INP
FROM IDEA TO PROTOTYPE

Verification and performance test of electric discharge modeling code developed in FEniCS

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FROM IDEA TO PROTOTYPE

Overview

- Description of the model
- FEniCS
- Code verification
  - Method of exact solutions
  - Benchmarking
- Performance testing
- Conclusion

Electric discharge modeling

- Governing equations
  - Poisson's equation

$$\nabla^2\phi = -\sum_\alpha \frac{q_\alpha n_\alpha}{\varepsilon}$$

  - Balance equations for particle number densities

$$\frac{\partial n_\alpha}{\partial t} + \nabla\cdot\boldsymbol{\Gamma}_\alpha = S_\alpha$$

where $\boldsymbol{\Gamma}_\alpha = -\mathrm{sgn}(q_\alpha) n_\alpha b_\alpha \nabla\phi - \nabla(D_\alpha n_\alpha)$

  - Electron energy balance equation

$$\frac{\partial w_e}{\partial t} + \nabla\cdot\boldsymbol{Q}_e = -e\boldsymbol{E}\cdot\boldsymbol{\Gamma}_e + \tilde{S}_e$$

where $\boldsymbol{Q}_e = n_e\tilde{b}_e\nabla\phi - \nabla(\tilde{D}_e n_e)$

- Boundary conditions:
  - Poisson's equation:
    - Dirichlet boundary condition
    - Neumann boundary condition
    - Robin boundary condition (e.g. on dielectrics for DBD modeling)
  - Particle balance equations [1,2]:
    - For heavy particles

$$\boldsymbol{\Gamma}_{\boldsymbol{h}}\cdot\boldsymbol{n} = \frac{1-r_h}{1+r_h}\left(|\mathrm{sgn}(q_h) b_h E n_h| + \frac{1}{2} v_{th,h} n_h\right)$$

