Adaptation of SPARK to atmospheric-pressure micro-plasma jet flow conditions

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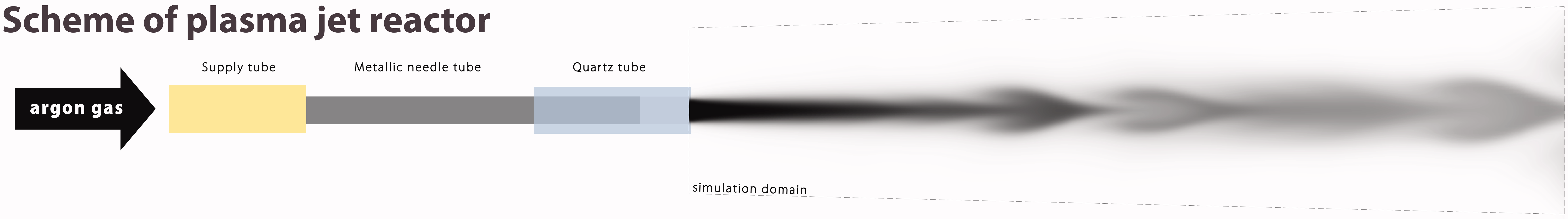
Scheme of plasma jet reactor



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Core adaptations to SPARK: Software Platform for Aerothermodynamics Radiation and Kinetics [1]

0 About SPARK, a CFD code

SPARK solves the **multi-component, multi-temperature, Navier-Stokes** equations which can be written as:

- ***s* mass conservation equations**, one for each of *s* species:

$$\frac{\partial \rho_s}{\partial t} + \vec{\nabla}\cdot(\rho_s \vec{u}) = \vec{\nabla}\cdot \boxed{\vec{J}_s} + \boxed{\dot{\omega}_s}$$

- **1 momentum conservation equation**:

$$\frac{\partial (\rho \vec{u})}{\partial t} + \vec{\nabla}\cdot(\rho \vec{u}\otimes\vec{u}) = \vec{\nabla}\cdot[\tau] - \vec{\nabla}P$$

- **1 total energy conservation equation**:

$$\frac{\partial (\rho E)}{\partial t} + \vec{\nabla}\cdot(\rho \vec{u} E) = \vec{\nabla}\cdot\left(\sum_k q_{C_k} + \sum_s \vec{J}_s h_s + \vec{u}\cdot[\tau] - Pu\right) + \dot{Q}$$

- ***k* non-equilibrium energy conservation equations**, one for each of k energy mode:

$$\frac{\partial (\rho \epsilon_k)}{\partial t} + \vec{\nabla}\cdot(\rho \vec{u} h_k) = \vec{\nabla}\cdot(q_{C_k} + q_{D_k}) + \boxed{\dot{Q}_k}$$

Species source terms (in blue) are calculated from rate coefficients following a prescribed **kinetic scheme**.

The mass diffusive fluxes (in red) ensure a **neutral fluid** by using **ambipolar diffusion coefficients**.

How is a plasma created?

With an **energy source** in the **free-electron energy equation** (green). This **increases electron temperature** which favours **electron-impact reactions** that in turn **create excited species**, e.g. Ar(4S) species.

