

# TP2: Poisson's equation

Antoine Tavant

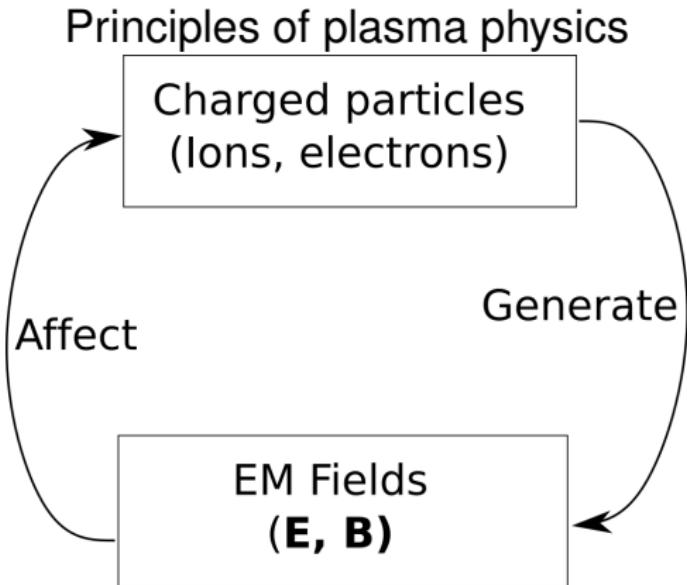
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TC5 : TP sur les méthodes numériques et simulations  
Séances du 27 octobre 2021 à CentraleSupélec



- For which plasma studies do we need to solve Poisson's equation and not Maxwell equations?
- What is the Poisson's equation ?
- Work to be done during this TP.

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



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

The Electrostatic Assumption can usually 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
- back-up slides for details

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

Maxwell's equations with electrostatic hypothesis:

$$\nabla \times \vec{E} = -\frac{\partial \vec{B}}{\partial t} = 0$$
$$\nabla \cdot \vec{B} = 0$$

$$\nabla \times \vec{B} = \mu_0 \left( \epsilon_0 \frac{\partial \vec{E}}{\partial t} + \vec{j} \right) = 0$$
$$\nabla \cdot \vec{E} = \frac{\rho}{\epsilon_0}$$

Becomes the Poisson Equation

$$\nabla \cdot \vec{E} = -\Delta \phi = \frac{\rho}{\epsilon_0}$$

With  $\vec{B} = \text{cst}$

- For which plasma studies do we need to solve Poisson's equation ?
- What is the Poisson's equation ?
- Work to be done during this TP.

# The Poisson's equation

The generic Poisson's equation  $\Delta\phi = f$  is found several times in physics:

- Newtonian gravity :  $\nabla \cdot \vec{g} = -\Delta\phi = 4\pi G\phi$
- Incompressible fluid dynamics:  $\Delta\vec{p} = -\rho\nabla\vec{v}$
- Heat equation:  $\Delta u = \alpha \frac{\partial u}{\partial t}$
- and many others

So it is an important equation, but **Why so Special about it?**

⇒ It is an *Elliptic* equation!

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So it is an important equation, but **Why so Special about it?**

⇒ It is an *Elliptic* equation!

Important aspects of the Elliptic equations : **There is not real characteristic curves**, hence

- Continuous derivatives
- No sense of information propagation

Hence only meaningful for static, steady state system.

**The source term impacts instantaneously the solution.**

In general plasmas:

$$\varepsilon_0 \nabla \cdot (\varepsilon_r \nabla V) = -q_e(n_p - n_n - n_e)$$

In this work, the source term will be defined as  $\rho$ , the charged density

$$\varepsilon_0 \nabla \cdot (\varepsilon_r \nabla V) = -\rho$$

We propose the following exercices:

- Exercice 1 : 1D poisson solver for a plasma between metallic walls ( $\varepsilon_r = 1$ )
- Exercice 2 : 1D poisson solver: performances
- Exercice 3 : 2D poisson solver for a plasma between metallic walls
- Exercice 4 (optional) : 1D poisson solver for a plasma between metallic walls covered by dielectric walls