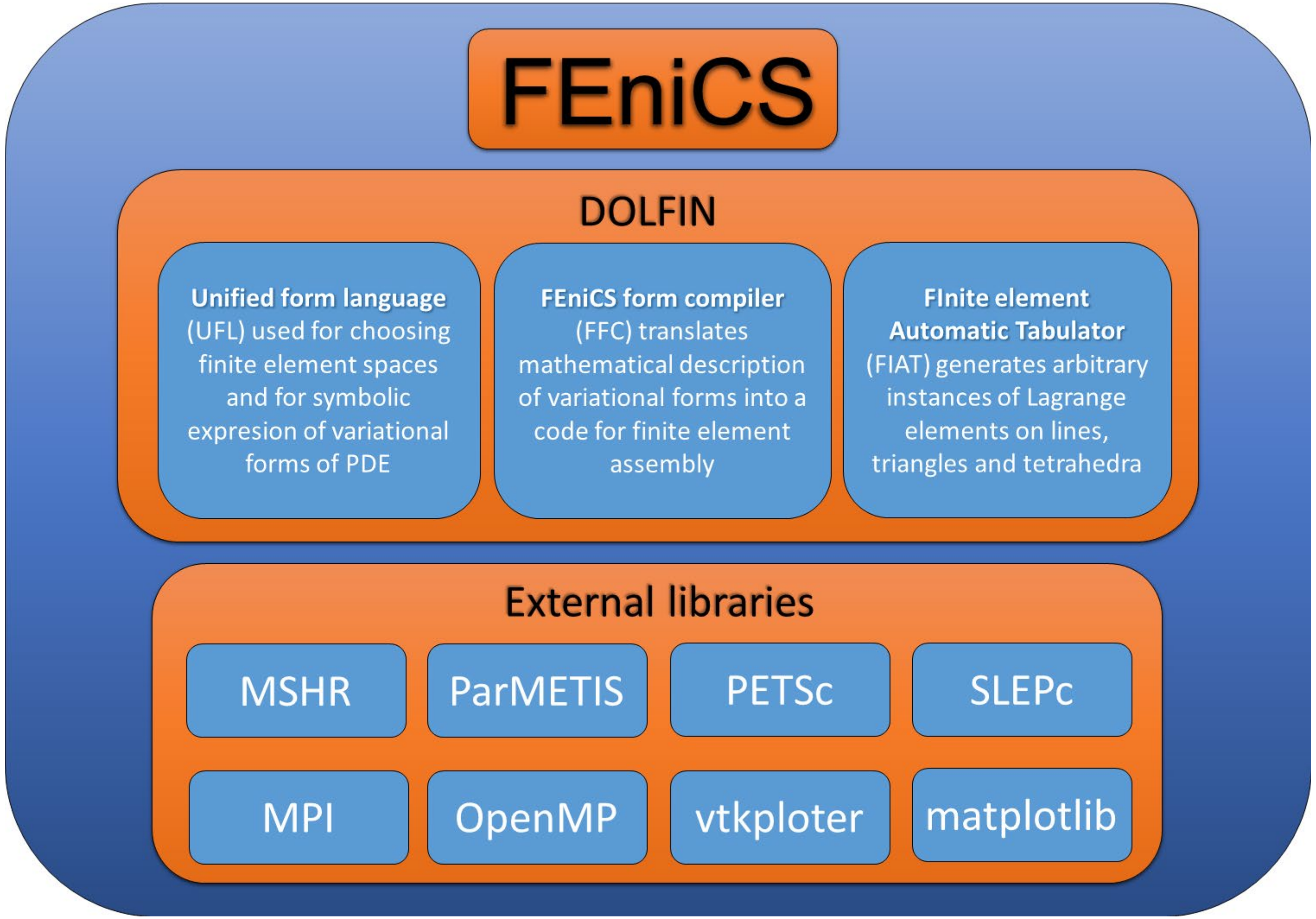
    - For electrons

$$\boldsymbol{\Gamma}_{\boldsymbol{e}}\cdot\boldsymbol{n} = \frac{1-r_e}{1+r_e}\left(|b_e E n_e| + \frac{1}{2} v_{th,e} n_e\right) - \frac{2}{1+r_e}\gamma \sum_i \max(\boldsymbol{\Gamma}_i\cdot\boldsymbol{n}, 0)$$

  - Electron energy balance equation [2]:
    - $\boldsymbol{Q}_{\boldsymbol{e}}\cdot\boldsymbol{n} = \frac{1-r_e}{1+r_e}\left(|\tilde{b}_e E_e| + \frac{1}{2}\tilde{v}_{th,e} n_e\right) - \frac{2}{1+r_e}\gamma\bar{\varepsilon}^\gamma \sum_i \max(\boldsymbol{\Gamma}_i\cdot\boldsymbol{n}, 0)$

[1] *G. J. M. Hagelaar et al., Phys. Rev. E* ***62*** *(2000) 1452*
[2] *Becker et al., J. Phys. D: Appl. Phys.* ***46*** *(2013) 355203*

FEniCS



FEniCS

DOLFIN

Unified form language (UFL) used for choosing finite element spaces and for symbolic expresion of variational forms of PDE

FEniCS form compiler (FFC) translates mathematical description of variational forms into a code for finite element assembly

FInite element Automatic Tabulator (FIAT) generates arbitrary instances of Lagrange elements on lines, triangles and tetrahedra

External libraries

MSHR

ParMETIS

PETSc

SLEPc

MPI

OpenMP

vtkploter

matplotlib

[1] *A. Logg et al. Automated Solution of Differential Equations by the Finite Element Method, Springer, Berlin 2012*

