{1}{V_c} \sum_f D_{Nf} \cdot S_f = -\bar{\rho} \tag{9}$$

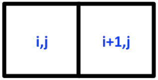


As an example: the EAST interface



$$\frac{D_{Ne} S_{fe}}{V_c} = \frac{1}{dx.dy} \epsilon_0 \epsilon_r E_{Ne} dy$$

As $\epsilon_r = 1$ and the mesh is uniform:



$$E_{Ne} = -\frac{V_{i+1} - V_i}{dx}$$

In doing the same on all interfaces, we obtain:

$$Ve_{i,j}.V_{i+1,j} + Vw_{i,j}.V_{i-1,j} + Vn_{i,j}.V_{i,j+1} + Vs_{i,j}.V_{i,j-1} - Vc_{i,j}.V_{i,j} = -\rho_{i,j} \tag{10}$$

where

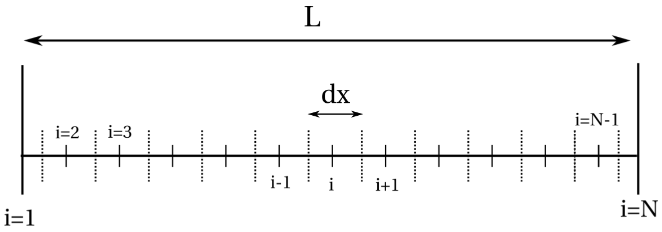
$$Vc_{i,j} = Ve_{i,j} + Vw_{i,j} + Vn_{i,j} + Vs_{i,j} \tag{11}$$

In 2D : The coefficients Ve,Vw,Vn and Vs are known : how to calculate $V_{i,j}$?
$\rightarrow$ exercice 3

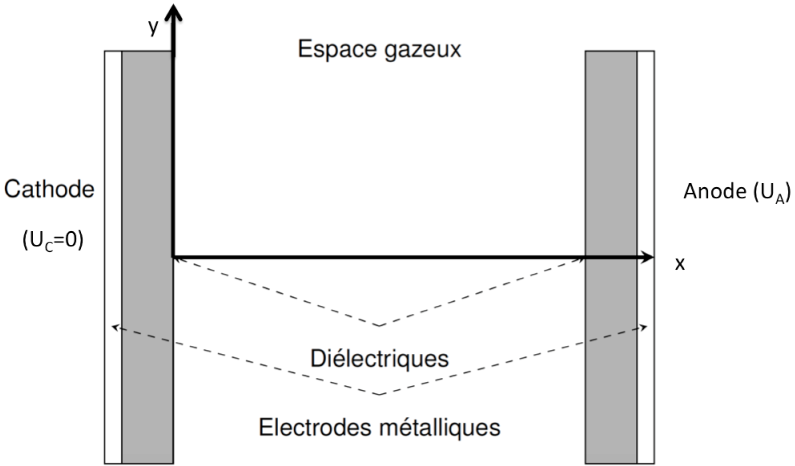
$\rightarrow$ First part of Exercice 1 : discretize Poisson's Equation in 1D
Similar to the discretization in 2D, be careful of the values of the vomule of the cell V_c and the surface of the borders S_f.

You can check with me the discretization, before starting the rest of the exercise. $\rightarrow$

Second part of Exercice 1 : Implementation.

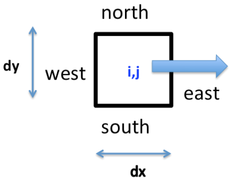


Exercice 3 : Studied configuration:

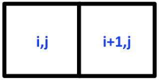


Exercice 4 : Integration of Poisson's equation with a permittivity that may vary from one cell to another