1 Testing SPARK in subsonic conditions

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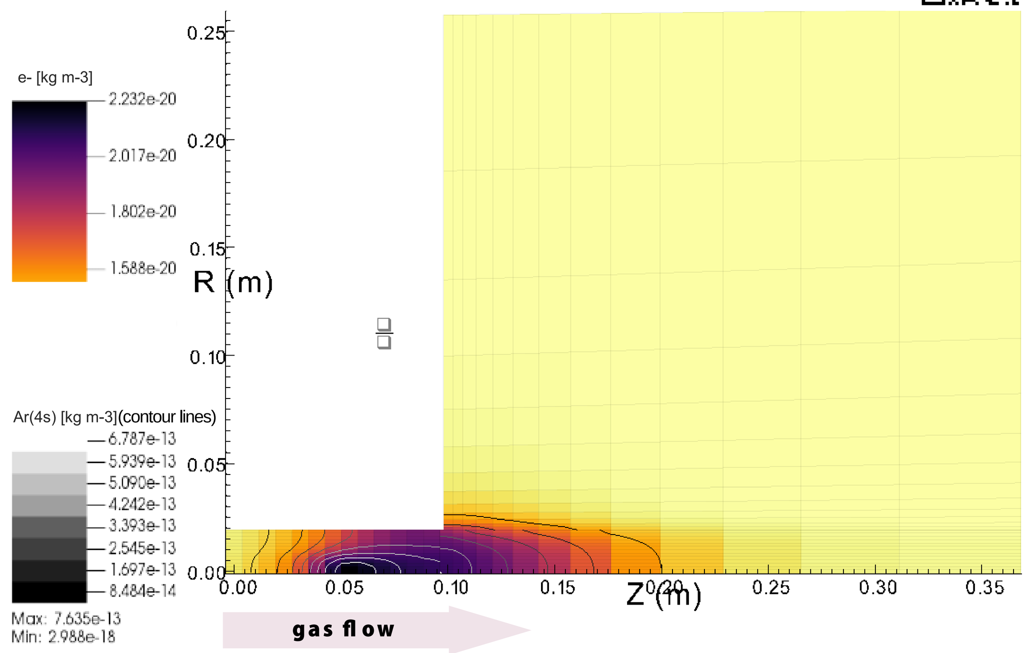
Electrons and Ar(4S) mass fraction



Simulations of inviscid jet, pure argon gas, argon kinetic scheme. An electron energy source was place at (R, Z)= (0, 0.05) m.

Demonstration that **SPARK can simulate**:

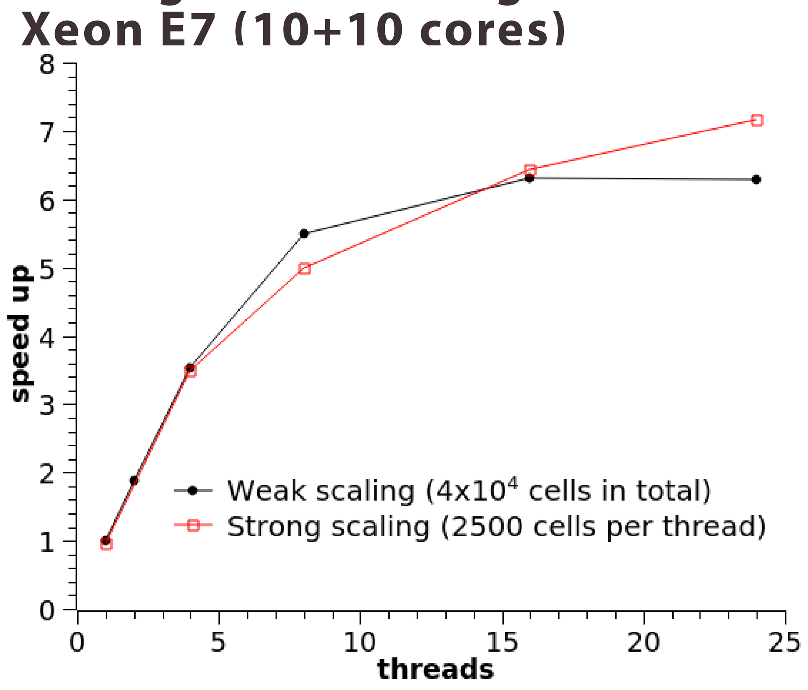
- Jet flows under **subsonic conditions**;
- **Non-equilibrium** between **gas** and free-**electron temperature**;
- **Chemical non-equilibrium**;

Problems include:

