Why we need a fast and accurate solution of Poisson's equation for low-temperature plasmas?

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Journée problème de Poisson, January 26, 2015, IHP, France

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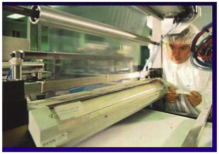
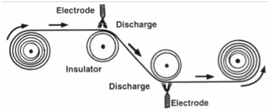
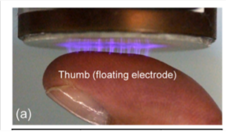
Non-thermal discharges at atmospheric pressure

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







Plasma assisted combustion

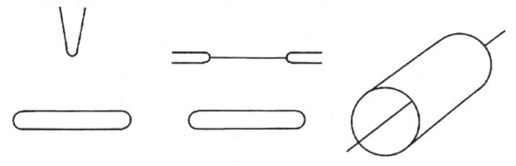
Φ= 0.8, Air flow rate = 15 m^3/h

Lean premixed burner

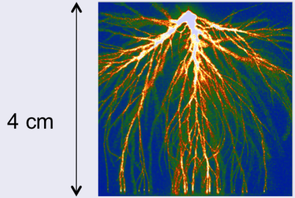
How to generate non-thermal discharges at atmospheric pressure ?

Between two metallic electrodes

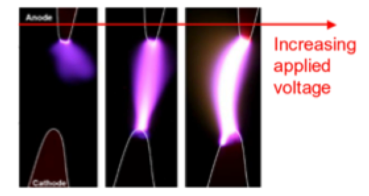
- Interelectrode gaps of a few mm to a few cm at P_{atm}



- Risk: If the voltage pulse is too long $\rightarrow$ transition to spark

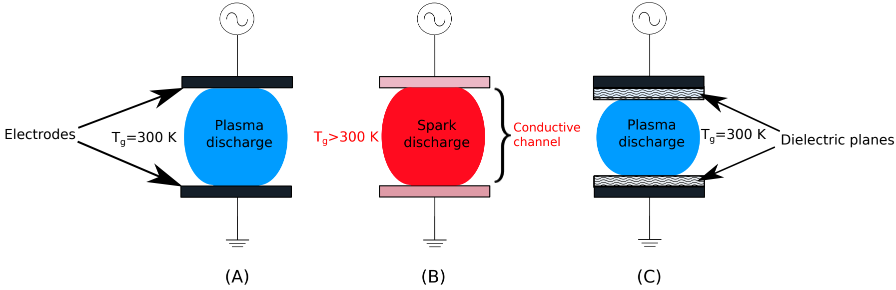


Briels, PhD (2007)



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

How to generate non-thermal discharges at atmospheric pressure ?



Dielectric Barrier Discharge (DBD)

- (A) Ignition of a discharge between electrodes
- (B) **Transition to spark** → high current, $T_g > 300K$
- (C) To prevent spark transition: **dielectric layers between the electrodes**

- $T_i = T_g = 300$K, $T_e > 10000K$ → **Cold plasma**
- O, OH, radicals and UV radiation

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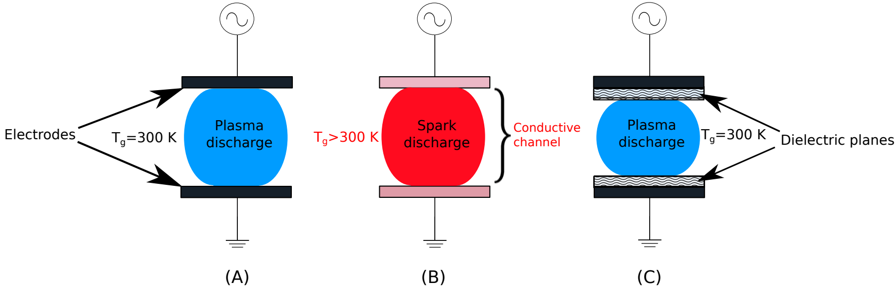

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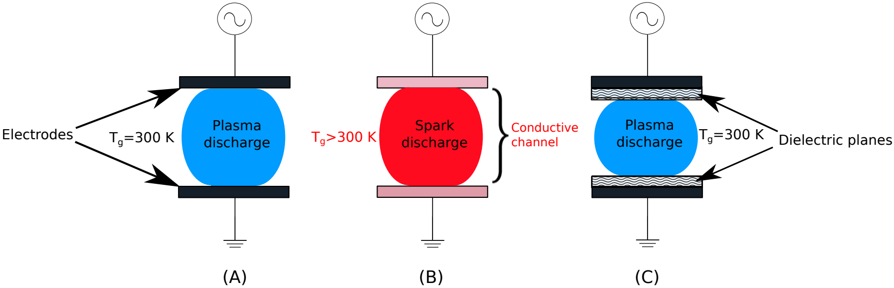