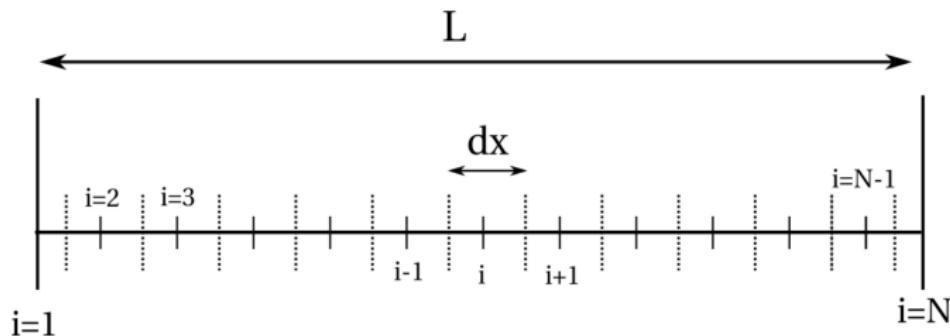
# Poisson's equation in 1D

In 1D:

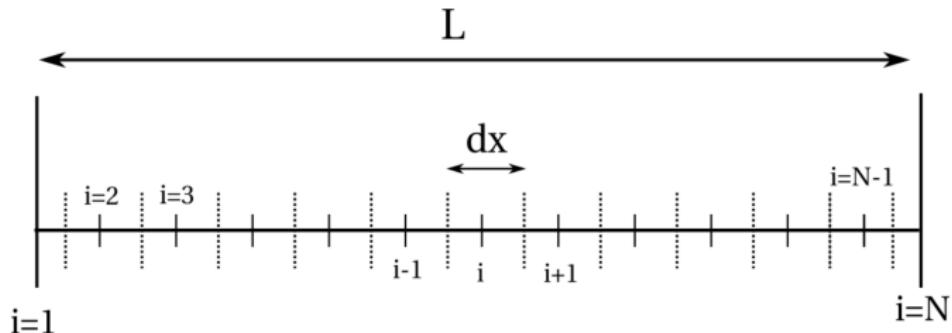
$$\varepsilon_0 \nabla_x \cdot (\varepsilon_r \nabla_x V(x)) = -\rho(x)$$

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 equation.



# Mesh in 1D

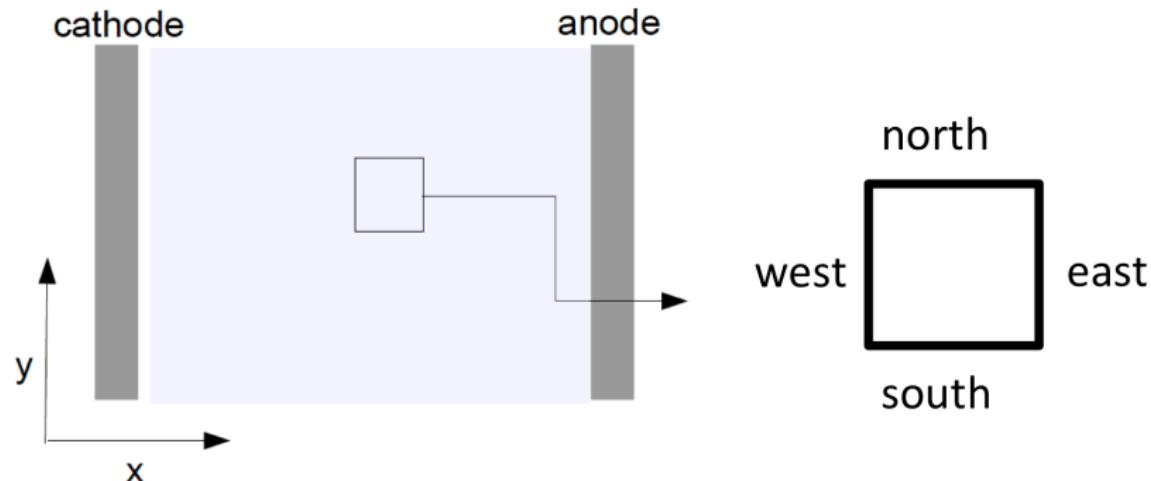


- We discretize the domain  $x = [0, L_x]$  in  $N - 2$  cells of size  $dx$  and 2 half-cells
- The center of each cell is defined by the index  $i$
- The unknown potential  $V(x)$  becomes  $V_i$  and the source term  $\rho(x)$  becomes  $\rho_i$
- The unknowns are **mean values at the center** of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