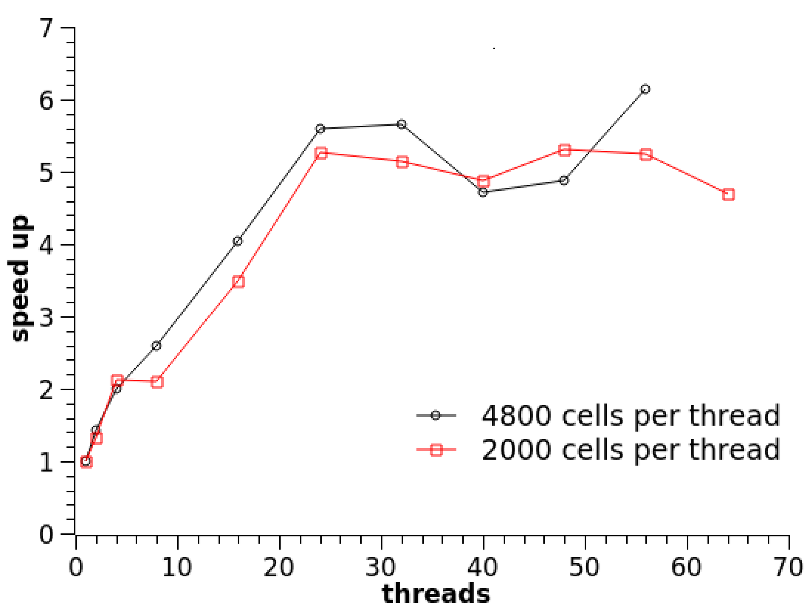
1. **Long computation times** for high resolution meshes;
2. **High numerical dissipation**;
3. **Slow convergence**.

2 Parallelizing SPARK with OpenMP [2]

Strong/weak scaling 2x Intel Xeon E7 (10+10 cores)



Strong scaling AMD EPYC 7552 (48 cores)



speed up = (simulation time with 1 thread) / (simulation time with # threads)

From the scaling tests we can see that:

- OpenMP is a **simple parallelization** method that leads to significant results;
- It is possible to consistently obtain **~6x speed ups**;
- If the computation servers have hyperthreading enabled, scaling test might show inconsistent results.

3 Lower dissipation: SLAU solver [3], WENO-5 reconstruction [4]

SLAU is a flux solver formulated to have the numerical dissipation term with better scaling for low-Mach flows.

WENO-5 is a 5th order spatial reconstruction method that allows for higher accuracy, or equivalently low dissipation, for lower cell count while reducing oscillations

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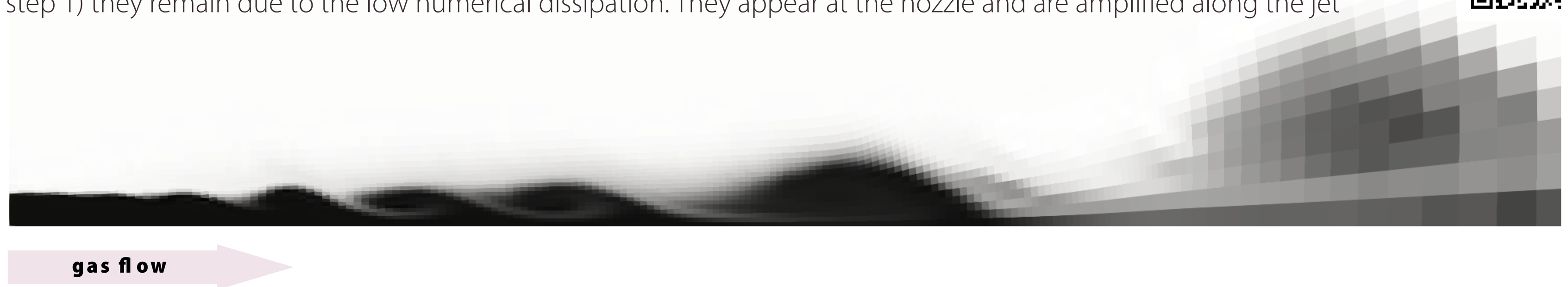
Simulation of inviscid jet flow, perfect gas model

Flow instabilities appear due to numerical oscillations or reflected acoustic waves, and instead of being dissipated (as in step 1) they remain due to the low numerical dissipation. They appear at the nozzle and are amplified along the jet