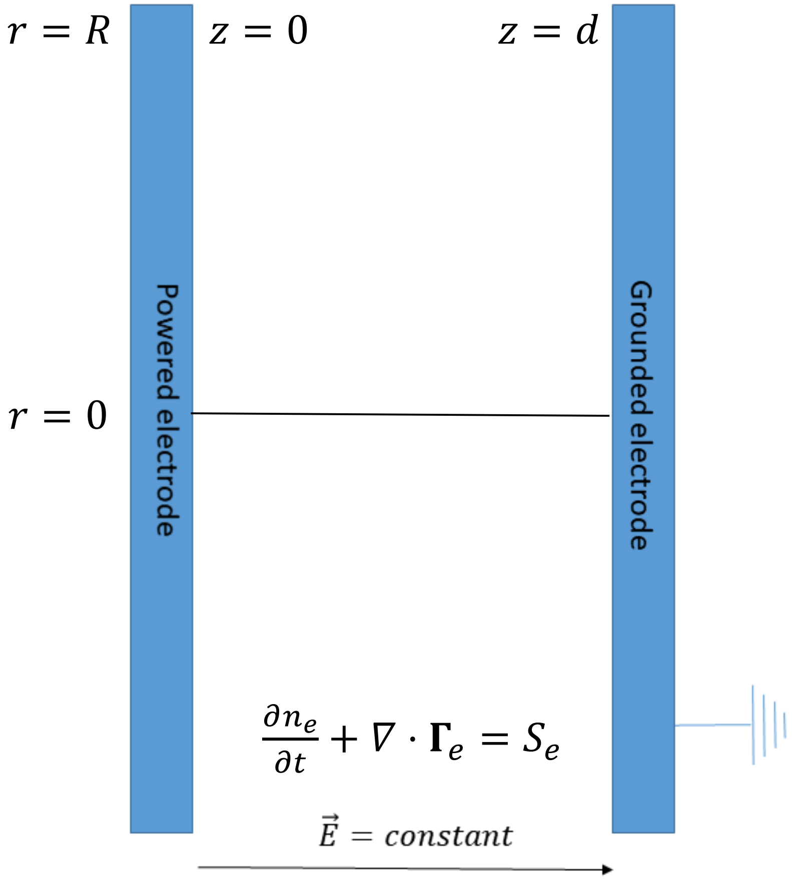
[2] *https://fenicsproject.org*

Verification of the FEniCS code

- Three examples of time-dependent, two-dimensional modeling
- Method of exact solutions
  - Modeling of the electron number density profile in time of flight (TOF) experiment
- Benchmarking
  - Modeling of an axisymmetric positive streamer in air
  - Modeling of a low pressure glow discharge in argon
- For all cases linear Lagrange (triangular) elements are used
- The mesh size depends on application requirements (finer for streamer, while coarser for glow discharge modeling)
- Backward differentiation formula (BDF) of the order of 2 is used for time discretization
- Adaptive time stepping control is done using proportional–integral–derivative (PID) controller

Method of Exact Solutions – Time of flight experiment

- Time of flight experiment in air at $760\ \mathrm{Torr}$ and $300\ \mathrm{K}$
- Planar electrodes in a square domain of 1 mm radius and gap distance
- Constant electric field is assumed, so only particle balance equation for the electrons is solved
- For this particular field, attachment is negligible
- The modeling is done in a time range between 3 and 6 ns



Method of Exact Solutions – Time of flight experiment

- Since electric field is constant, only particle balance equation for the electrons is solved

$$\frac{\partial n_e}{\partial t} + \nabla \cdot \mathbf{\Gamma}_e = (\alpha - \eta) n_e v_e$$

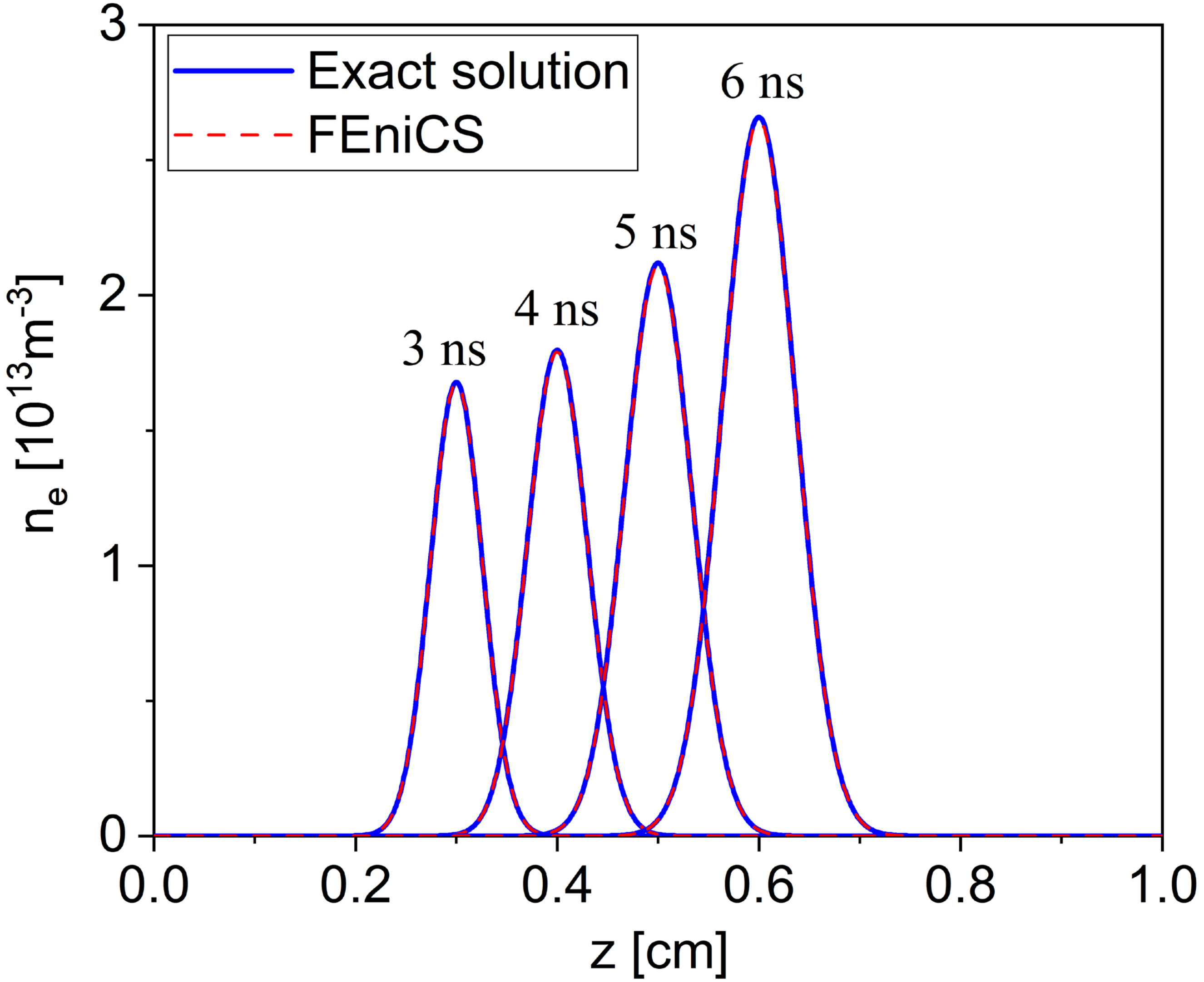
- The analytic solution of this equation is 2D Gaussian profile [1, 2]