→ exercices 1, 2 and 4

# Discretization: Finite volume method in 2D

Finite volume discretization in 2D (easier to get than the 1D)  
Volume of the discharge =  $\sum$  elementary cells



# Discretization: Integration of Poisson's equation in 2D

$$\varepsilon_0 \nabla \cdot (\varepsilon_r \nabla V) = -\rho \quad (1)$$

Poisson's equation can be written as :

$$\nabla \cdot D = -\rho \quad (2)$$

with

$$D = -\varepsilon_0 \varepsilon_r \nabla V = \varepsilon_0 \varepsilon_r E \quad (3)$$

# Discretization: Integration of Poisson's equation in 2D

$$\nabla \cdot \mathbf{D} = -\rho \quad (4)$$

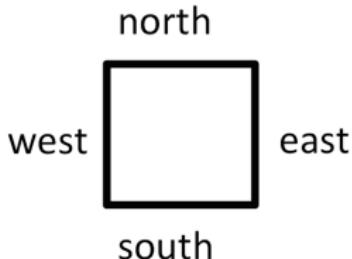
$$\iint_{V_c} \nabla \cdot \mathbf{D} dV = - \iint_{V_c} \rho dV \quad (5)$$

using the Divergence Theorem (aka Green-Ostrogradsky's, aka Gausse's theorem)

$$\oint_S \mathbf{D} \cdot d\mathbf{S} = -\bar{\rho} V_c \quad (6)$$

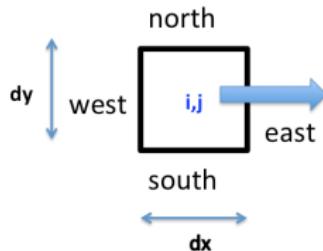
with  $\bar{\rho}$  the mean charge density in the cell, and  $V_c$  the Volume of the cell

$$\frac{1}{V_c} \sum_f D_{Nf} \cdot S_f = -\bar{\rho} \quad (7)$$



# Discretization: Integration of Poisson's equation in 2D

As an example: the EAST interface



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

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



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

# Discretization: Integration of Poisson's equation in 2D on a control volume

In doing the same on all interfaces, we obtain:

$$V_{e,i,j} \cdot V_{i+1,j} + V_{w,i,j} \cdot V_{i-1,j} + V_{n,i,j} \cdot V_{i,j+1} + V_{s,i,j} \cdot V_{i,j-1} - V_{c,i,j} \cdot V_{i,j} = -\rho_{i,j} \quad (8)$$

where

$$V_{c,i,j} = V_{e,i,j} + V_{w,i,j} + V_{n,i,j} + V_{s,i,j} \quad (9)$$

The coefficients  $V_e, V_w, V_n$  and  $V_s$  are now known : how to solve for  $V_{i,j}$ ?  
→ exercice 3

# Numerical solution of Poisson's equation

In 1D:

$$V\mathbf{e}_i \cdot V_{i+1} + V\mathbf{w}_i \cdot V_{i-1} - V\mathbf{c}_i \cdot V_i = -\rho_i \quad (10)$$

where  $V\mathbf{c}_i = V\mathbf{e}_i + V\mathbf{w}_i$

And in 2D:

$$V\mathbf{e}_{i,j} \cdot V_{i+1,j} + V\mathbf{w}_{i,j} \cdot V_{i-1,j} + V\mathbf{n}_{i,j} \cdot V_{i,j+1} + V\mathbf{s}_{i,j} \cdot V_{i,j-1} - V\mathbf{c}_{i,j} \cdot V_{i,j} = -\rho_{i,j} \quad (11)$$

where  $V\mathbf{c}_{i,j} = V\mathbf{e}_{i,j} + V\mathbf{w}_{i,j} + V\mathbf{n}_{i,j} + V\mathbf{s}_{i,j}$

The coefficients  $V\mathbf{e}, V\mathbf{w}, V\mathbf{n}$  and  $V\mathbf{s}$  are known, the source term is also known. We want to calculate  $V_{i,j}$

→ The system to be solved can be written as  $\mathbf{A}\mathbf{x}=\mathbf{B}$ .