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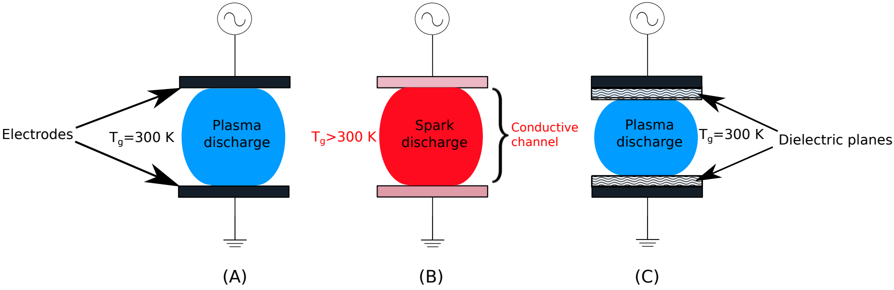

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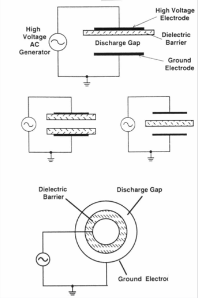
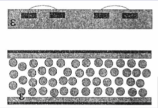
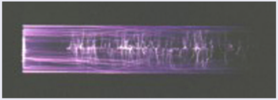
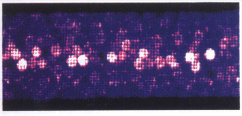




Plane-plane reactor (LPGP Orsay)



Wire-cylinder (GREMI Orléans)

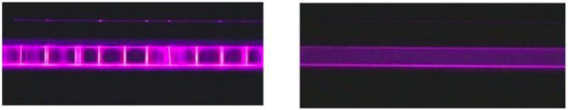


H.Russ et al , *IEEE Trans. Plasma Sci.* **27** (1999) 38

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

- 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). However, local heating may be significant

Diffusive discharges

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

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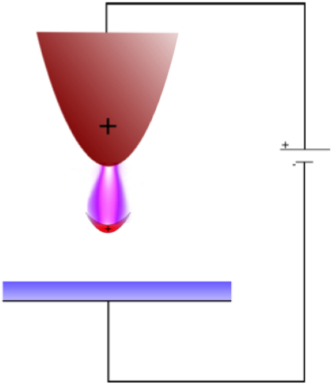
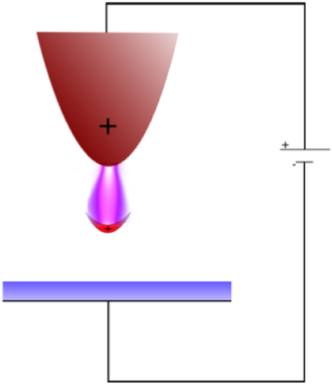
Streamer propagation in air at atmopsheric pressure



Streamer propagation

- In air at P_{atm}, the beakdown field is 30 kV/cm
- In a point to plane geometry, the electric field is enhanced close to the point electrode
- At first, the discharge will start from the point electrode and will propagate towards the grounded plane

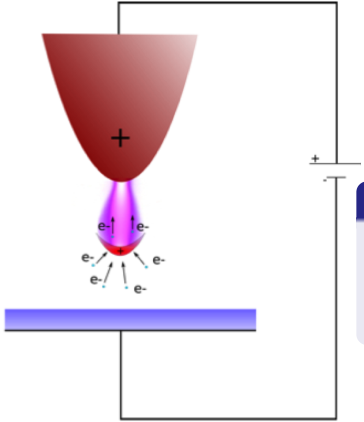
Streamer propagation in air at atmopsheric pressure



Streamer propagation

- Typical radius of the filament = 100 μm, velocity = 10^8 cm/s so 10 ns for 1 cm
- Almost neutral channel and charged streamer head
- In the conductive channel: low electric field (5 kV/cm) and a charged species density of 10^{13}-10^{14} cm^{-3}
- In the streamer head peak: peak electric field (140 kV/cm)
- Ions are almost immobile during propagation: streamer velocity > drift velocity of electrons
- A streamer discharge is an ionization wave