As an example: the EAST interface



$$\frac{D_{Ne}S_{fe}}{V_c} = \frac{1}{dx.dy}\epsilon_{i,j}E_{Ne}dy \qquad (12)$$

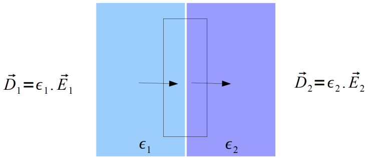


with $\epsilon = \epsilon_0\epsilon_r(x,y)$

$$E_{Ne} = -\frac{V_{i+1/2} - V_i}{dx/2} \qquad (13)$$

Exercice 4 : Integration of Poisson's equation on a control volume

Case of the interface of two materials with different dielectric properties:
The mesh is done such that the interface between materials corresponds to an interface between cells



$$\iiint_V \nabla \cdot \boldsymbol{D} dV = - \iiint_V \rho dV \tag{14}$$

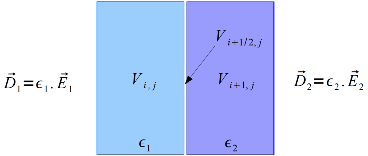
$$\oiint_S \boldsymbol{D} \cdot \boldsymbol{dS} = -\bar{\rho} V \tag{15}$$

with no surface charges on the dielectric surface

$$D_{N1} = D_{N2} \tag{16}$$

Exercice 4 : Integration of Poisson's equation on a control volume

Case of the interface of two materials with different dielectric properties:



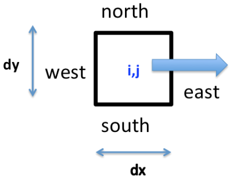
$$D_{N1} = D_{N2} \tag{17}$$

$$\epsilon_i \frac{V_{i+1/2} - V_i}{dx/2} = \epsilon_{i+1} \frac{V_{i+1} - V_{i+1/2}}{dx/2} \tag{18}$$

$$V_{i+1/2} = \frac{\epsilon_{i+1}}{\epsilon_i + \epsilon_{i+1}} V_{i+1} + \frac{\epsilon_i}{\epsilon_i + \epsilon_{i+1}} V_i \tag{19}$$

Exercice 4 : Integration of Poisson's equation on a control volume

As an example: the EAST interface



$$\frac{D_{Ne}S_{fe}}{V_c} = \frac{1}{dx.dy}\epsilon_{i,j}E_{Ne}dy \quad (20)$$

$$E_{Ne} = -\frac{V_{i+1/2,j} - V_{i,j}}{dx/2} = -\frac{2\epsilon_{i+1,j}(V_{i+1,j} - V_{i,j})}{dx(\epsilon_{i,j} + \epsilon_{i+1,j})} \quad (21)$$

$$\frac{D_{Ne}S_{fe}}{V_c} = -\frac{2\epsilon_{i,j}\epsilon_{i+1,j}}{dx^2(\epsilon_{i,j} + \epsilon_{i+1,j})}(V_{i+1,j} - V_{i,j}) \quad (22)$$

Exercice 4 : Integration of Poisson's equation on a control volume

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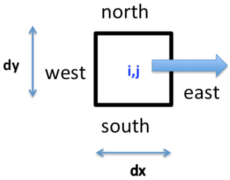

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$$\frac{D_{Ne}S_{fe}}{V_c} = \underbrace{-\frac{2\epsilon_{i,j}\epsilon_{i+1,j}}{dx^2(\epsilon_{i,j} + \epsilon_{i+1,j})}}_{\downarrow \; Ve_{i,j}}(V_{i+1,j} - V_{i,j}) \tag{22}$$

back-up slides

For which plasma studies do we need to solve Poisson's equation?