# Numerical solution of Poisson's equation

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where  $V\mathbf{c}_i = V\mathbf{e}_i + V\mathbf{w}_i$

And in 2D:

$$V\mathbf{e}_{i,j} \cdot V_{i+1,j} + V\mathbf{w}_{i,j} \cdot V_{i-1,j} + V\mathbf{n}_{i,j} \cdot V_{i,j+1} + V\mathbf{s}_{i,j} \cdot V_{i,j-1} - V\mathbf{c}_{i,j} \cdot V_{i,j} = -\rho_{i,j} \quad (11)$$

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The coefficients  $V\mathbf{e}, V\mathbf{w}, V\mathbf{n}$  and  $V\mathbf{s}$  are known, the source term is also known. We want to calculate  $V_{i,j}$

→ The system to be solved can be written as  $\mathbf{A}\mathbf{x}=\mathbf{B}$ .

# Numerical solution of Poisson Equation

→ 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 1 direct and 2 iterative methods:

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

Thomas solver to use in 1D to solve any tridiagonal systems:  
This is a rather direct usage of the Gauss pivot method,  
simplified for the matrix type.

→ See Exercie 1 and the notebook linear\_system.ipynb for  
more information on Thomas' solver.

$$V_{e,i,j} \cdot V_{i+1,j} + V_{w,i,j} \cdot V_{i-1,j} + V_{n,i,j} \cdot V_{i,j+1} + V_{s,i,j} \cdot V_{i,j-1} - V_{c,i,j} \cdot V_{i,j} = -\rho_{i,j} \quad (12)$$

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

$$V_{i,j} = (-V_{e,i,j} \cdot V_{i+1,j} - V_{w,i,j} \cdot V_{i-1,j} - V_{n,i,j} \cdot V_{i,j+1} - V_{s,i,j} \cdot V_{i,j-1} + \rho_{i,j}) / V_{c,i,j} \quad (13)$$

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:

$$V_{i,j} = (1 - \omega)V_{i,j}^{old} + (-Ve_{i,j} \cdot V_{i+1,j} - Vw_{i,j} \cdot V_{i-1,j} - Vn_{i,j} \cdot V_{i,j+1} - Vs_{i,j} \cdot V_{i,j-1} + \rho_{i,j})\omega / Vc_{i,j} \quad (14)$$

until convergence

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

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

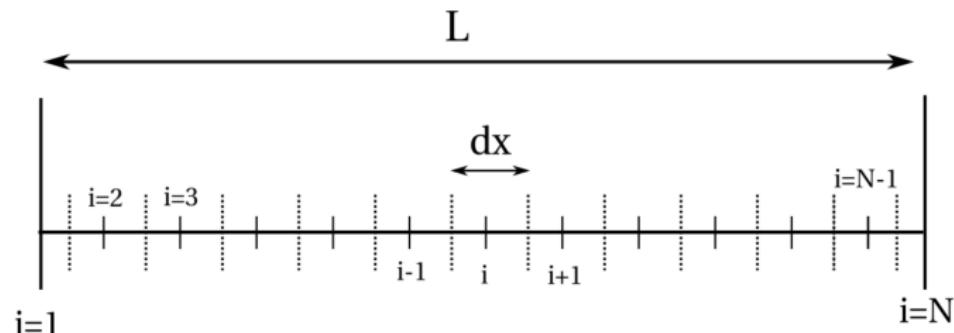
A good compromise for the SOR method is to use  $\omega = 1.5$

→ First part of Exercie 1: Discretize Poisson's equation in 1D

Similar to the 2D process, but be careful for the value of the cell "volume"  $V_c$  and the border surface  $S_f$ ,