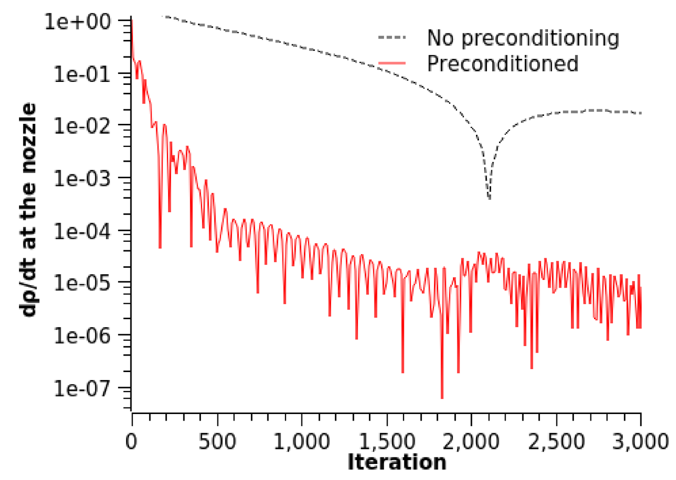
4 Preconditioning [5]

For inviscid flows: $\lambda_{max} = \mathbf{u} + \mathbf{c}$ — **u: flow velocity**

$\lambda_{min} = \mathbf{u}$ — **c: speed of sound**

If $\mathbf{u} << \mathbf{c}$ the equations become stiff and convergence is slow

Preconditioning speeds up convergence by making $\lambda_{max} \approx \lambda_{min}$



5 Uniform grouping in Ar kinetic scheme

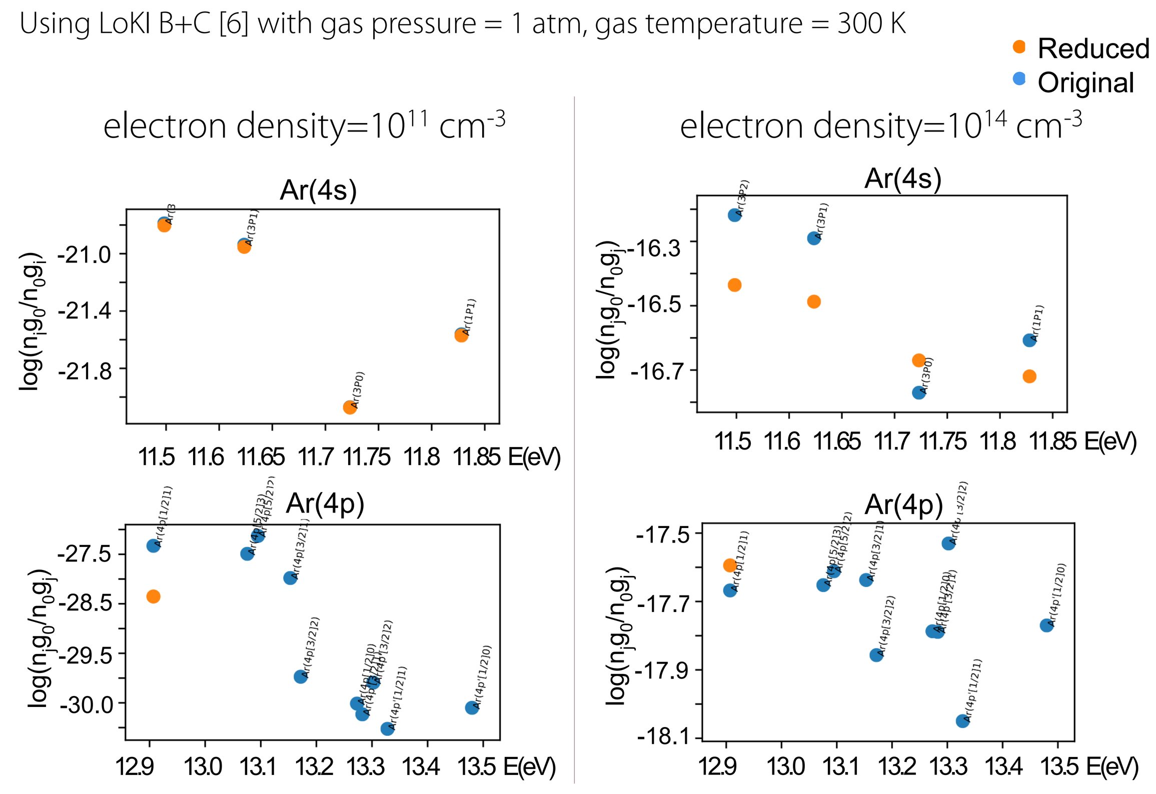
A **macro state** is created by grouping some states weighted by their statistical weights. Forward rate and backward rate coefficients are calculated, respectively, by simple and weighted sum of the original rate coefficients.