For low-temperature plasmas:

- Electrostatic Particle-In-Cell (PIC) simulations for low-pressure plasmas with static magnetic fields
- Non magnetized plasmas : Fluid simulations of low-temperature plasmas at atmospheric pressure

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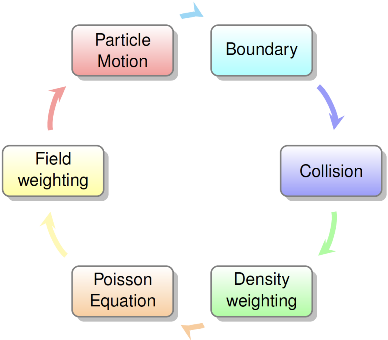
Electrostatic PIC simulations for low-temperature plasmas at low pressure

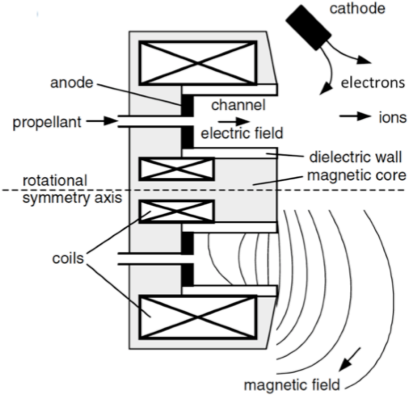
Standard Particle in Cell simulation:

- Explicit
- Electrostatic
- Numerous gases
  - Helium
  - Argon
  - Krypton
  - Xenon



Example : Electrostatic PIC simulations for electric propulsion applications

Figure: Example of HET - PPS© 1350 Safran



Hall effect thruster (HET) :
A low-temperature low-pressure plasma with a fixed magnetic field
Plasma interaction with dielectric walls

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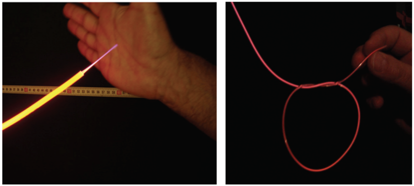
What is a low-temperature plasma at P_{atm} ?

- Electron density $\ll$ neutral density : ionization degree of about 10^{-4}-10^{-5}
- T_e (10 000 to 50 000 K) $\gg$ T_N=300 K
- Interest of low-temperature plasmas at P_{atm}: nonequilibrium chemistry at room temperature

Non-thermal discharges at atmospheric pressure

Applications of non-thermal discharges at P_{atm} ?

- Since a few years, many studies on non-thermal discharges at atmospheric ground pressure
- Wide range of applications at low pressure $\rightarrow$ possible at ground pressure to reduce costs (no need for pumping systems) ?
- New applications as biomedical applications, plasma assisted combustion



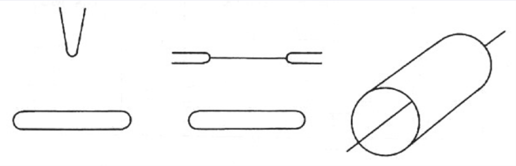
Robert *et al.*, Plasma Process. Polym. 2009, 6, 795-802

G. Pilla, PhD thesis (2008)

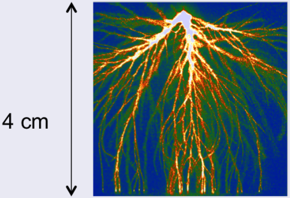
How to generate non-thermal discharges at atmospheric pressure ?

Between two metallic electrodes

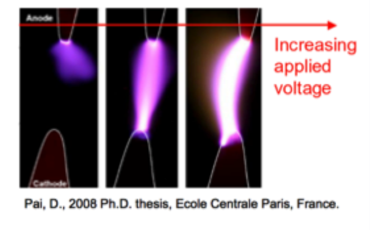
- Interelectrode gaps of a few mm to a few cm at P_{atm}



- If the gap distance > 1cm → complex discharge structure



Briels, PhD (2007)

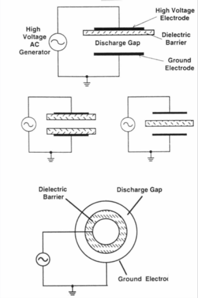


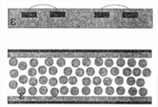
- Risk: If the voltage pulse is too long → transition to spark (thermal plasma!)

How to generate non-thermal discharges at atmospheric pressure ?