$$n_e = (4\pi D t)^{-3/2} e^{-\frac{(z-vt)^2 + r^2}{4Dt} + (\alpha-\eta)vt}$$

- The mesh consists of approx. 100 000 elements

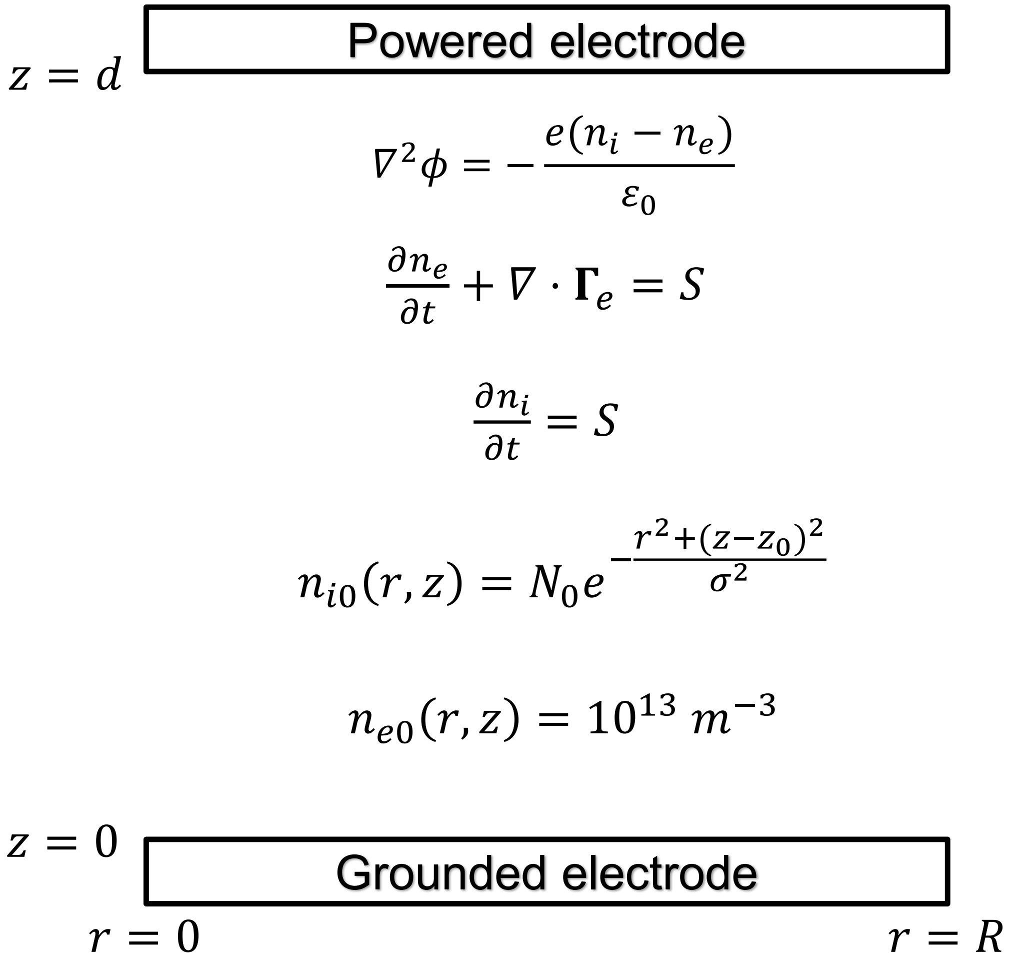
- Time step was constant $\Delta t = 10^{-12}$ s

[1] *Yu. P. Raizer, Gas discharge physics, Springer, Berlin 1991*
[2] *H. A. Blevin et al., Aust. J. Phys.,* ***37*** *(1984) 593*