→ Second part of Exercie 1: Solve for  $V_i$

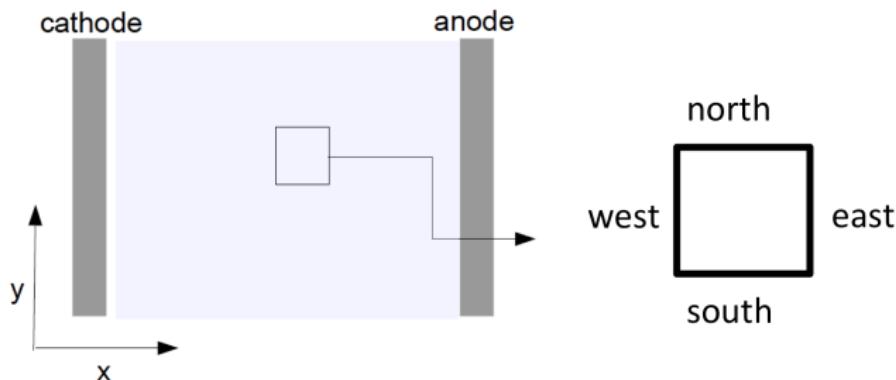
Implementation of a direct solver



→ Exercie 2: Analyse the performances of the solver

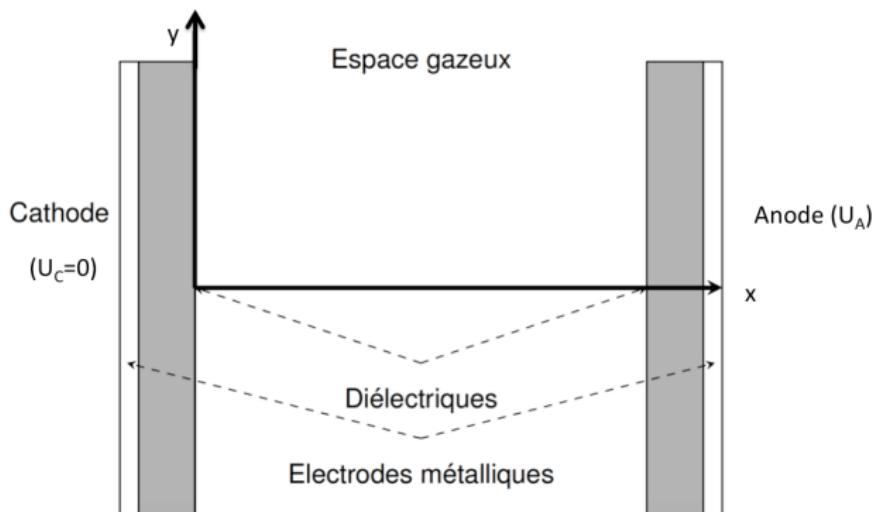
# Finite volume in 2D

- the discretisation is already done
- Solving using an iterative solver: SOR



# Exercice 4 : Studied configuration:

Exercie 4 is **OPTIONAL**: first master the previous exercie befor even trying this one



# Getting started with the exercies

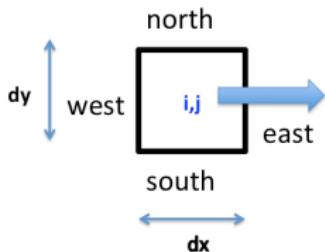
- Download the sources on GH :  
[https://github.com/antoinetavant/TP\\_M2](https://github.com/antoinetavant/TP_M2)
- Use a jupyter environement :
  - Your local computer
  - The JupyterHub  
<https://jupytercloud.idcs.polytechnique.fr/jupyter>
  - Google Colab (best for collaboration)
- **Write the answers and the code directly in the notebooks**
- Use the learntool package to get hints and check some of the answers

# Rules for this exercices

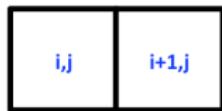
- Deadline : 17th December 2021 at 23h59. 0/20 after the deadline
- Better to send an unfinished work than no work at all
- Send me all the notebooks completed by email (attached in the mail, WeTransfer, or by other tools)
- You can work in group, but everyone needs to send me a report
- 3 sessions with me : 27/10, 3/11 & 15/11
- After this, I am available to discuss by email, and by visio if the emails are not enough

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

As an example: the EAST interface



$$\frac{D_{Ne} S_{fe}}{V_c} = \frac{1}{dx \cdot dy} \epsilon_{i,j} E_{Ne} dy \quad (15)$$