The macro states in our argon kinetic scheme are:

- Ar(4p) from the grouping of Ar(4pi) states;
- Ar* from the grouping of Ar(5pi), Ar(3d+5s), Ar(3d'+5s').

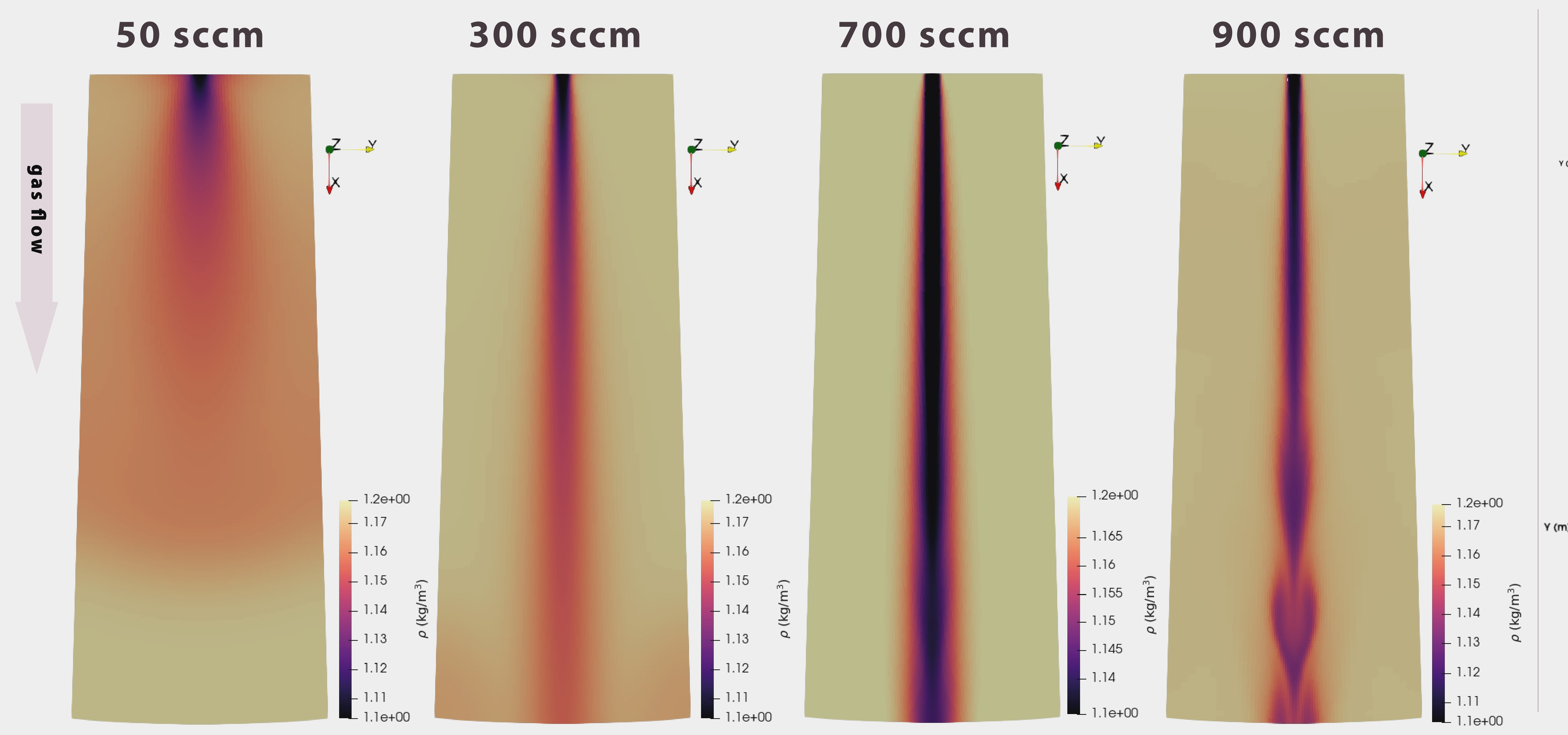
Comparison between reduced and original scheme