Benchmarking – Modeling of an axisymmetric positive streamer in air

- Positive streamer in air at $760\ \mathrm{Torr}$ and $300\ \mathrm{K}$
- Planar electrodes in a square domain of $1.25\ \mathrm{cm}$ radius and gap distance
- Background electric field is $15\ \mathrm{kV/cm}$, which is below breakdown field
- Initial Gaussian seed is introduced near the powered electrode to locally enhance the field and start the streamer



$$\nabla^2\phi = -\frac{e(n_i - n_e)}{\varepsilon_0}$$

$$\frac{\partial n_e}{\partial t} + \nabla \cdot \boldsymbol{\Gamma}_e = S$$

$$\frac{\partial n_i}{\partial t} = S$$

$$n_{i0}(r,z) = N_0 e^{-\frac{r^2+(z-z_0)^2}{\sigma^2}}$$

$$n_{e0}(r,z) = 10^{13}\ m^{-3}$$

[1] *B. Bagheri et al., Plasma Sources Sci. Technol.* ***27*** *(2018) 09500*

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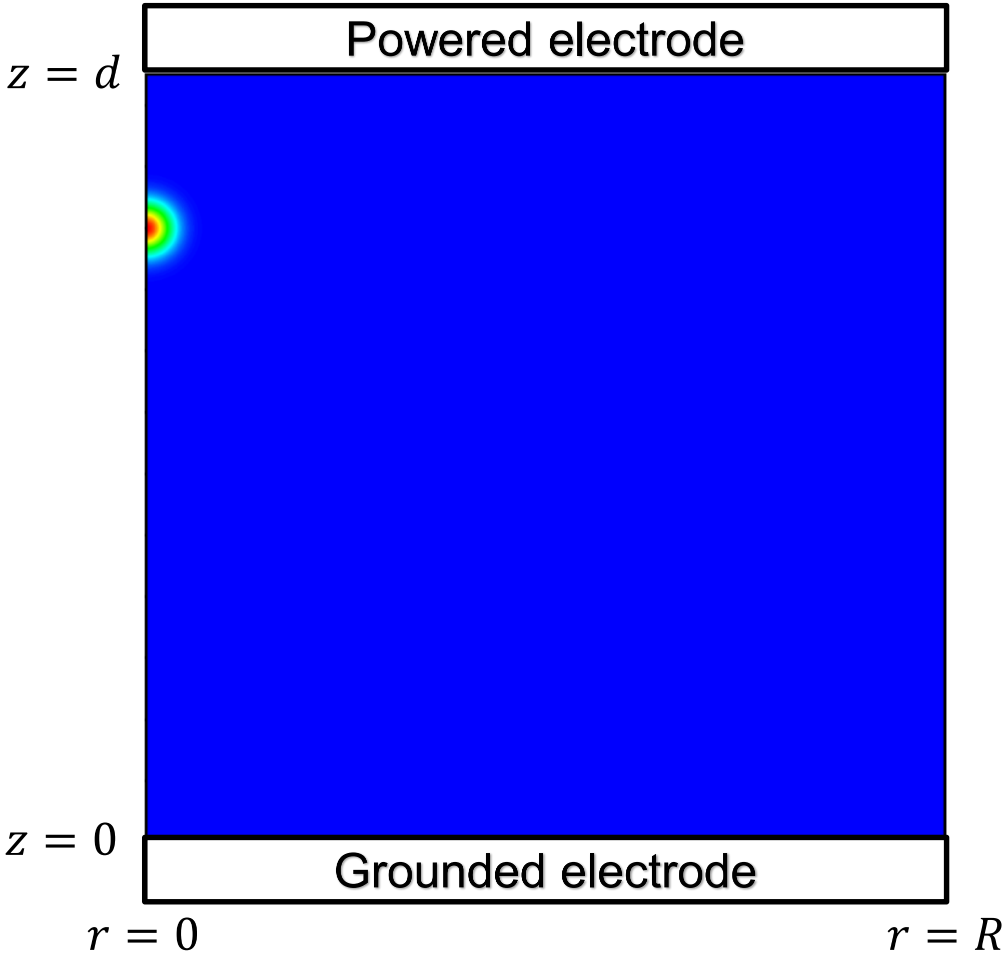