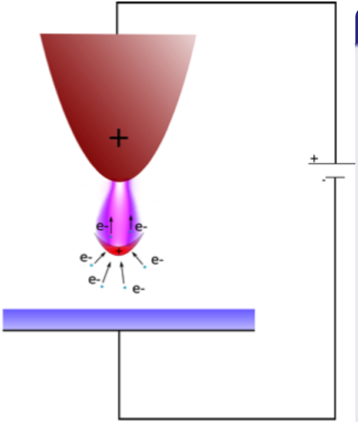
Streamer propagation in air at atmopsheric pressure



Streamer propagation

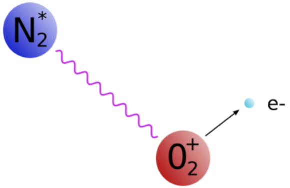
- The discharge move towards the cathode, whereas electrons move towards the anode
- Need for seed electrons for the discharge propagation

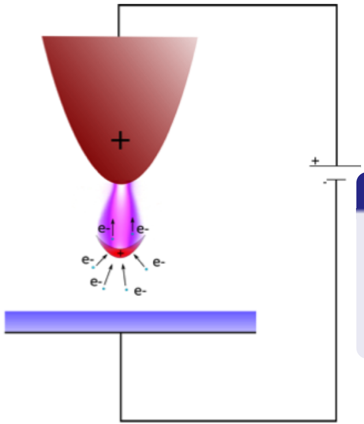
Streamer propagation in air at atmopsheric pressure



Origin of seed electrons

- Cosmic rays (up to 10^4 cm^{-3}), preionization from previous discharges
- Photoionization (depends on the gas mixture) in air

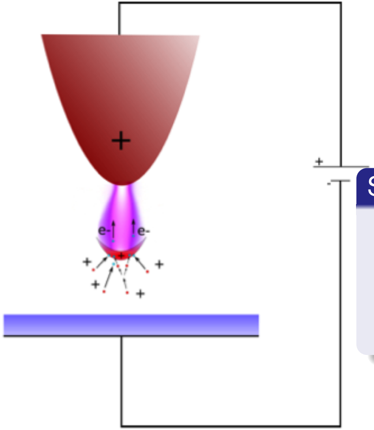




Streamer propagation

- Seed electrons in front of the streamer
- Transport of charged species
- Screening of the streamer head by electrons
- Streamer moves forward

Streamer propagation in air at atmopsheric pressure



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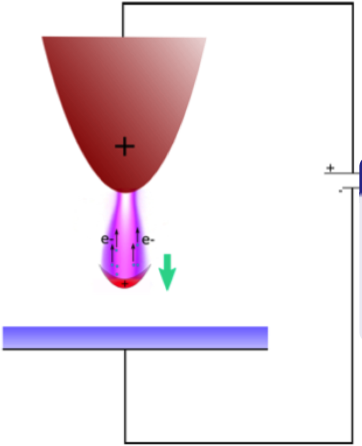

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How to simulate non-thermal discharges at P_{atm}?

Complex medium

- Charged species (ions, electrons), atoms and molecules (excited or not) and photons
- Simplest models take into account only charged species (and photons)
- Magnetic effects are negligible: electric field derived from Poisson's equation

Different models

- Microscopic model for charged particles coupled with Poisson's equation (PIC-MCC model (Chanrion and Neubert JCP (2008) and JGR (2010))
- Most popular: macroscopic fluid model coupled to Poisson's equation
- Hybrid models:
  - Particle model in the high field region
  - Fluid model in the streamer channel (low field, high electron densities)
  - Transition between both models:
    - In space: Li, Ebert and Brook IEEE Trans. Plasma Sci. (2008), Li, Ebert, Hundsdorfer, JCP (2012)
    - In energy: *bulk-model* (Bonaventura et al., ERL (2014))

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

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

$$\frac{\partial n_i}{\partial t} + \mathrm{div}\, \boldsymbol{j}_i = S_i \tag{1}$$

- Drift-diffusion approximation

$$\boldsymbol{j}_i = \mu_i\, n_i\, \boldsymbol{E} - D_i\, \mathbf{grad}\, n_i \tag{2}$$

- Poisson's equation:

$$\varepsilon_0 \boldsymbol{\nabla} \cdot (\varepsilon_{\mathrm{r}} \boldsymbol{\nabla} V) = -q_{\mathrm{e}}(n_{\mathrm{p}} - n_{\mathrm{n}} - n_{\mathrm{e}}) \tag{3}$$

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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

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

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

$$\frac{\partial n_i}{\partial t} + \mathrm{div}\, \boldsymbol{j}_i = S_i \tag{4}$$