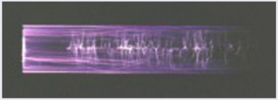
Dielectric Barrier Discharge (DBD)

- Interelectrode gaps of a few mm to a few cm at P_{atm}

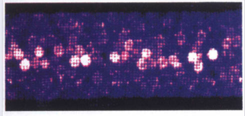




Plane-plane reactor (LPGP Orsay)



Wire-cylinder (GREMI Orléans)

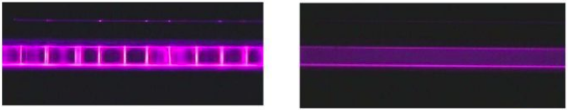


H.Russ et al , *IEEE Trans. Plasma Sci.* **27** (1999) 38

Non-thermal discharges at atmospheric pressure

Structure of P_{atm} discharges

- At P_{atm}, non-thermal atmospheric pressure discharges may have filamentary or diffuse structures



Filamentary discharges: most frequent

- High electron density (10^{14} cm^{-3}) in a filament with a radius of the order of 100 μm $\rightarrow$ high density of active species (radicals, excited species). In some cases, local heating may occur

Diffuse discharges

- Low density of electrons, large volume of the discharge and negligible heating

Simplest 2D Fluid model for discharge in air at $\mathrm{P_{atm}}$

- Continuity equation is solved for electrons, positive and negative ions

$$\frac{\partial n_i}{\partial t} + \mathrm{div}\, \boldsymbol{j}_i = S_i \tag{23}$$

- Drift-diffusion approximation

$$\boldsymbol{j}_i = \mu_i\, n_i\, \boldsymbol{E} - D_i\, \mathbf{grad}\, n_i \tag{24}$$

- Poisson's equation:

$$\varepsilon_0 \boldsymbol{\nabla} \cdot (\varepsilon_\mathrm{r} \boldsymbol{\nabla} V) = -q_\mathrm{e}(n_\mathrm{p} - n_\mathrm{n} - n_\mathrm{e}) \tag{25}$$

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- Strong non-linear coupling between drift-diffusion and Poisson's equations
- The species densities have to be calculated accurately as their difference is used to compute the potential and then the electric field $\rightarrow$ crucial to simulate the propagation of ionization fronts

2D Fluid model for discharge in air at $\mathrm{P_{atm}}$

- Continuity equation is solved for electrons, positive and negative ions

$$\frac{\partial n_i}{\partial t} + \mathrm{div}\, \boldsymbol{j}_i = S_i \tag{26}$$

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$$\boldsymbol{j}_i = \mu_i \, n_i \, \boldsymbol{E} - D_i \, \mathbf{grad} \, n_i \tag{27}$$

- Source terms for air:

$$\begin{cases} \mathrm{S_e} = (\partial_t n_e)_{chem} = (\nu_\alpha - \nu_\eta - \beta_{ep} n_p)\, n_e + \nu_{det} n_n + S_{ph} \,, \\ \mathrm{S_n} = (\partial_t n_n)_{chem} = -(\nu_{det} + \beta_{np} n_p)\, n_n + \nu_\eta n_e \,, \\ \mathrm{S_p} = (\partial_t n_p)_{chem} = -(\beta_{ep} n_e + \beta_{np} n_n)\, n_p + \nu_\alpha n_e + S_{ph} \,. \end{cases} \tag{28}$$

- Local field approximation: $\nu_\alpha(|\vec{E}|/N)$, $\nu_\eta(|\vec{E}|/N)$, $\mu_i(|\vec{E}|/N)$, $D_i(|\vec{E}|/N)$
Morrow et al., *J.Phys. D:Appl. Phys.* **30**,(1997)
- Transport parameters and source terms are pre-calculated (Bolsig+ solver - http://www.bolsig.laplace.univ-tlse.fr/)

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2D Fluid model for discharge in air at $\mathrm{P_{atm}}$

- Poisson's equation

$$\varepsilon_0 \nabla \cdot (\varepsilon_\mathrm{r} \nabla V) = -q_\mathrm{e}(n_\mathrm{p} - n_\mathrm{n} - n_\mathrm{e}) \tag{29}$$