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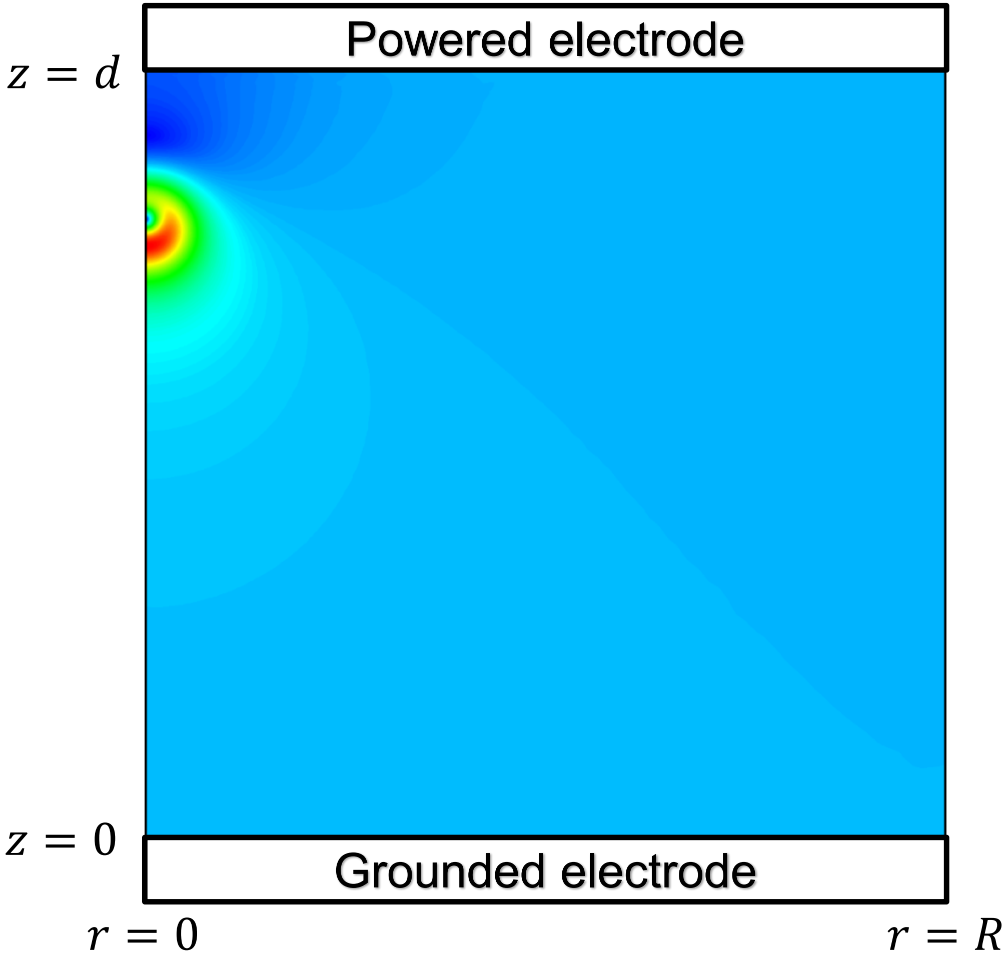

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Benchmarking – Modeling of an axisymmetric positive streamer in air

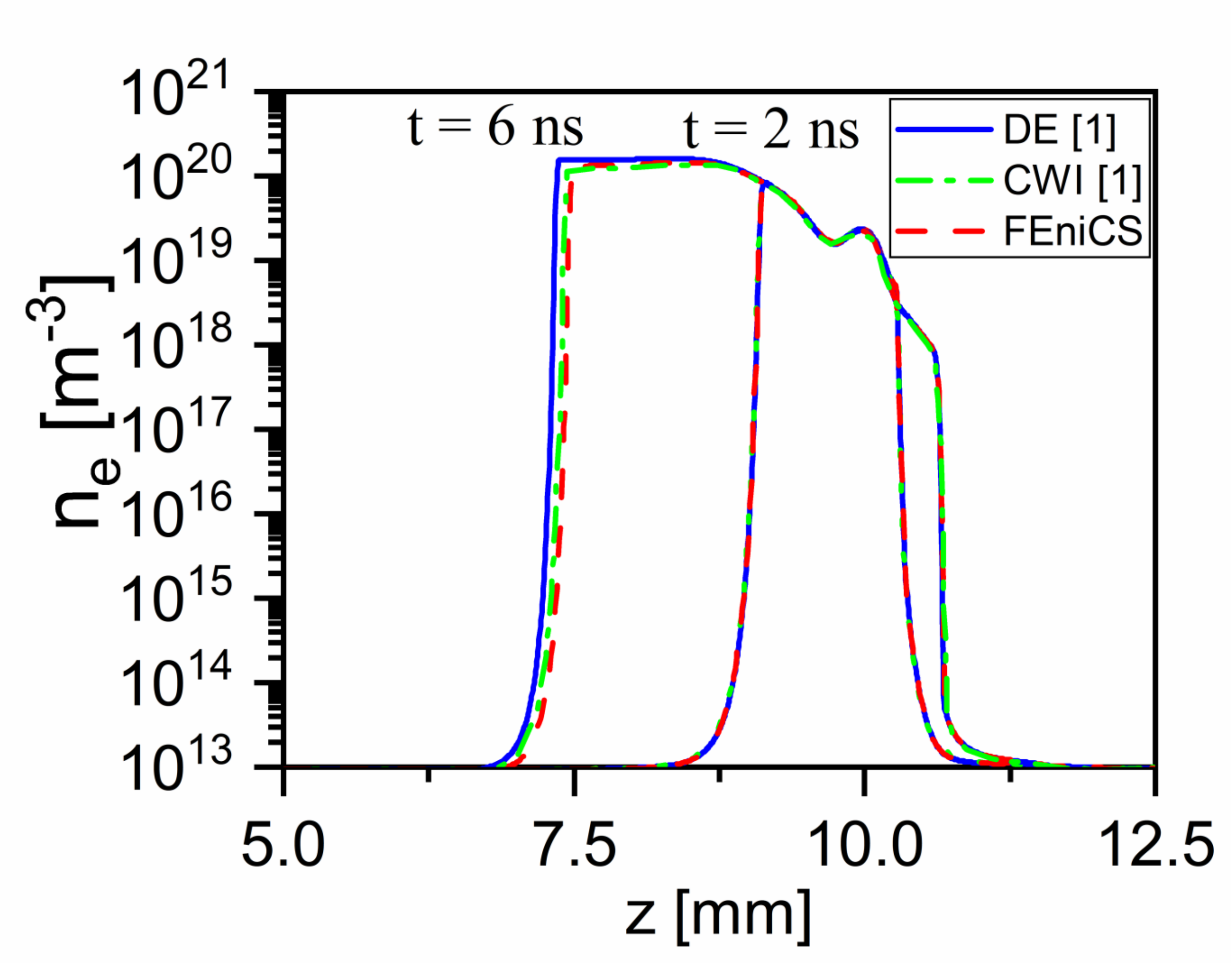
- Poisson’s equation and particle balance equation for electrons and ions are solved