- Drift-diffusion approximation

$$\boldsymbol{j}_i = \mu_i \, n_i \, \boldsymbol{E} - D_i \, \mathbf{grad} \, n_i \tag{5}$$

- Source terms for air:

$$\begin{cases} \mathrm{S_e} = (\partial_t n_e)_{\mathrm{chem}} = (\nu_\alpha - \nu_\eta - \beta_{\mathrm{ep}} n_{\mathrm{p}})\, n_{\mathrm{e}} + \nu_{\mathrm{det}} n_{\mathrm{n}} + S_{ph} \,, \\ \mathrm{S_n} = (\partial_t n_n)_{\mathrm{chem}} = -(\nu_{\mathrm{det}} + \beta_{\mathrm{np}} n_{\mathrm{p}})\, n_{\mathrm{n}} + \nu_\eta n_{\mathrm{e}} \,, \\ \mathrm{S_p} = (\partial_t n_p)_{\mathrm{chem}} = -(\beta_{\mathrm{ep}} n_{\mathrm{e}} + \beta_{\mathrm{np}} n_{\mathrm{n}})\, n_{\mathrm{p}} + \nu_\alpha n_{\mathrm{e}} + S_{ph} \,. \end{cases} \tag{6}$$

- 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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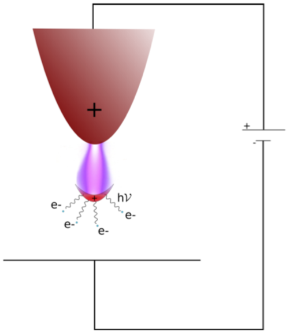
Photoionization in air



Photoionization model in air

- Non-local phenomenon
- Photoionization rate at one position depends on all the emitters positions
- Reference model derived from experimental results *[Zheleznyak, et al., High Temp., 20, 357 (1982)]* and confirmed by recent experiments *[Aints, et al., Plasma Process. and Polym. 5, 672 (2008)]*
- Original model requires to calculate a 3D integral for each point at each time step
- New model based on a third order approximation of the radiative transfer equation $\rightarrow$ differential model *[Bourdon et al. PSST, 16, 656 (2007), Liu et al. APL 91, 211501 (2007)]*

- Poisson's equation

$$\varepsilon_0 \boldsymbol{\nabla} \cdot (\varepsilon_\mathrm{r} \boldsymbol{\nabla} V) = -q_\mathrm{e}(n_\mathrm{p} - n_\mathrm{n} - n_\mathrm{e}) \tag{7}$$

- Photoionization source term S_{ph}: SP3 model
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- It leads to solve 18+1 Poisson's equation !

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$\lambda_{j=1,3} \rightarrow$ 2 Poisson's equation ($\phi_{1,j}$ and $\phi_{2,j}$) $\times$ 3 iterations for BC

$$\downarrow$$

$$\boxed{6 \times 3 \text{ Poisson's equations}} \rightarrow S_{ph} = \sum_{\mathrm{j}} = f(\phi_{1,j}(\vec{r}), \phi_{2,j}(\vec{r}))$$

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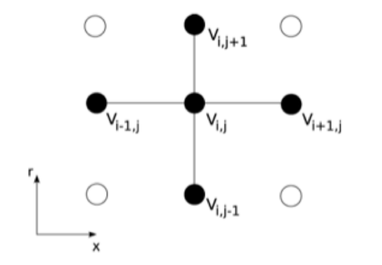
2nd order finite volume discretization in 2D

- In cylindrical coordinates, Poisson's equation can be written as

$$-\frac{\partial}{\partial x}\left(\epsilon\frac{\partial V}{\partial x}\right)-\frac{1}{r}\frac{\partial}{\partial r}\left(\epsilon r\frac{\partial V}{\partial r}\right)=\rho(x,r)\ , \tag{9}$$

- After integration it leads to

$$V^E_{i,j}V_{i+1,j}+V^W_{i,j}V_{i-1,j}+V^S_{i,j}V_{i,j-1}+V^N_{i,j}V_{i,j+1}+V^C_{i,j}V_{i,j}=\rho_{i,j}\Omega_{i,j}\ , \tag{10}$$



Discretization of Poisson's equation

We need to solve Poisson's equation at each timestep

Linear solver coupled with Poisson's equation

- Algorithm based on fast fourier transform
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- Streamer discharge simulation are known to be computationally **expensive**
- Temporal multiscale nature of **explicit** streamer simulation: Δt=$10^{-12} - 10^{-14}$s

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Characteristics of the initial discharge code