- Surface charges on the dielectric surface are obtained by time integrating charged particle fluxes to the surface.
- At the dielectric surface, secondary emission of electrons by ion bombardment

Specificities of the simulation of low-temperature plasmas at atmospheric pressure

- Simulation of ionization front propagation is known to be computationally **expensive**
- Temporal multiscale nature of **explicit** simulation: Δt=$10^{-12} - 10^{-14}$s

$$\underline{\text{Convection:}} \quad \Delta t_c = \min\left[\frac{\Delta x_i}{v_{x(i,j)}}, \frac{\Delta r_j}{v_{r(i,j)}}\right] \qquad \underline{\text{Diffusion:}} \quad \Delta t_d = \min\left[\frac{(\Delta x_i)^2}{D_{x(i,j)}}, \frac{(\Delta r_j)^2}{D_{r(i,j)}}\right]$$

$$\underline{\text{Chemistry:}} \quad \Delta t_l = \min\left[\frac{n_{k(i,j)}}{S_{k(i,j)}}\right] \qquad \underline{\text{Diel. relaxation:}} \quad \Delta t_{Diel} = \min\left[\frac{\varepsilon_0}{q_e \mu_{e(i,j)} n_{e(i,j)}}\right]$$

- Time scale of discharge propagation in centimeter gaps is $\sim$ 10 ns, $\rightarrow \sim 10^4$ time steps
- For a gap of 1 cm, Δx,r=$10 - 1$ μm $\rightarrow$ nbre of points > 1×10^6

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Numerical solution of Poisson's equation

$$Ve_{i,j}.V_{i+1,j} + Vw_{i,j}.V_{i-1,j} + Vn_{i,j}.V_{i,j+1} + Vs_{i,j}.V_{i,j-1} - Vc_{i,j}.V_{i,j} = -\rho_{i,j} \quad (30)$$

where

$$Vc_{i,j} = Ve_{i,j} + Vw_{i,j} + Vn_{i,j} + Vs_{i,j} \quad (31)$$

The coefficients Ve,Vw,Vn and Vs are known, the source term is also known.
We want to calculate $V_{i,j}$
$\rightarrow$ The system to be solved can be written as Ax=B.

Different methods can be used (iterative or direct methods).
In this work, we propose to use 2 iterative methods:

- Gauss-Seidel
- SOR (successive over-relaxation)

Numerical solution - Gauss-Seidel

$$Ve_{i,j}.V_{i+1,j} + Vw_{i,j}.V_{i-1,j} + Vn_{i,j}.V_{i,j+1} + Vs_{i,j}.V_{i,j-1} - Vc_{i,j}.V_{i,j} = -\rho_{i,j} \quad (32)$$

If we write the Gauss-Seidel algorithm, we have to calculate:

$$V_{i,j} = (-Ve_{i,j}.V_{i+1,j} - Vw_{i,j}.V_{i-1,j} - Vn_{i,j}.V_{i,j+1} - Vs_{i,j}.V_{i,j-1} + \rho_{i,j})/Vc_{i,j} \quad (33)$$

and iterate until convergence.

Numerical solution - successive over-relaxation (SOR)

The SOR method is a slight modification of the Gauss-Seidel method.

In the SOR, we define $0 < \omega < 2$ and calculate iteratively:

$$V_{i,j} = (1-\omega)V_{i,j}^{old} +$$

$$(-Ve_{i,j}.V_{i+1,j} - Vw_{i,j}.V_{i-1,j} - Vn_{i,j}.V_{i,j+1} - Vs_{i,j}.V_{i,j-1} + \rho_{i,j})\omega/Vc_{i,j} \qquad (34)$$

until convergence

$V_{i,j}^{old}$ is the solution obtained at the last iteration.

If $\omega = 1$ we have the Gauss-Seidel method.

A good compromise for the SOR method is to use $\omega = 1.5$