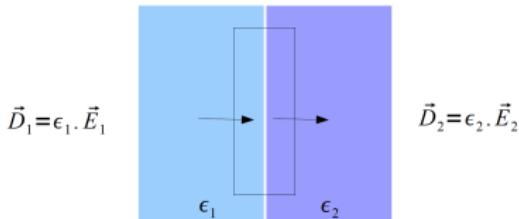
with  $\epsilon = \epsilon_0 \epsilon_r(x, y)$

$$E_{Ne} = -\frac{V_{i+1/2} - V_i}{dx/2} \quad (16)$$

# 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



$$\vec{D}_1 = \epsilon_1 \cdot \vec{E}_1$$

$$\vec{D}_2 = \epsilon_2 \cdot \vec{E}_2$$

$$\iiint_V \nabla \cdot \mathbf{D} dV = - \iiint_V \rho dV \quad (17)$$

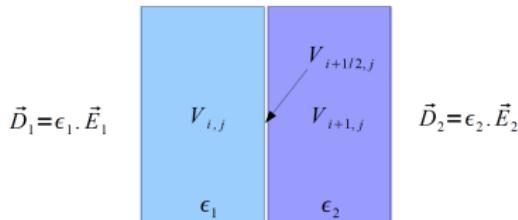
$$\iint_S \mathbf{D} \cdot d\mathbf{S} = -\bar{\rho}V \quad (18)$$

with no surface charges on the dielectric surface

$$D_{N1} = D_{N2} \quad (19)$$

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

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



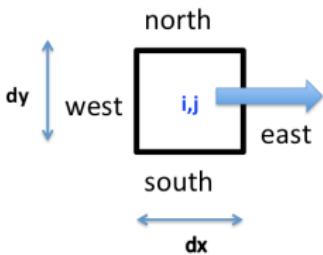
$$D_{N1} = D_{N2} \quad (20)$$

$$\epsilon_i \frac{V_{i+1/2} - V_i}{dx/2} = \epsilon_{i+1} \frac{V_{i+1} - V_{i+1/2}}{dx/2} \quad (21)$$

$$V_{i+1/2} = \frac{\epsilon_{i+1}}{\epsilon_i + \epsilon_{i+1}} V_{i+1} + \frac{\epsilon_i}{\epsilon_i + \epsilon_{i+1}} V_i \quad (22)$$

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

As an example: the EAST interface



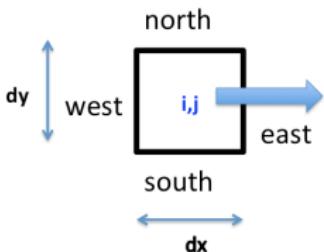
$$\frac{D_{Ne} S_{fe}}{V_c} = \frac{1}{dx \cdot dy} \epsilon_{i,j} E_{Ne} dy \quad (23)$$

$$E_{Ne} = -\frac{V_{i+1/2,j} - V_{i,j}}{dx/2} = -\frac{2\epsilon_{i+1,j}(V_{i+1,j} - V_{i,j})}{dx(\epsilon_{i,j} + \epsilon_{i+1,j})} \quad (24)$$

$$\frac{D_{Ne} S_{fe}}{V_c} = -\frac{2\epsilon_{i,j}\epsilon_{i+1,j}}{dx^2(\epsilon_{i,j} + \epsilon_{i+1,j})}(V_{i+1,j} - V_{i,j}) \quad (25)$$

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$$\downarrow \\ Ve_{i,j}$$

# 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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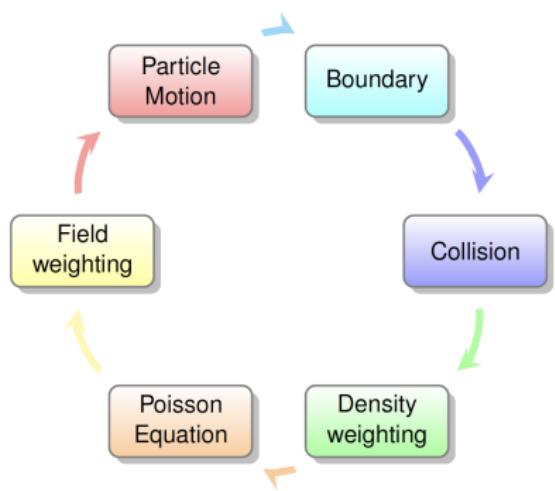
For low-temperature plasmas:

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# Electrostatic PIC simulations for low-temperature plasmas at low pressure

Standard Particle in Cell simulation:

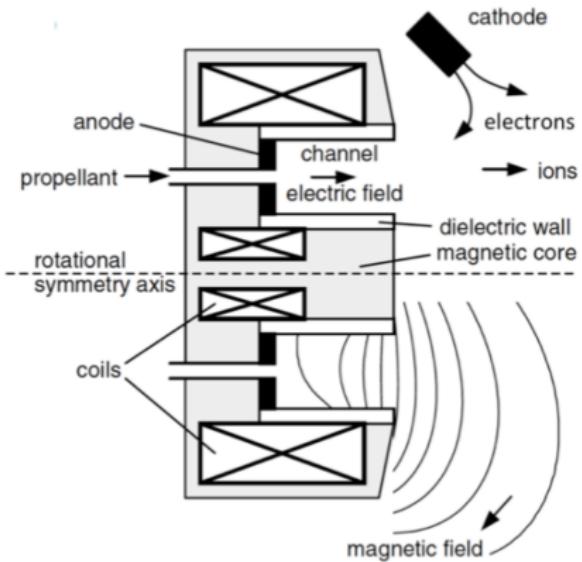
- ▶ Explicit
- ▶ Electrostatic
- ▶ Numerous gases
  - Helium
  - Argon
  - Krypton
  - Xenon



# Example : Electrostatic PIC simulations for electric propulsion applications



Figure: Example of HET - PPS<sup>©</sup> 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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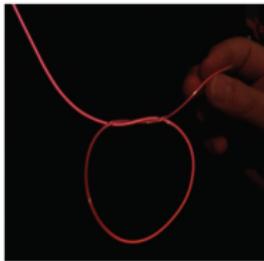
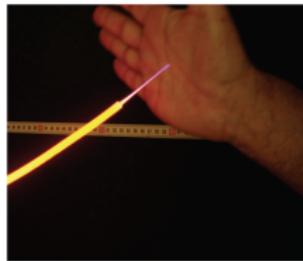
# What is a low-temperature plasma at $P_{atm}$ ?

- ▶ 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 → possible at ground pressure to reduce costs (no need for pumping systems) ?
- ▶ New applications as biomedical applications, plasma assisted combustion

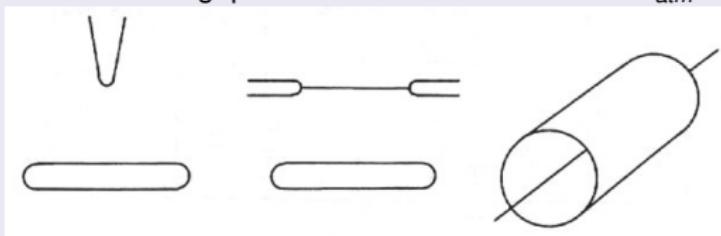


Robert *et al.*, Plasma Process. Polym. 2009, 6, 795-802

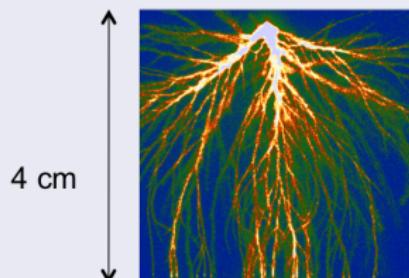
# How to generate non-thermal discharges at atmospheric pressure ?

Between two metallic electrodes

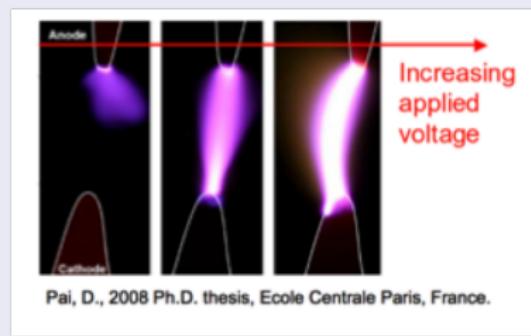
- ▶ Interelectrode gaps of a few mm to a few cm at  $P_{atm}$



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



Briels, PhD (2007)



Pai, D., 2008 Ph.D. thesis, Ecole Centrale Paris, France.