- 2D-axisymmetric discharge code
- Full explicit sequential code using Cartesian non-uniform static mesh
- MUMPS direct solver for Poisson's equation and photo-ionization source term
- Explicit Improved Scharfettel-Gummel (ISG) exponential scheme for the convection-diffusion equation
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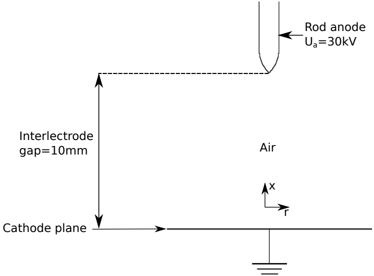

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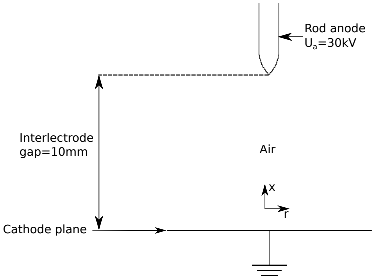

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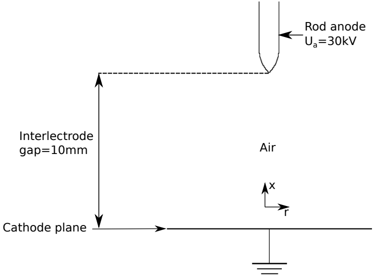

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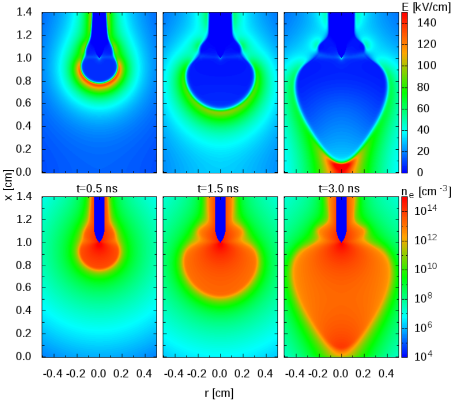
- Simulation time : $\sim$ **one month** with original code (memory used > 30 Go)



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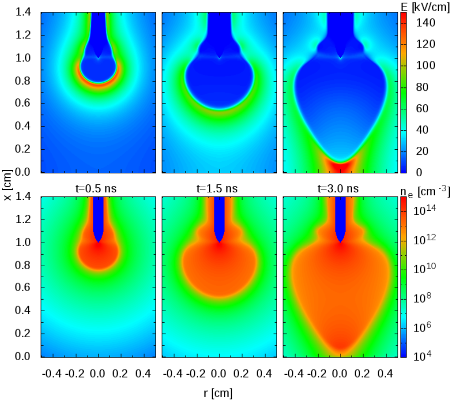

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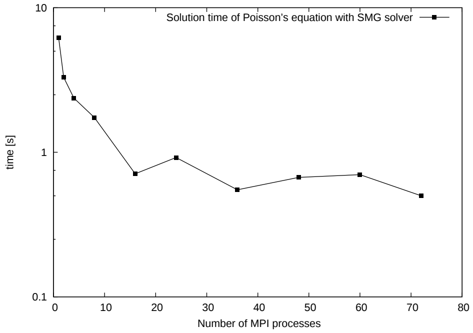

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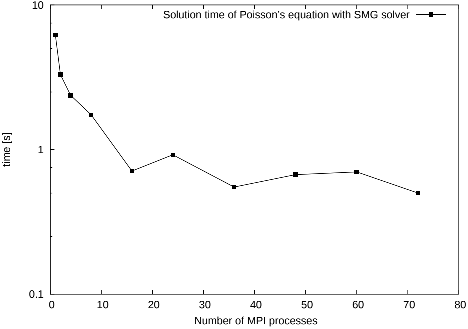

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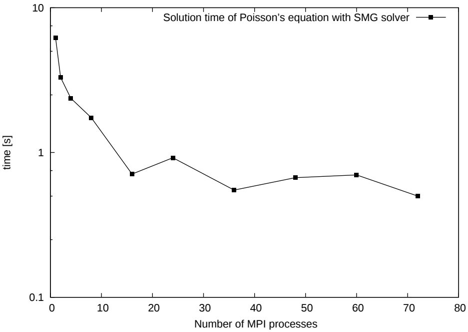