Using LoKI B+C [6] with gas pressure = 1 atm, gas temperature = 300 K

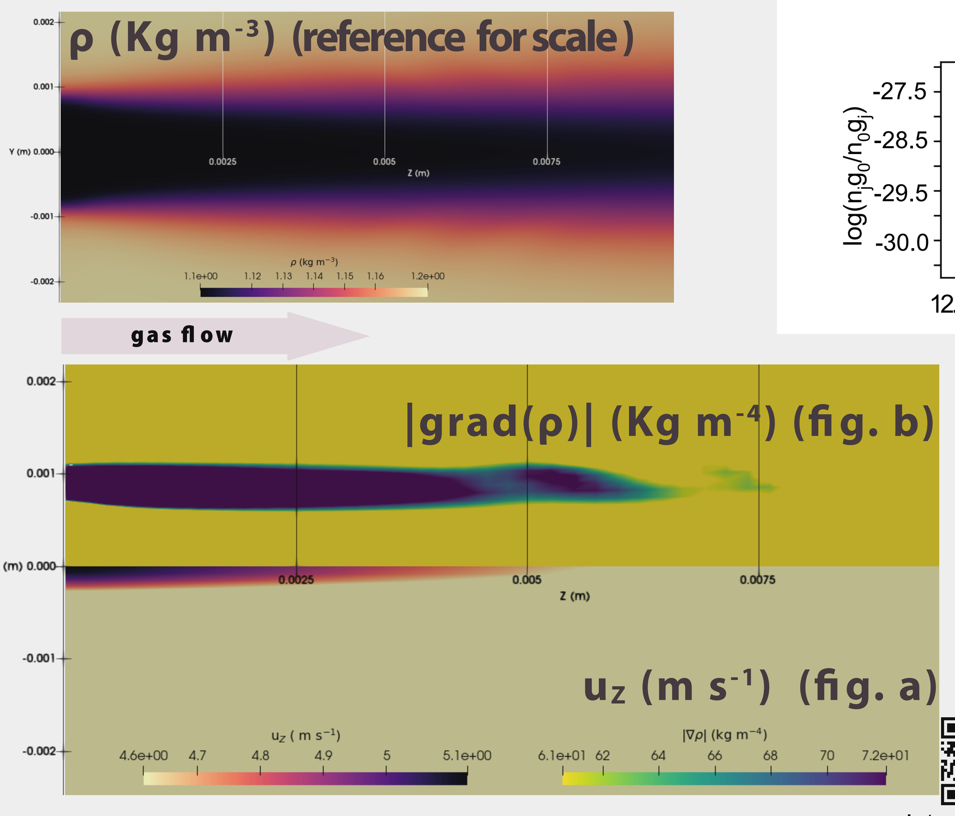


Simulations after improvements 1 to 5

From a diffusive to an unstable jet, ρ (Kg m⁻³)



Appearance of axisymmetric instabilities at 900 sccm



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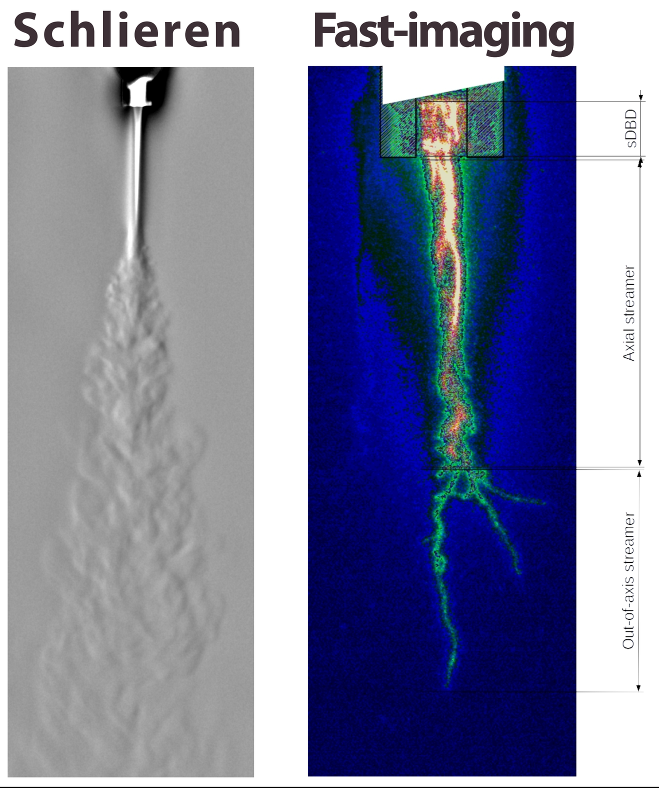
With varying flow rate we observe the **same qualitative behavior** as with Schlieren experiments performed at LPGP. For low flow rates, below 100sccm, we obtain a **diffusive jet**. At intermediate flow rates a long **laminar jet** is present. At high flow rates +600sccm coherent structures appear and are amplified along the **unstable jet**.