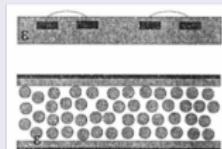
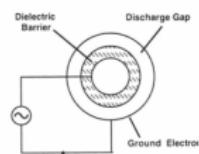
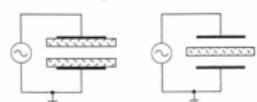
- ▶ Risk: If the voltage pulse is too long → transition to **spark** (thermal plasma!)



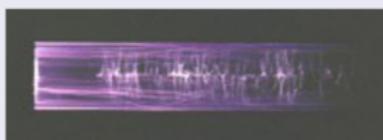
# How to generate non-thermal discharges at atmospheric pressure ?

## Dielectric Barrier Discharge (DBD)

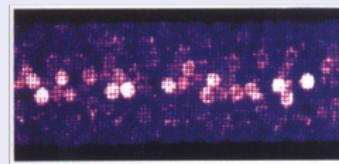
- ▶ Interelectrode gaps of a few mm to a few cm at  $P_{atm}$



Plane-plane reactor (LPGP Orsay)



Wire-cylinder (GREMI Orléans)



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

## 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 ( $10^{14} \text{ cm}^{-3}$ ) in a filament with a radius of the order of  $100 \mu\text{m}$  → 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

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

$$\frac{\partial n_i}{\partial t} + \operatorname{div} \mathbf{j}_i = S_i \quad (26)$$

- Drift-diffusion approximation

$$\mathbf{j}_i = \mu_i n_i \mathbf{E} - D_i \operatorname{grad} n_i \quad (27)$$

- Poisson's equation:

$$\varepsilon_0 \nabla \cdot (\varepsilon_r \nabla V) = -q_e(n_p - n_n - n_e) \quad (28)$$

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

$$\frac{\partial n_i}{\partial t} + \operatorname{div} \mathbf{j}_i = S_i \quad (26)$$

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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 → crucial to simulate the propagation of ionization fronts

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$$\mathbf{j}_i = \mu_i n_i \mathbf{E} - D_i \operatorname{grad} n_i \quad (30)$$

- Source terms for air:

$$\begin{cases} S_e = (\partial_t n_e)_{\text{chem}} &= (\nu_\alpha - \nu_\eta - \beta_{ep} n_p) n_e + \nu_{det} n_n + S_{ph} , \\ S_n = (\partial_t n_n)_{\text{chem}} &= -(\nu_{det} + \beta_{np} n_p) n_n + \nu_\eta n_e , \\ S_p = (\partial_t n_p)_{\text{chem}} &= -(\beta_{ep} n_e + \beta_{np} n_n) n_p + \nu_\alpha n_e + S_{ph} . \end{cases} \quad (31)$$

- 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)
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- 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:  $\Delta t = 10^{-12} - 10^{-14}$  s

$$\text{Convection: } \Delta t_c = \min \left[ \frac{\Delta x_j}{v_{X(i,j)}}, \frac{\Delta r_j}{v_{r(i,j)}} \right]$$

$$\text{Diffusion: } \Delta t_d = \min \left[ \frac{(\Delta x_j)^2}{D_{X(i,j)}}, \frac{(\Delta r_j)^2}{D_{r(i,j)}} \right]$$

$$\text{Chemistry: } \Delta t_l = \min \left[ \frac{n_{K(i,j)}}{S_{K(i,j)}} \right]$$

$$\text{Diel. relaxation: } \Delta t_{Diel} = \min \left[ \frac{\epsilon_0}{q_e \mu e_{(i,j)} n_e(i,j)} \right]$$

- ▶ Time scale of discharge propagation in centimeter gaps is  $\sim 10$  ns,  $\rightarrow \sim 10^4$  time steps
- ▶ For a gap of 1 cm,  $\Delta x, r = 10 - 1 \mu\text{m} \rightarrow$  nbre of points  $> 1 \times 10^6$

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