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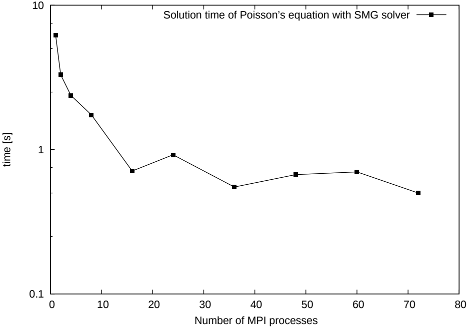

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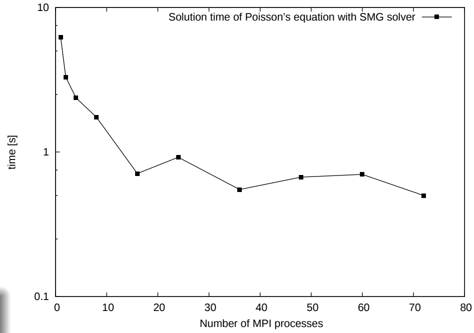

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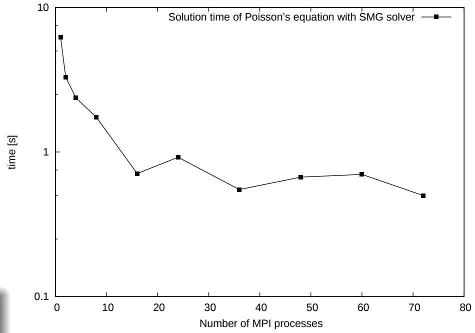

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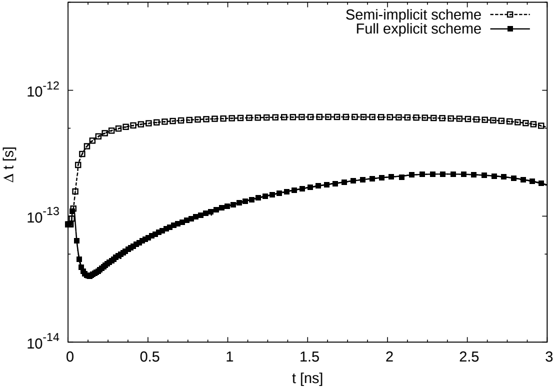

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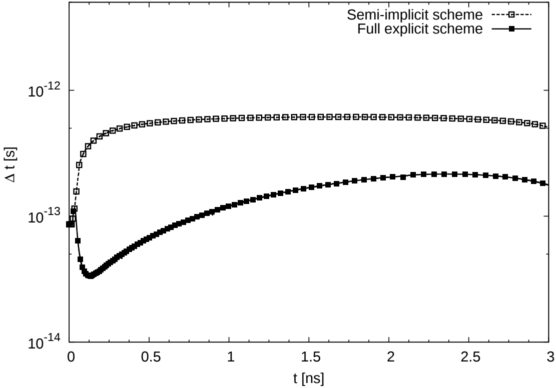

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Improvements of the discharge code: UNO3 convection scheme

To improve the computational efficiency, we need a transport scheme that is accurate with less points

- Is the ISG exponential transport scheme (drift+diffusion) accurate with less points?
  - Test-case 2: E_{axis} profile with close to the point Δx=1 μm,Δr=1 μm
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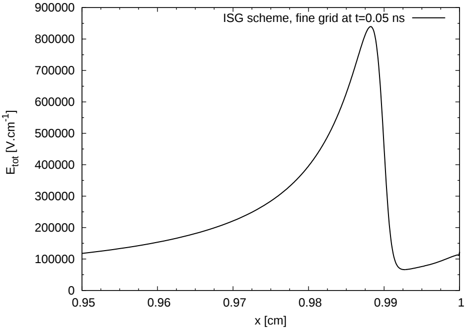

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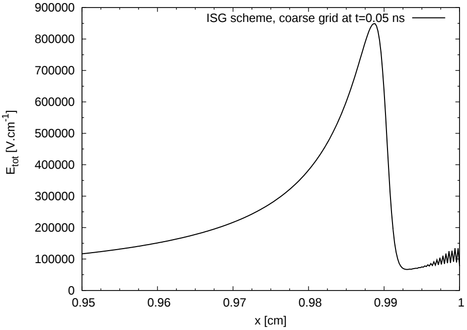

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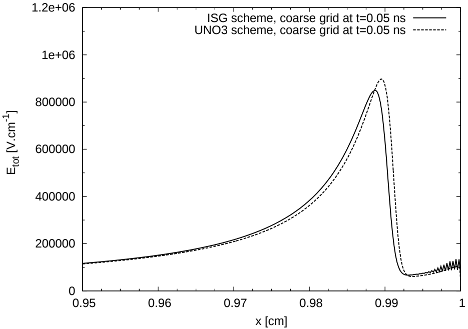