Near the nozzle the simulated jet depicts a **"cone" velocity** profile (see fig. a) in which the velocity drops slowly. The axisymmetric instabilities seem to become more noticeable closer to the end of the velocity "cone" (see fig. b).

Macroscopic streamer model to couple to SPARK

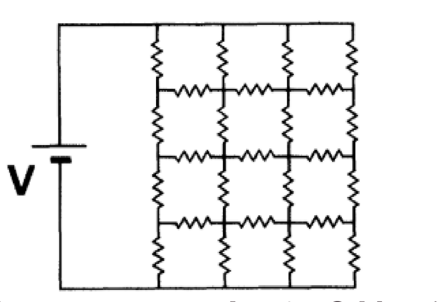
Streamers in APMPJs

Schlieren — Fast-imaging



Resistor percolation model [7]: light to compute, similar spatial profile

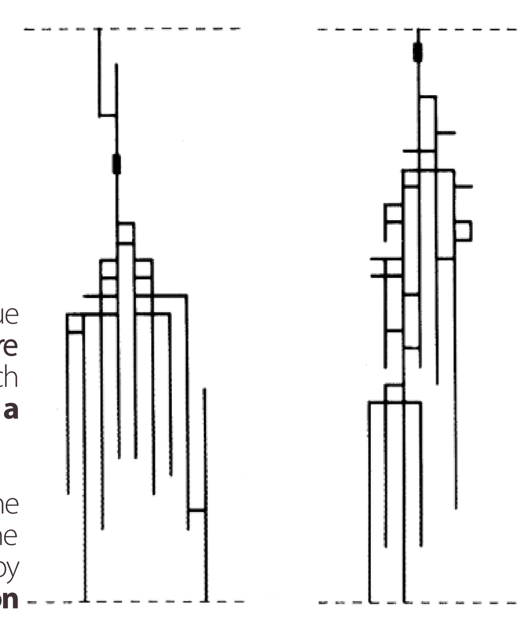
Electric circuit model



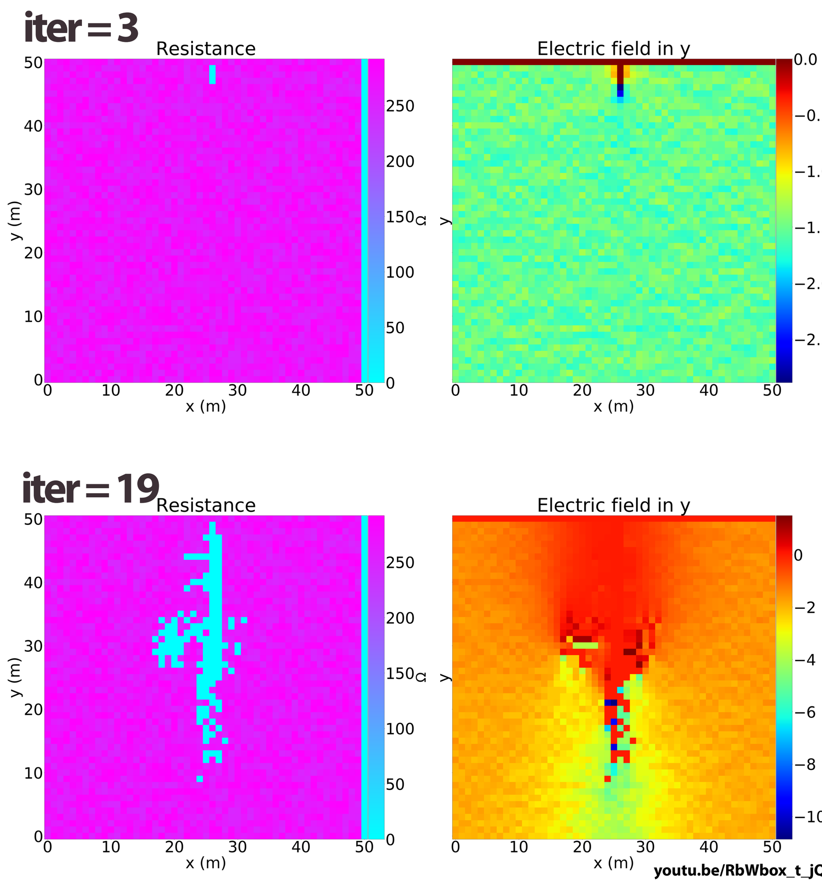
Above a certain **electric field** value between two nodes, the **resistors are** converted to **"short-circuits"** which mimics the behaviour of a **streamer in a dielectric medium**.