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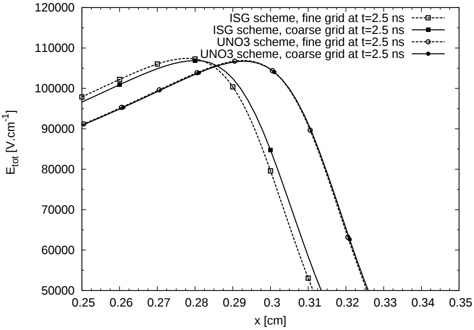
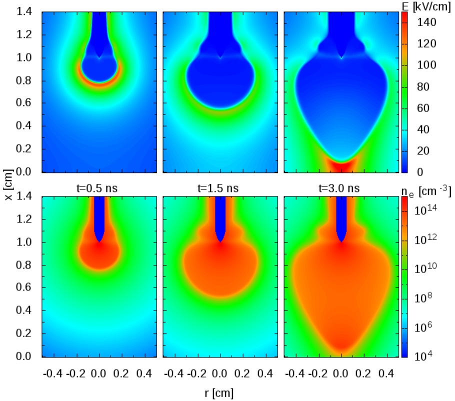


Improvements of the discharge code: MPI-OPENMP discharge code

- **Full parallel MPI-OPENMP discharge code**
- Poisson's equation: MPI-OPENMP iterative solver SMG
- Small time-steps: Semi-implicit scheme (to remove Δt_{Diel})
- Robustness: Explicit UNO3 scheme 3^{rd} order for convection + Explicit 2^{nd} order for diffusion (not shown here)
- Test on TC one time-step:
- Test on TC one time-step: 24 MPI$\times$3 OPENMP: 17.05 s $\searrow$ 0.86 s
- TC is computed in $\sim$ **3 hours**

  (**one month** with initial code)



Improvements of the discharge code: MPI-OPENMP discharge code

- **Full parallel MPI-OPENMP discharge code**
- Poisson's equation: MPI-OPENMP iterative solver SMG
- Small time-steps: Semi-implicit scheme (to remove Δt_{Diel})
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- Test on TC one time-step:
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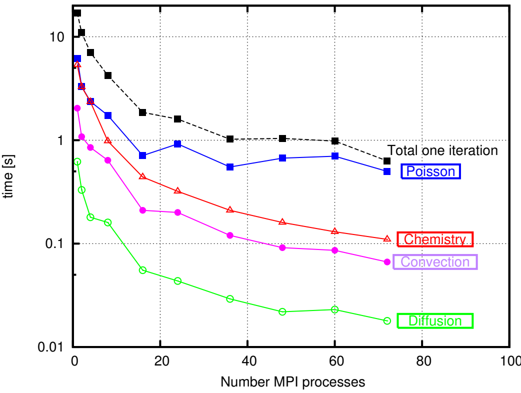

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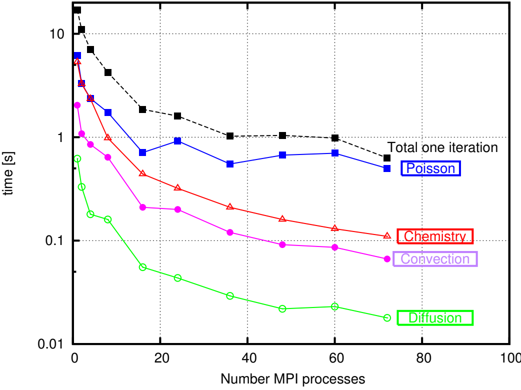

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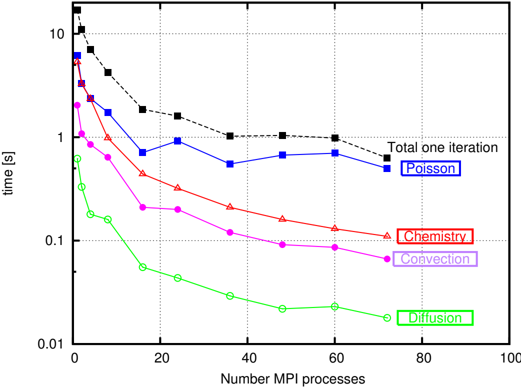
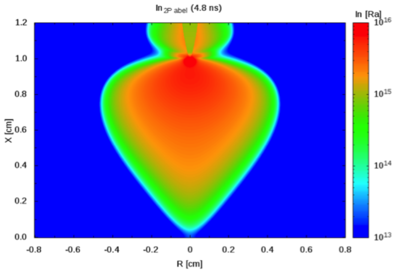