Compared with streamers in plasma, one major limitation is the **exclusion** of the **displacement field**. This can be solved by using a **resistor-capacitor percolation model [8].**

Streamer trajectory



2D resistive model example



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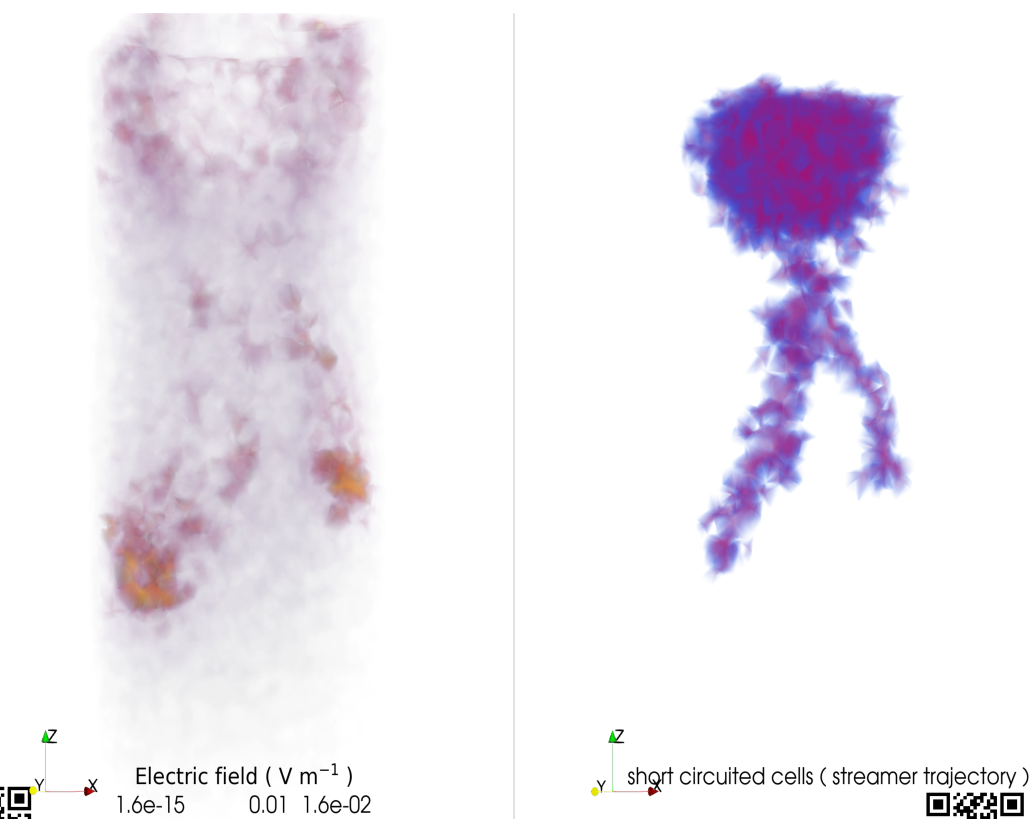
3D resistive model example



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