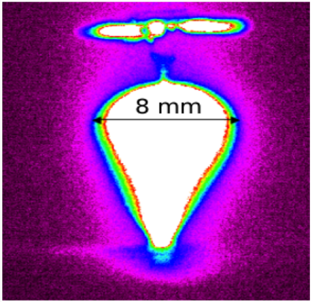
Comparison of results with experiments

Numerical/Experimental comparison

- Diameter of the discharge:
  8 mm / 8 mm
- Velocity of the discharge:
  $v_{num} = 2.6\ 10^8\ \mathrm{cm.s}^{-1}$ /
  $v_{exp} = 2.6 - 3.2\ 10^8\ \mathrm{cm.s}^{-1}$

Good agreement with experiments





Pierre Le Delliou PhD. Thesis.

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Conclusions

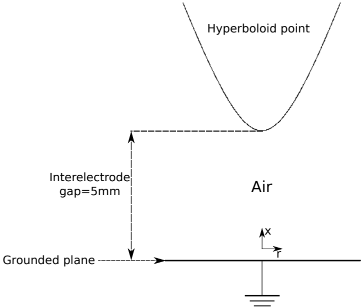
- For plasma applications, we need of course fast, robust and parallel iterative solvers (HYPRE is used for now)
- Even on 2D structured grids the computation can be very intensive
- Next step is mostly to use AMR meshes as well as improving the physical model (hybrid models)
- Currently in a joint project between LPP, CERFACS and SNECMA that just started, we also need to solve Poisson's equation to do a 3D simulation of a Hall thruster
- We are modifying a 3D massively parallel code AVBP to carry out these simulations but as of now this code does not solve Poisson's equation
- We are implementing now a laplacian operator in a 3D unstructured mesh framework based on a finite volume discretization coupled with the HYPRE library for the solving part
- Unstructured or not we need to implement accurate discretization and fast, robust and parallel library to solve Poisson's equation

Thanks

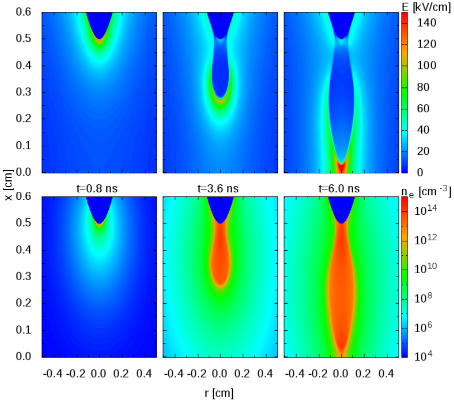
Thank you for your attention.

Improvements of the discharge code: Test-case 1

- 5 mm gap with a point to plane geometry with a stump point electrode
- Constant voltage applied at the anode, V_{anode} **= +13 kV**
- Computational domain is 1 cm $\times$ 17 cm with Cartesian grid
- Small domain size $n_x \times n_r = 1287 \times 1000$ so 1.3$\times$ 10^6 points



- Propagation of a cathode directed streamer from the point anode to the cathode plane
- At t= 3.6 ns, E_{axis}= 110 kV.cm^{-1} and $n_e = 3 \times 10^{13}$ cm^{-3}
- At t_c=6.0 ns, discharge impacts the cathode plane
- General time step: $\Delta t=10^{-12}$s
- Simulation time : $\sim$ 4 hours
- Improvements of computational time: introduce parallel protocols



Improvements of the discharge code: Test-case 1

- Poisson's equation is the most expensive equation to solve
- 1 for Poisson's equation and 6 (each iterated $\times$ 3) for photoionisation source term
- First step: introduction of **shared memory OPENMP** protocols:
  - Change of direct solver: MUMPS (MPI only) to PaStiX (MPI-OPENMP)
  - OPENMP protocols in the rest of the code

Code with:	MUMPS	PaStiX			
Memory:	664 Mo	886 Mo			
Nb thread	1	1	2	4	6
Factorization (s)	64.12	24.87	21.55	19.91	19.48
Solution (s)	1.27	0.64	0.38	0.25	0.22
One time-step (s)	5.76	2.71	1.76	1.51	1.36

- With 6 threads:
  - Speed up Poisson's equation: 5.77
  - Speed up one time step: 4.2
- Computational time for TC-1: 4 hours $\rightarrow \sim$ 40 minutes