$$\nabla^2\phi = -\frac{e(n_i - n_e)}{\varepsilon_0}$$

$$\frac{\partial n_e}{\partial t} + \nabla \cdot \mathbf{\Gamma}_e = S$$

$$\frac{\partial n_i}{\partial t} = S$$

- The mesh consisted of 500 000 elements (approximately equal as in COMSOL)
- Mesh was refined towards the axis and streamer region
- Time step was constant $\Delta t = 5 \times 10^{-12}$ s



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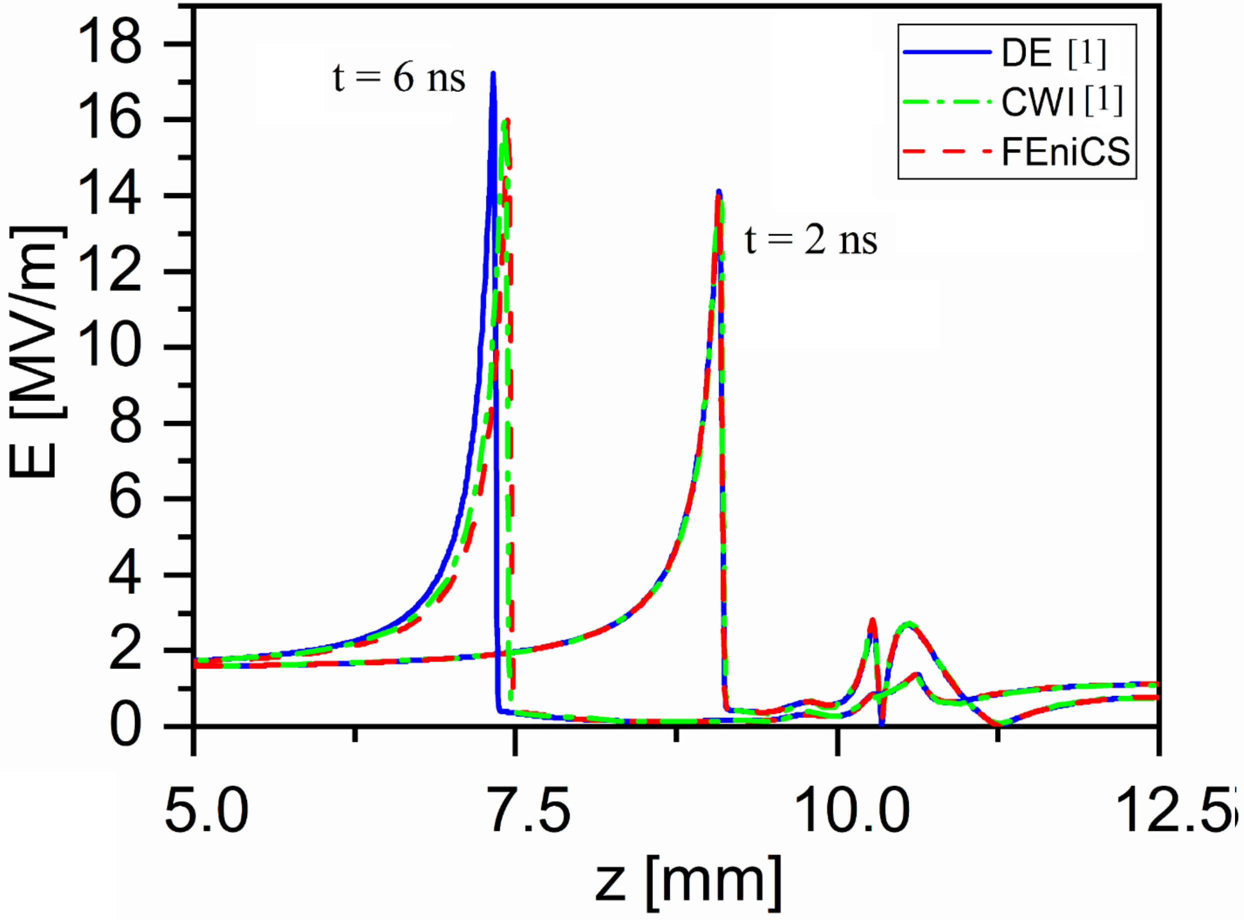
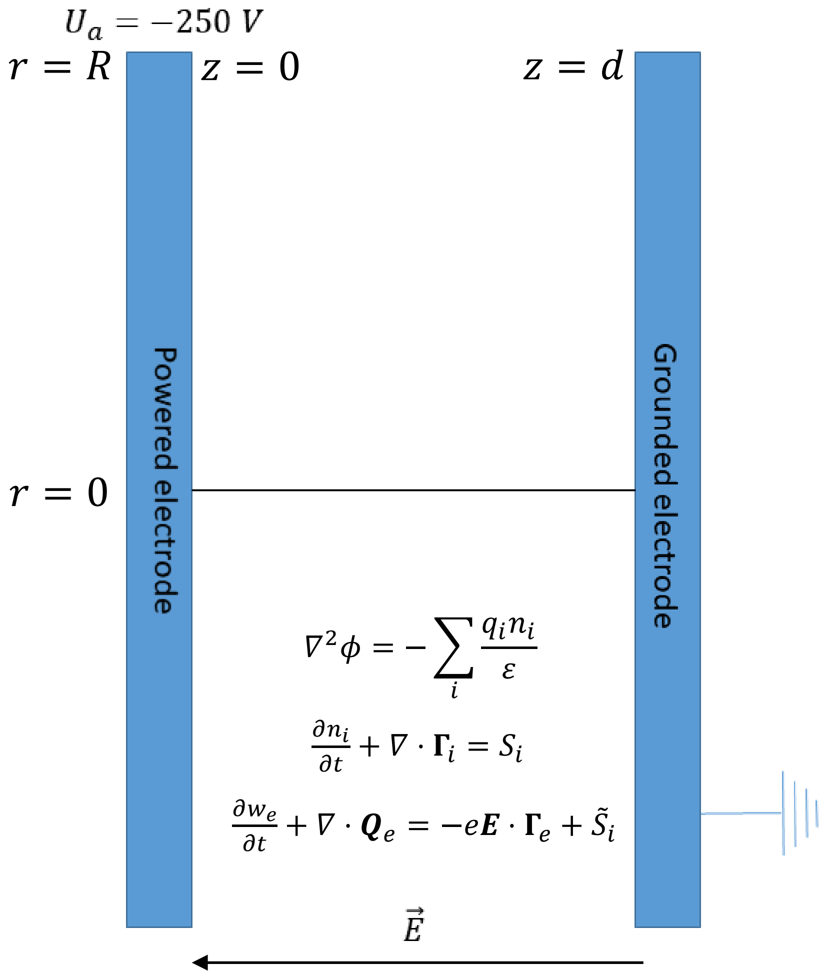


[1] *B. Bagheri et al., Plasma Sources Sci. Technol.* ***27*** *(2018) 09500*

Benchmarking – Modeling of a low pressure glow discharge in argon

- Glow discharge in argon at 1 Torr and 300 K
- Planar electrodes in a square domain of 1 cm radius and gap distance
- Voltage $U_a = -250\ \mathrm{V}$ is applied to the cathode

[1] Becker M M et al., Comput. Phys. Commun. **180** (2009) 1230



$$\nabla^2 \phi = -\sum_i \frac{q_i n_i}{\varepsilon}$$

$$\frac{\partial n_i}{\partial t} + \nabla \cdot \mathbf{\Gamma}_i = S_i$$

$$\frac{\partial w_e}{\partial t} + \nabla \cdot \boldsymbol{Q}_e = -e\boldsymbol{E} \cdot \mathbf{\Gamma}_e + \tilde{S}_i$$

Benchmarking – Modeling of a low pressure glow discharge in argon

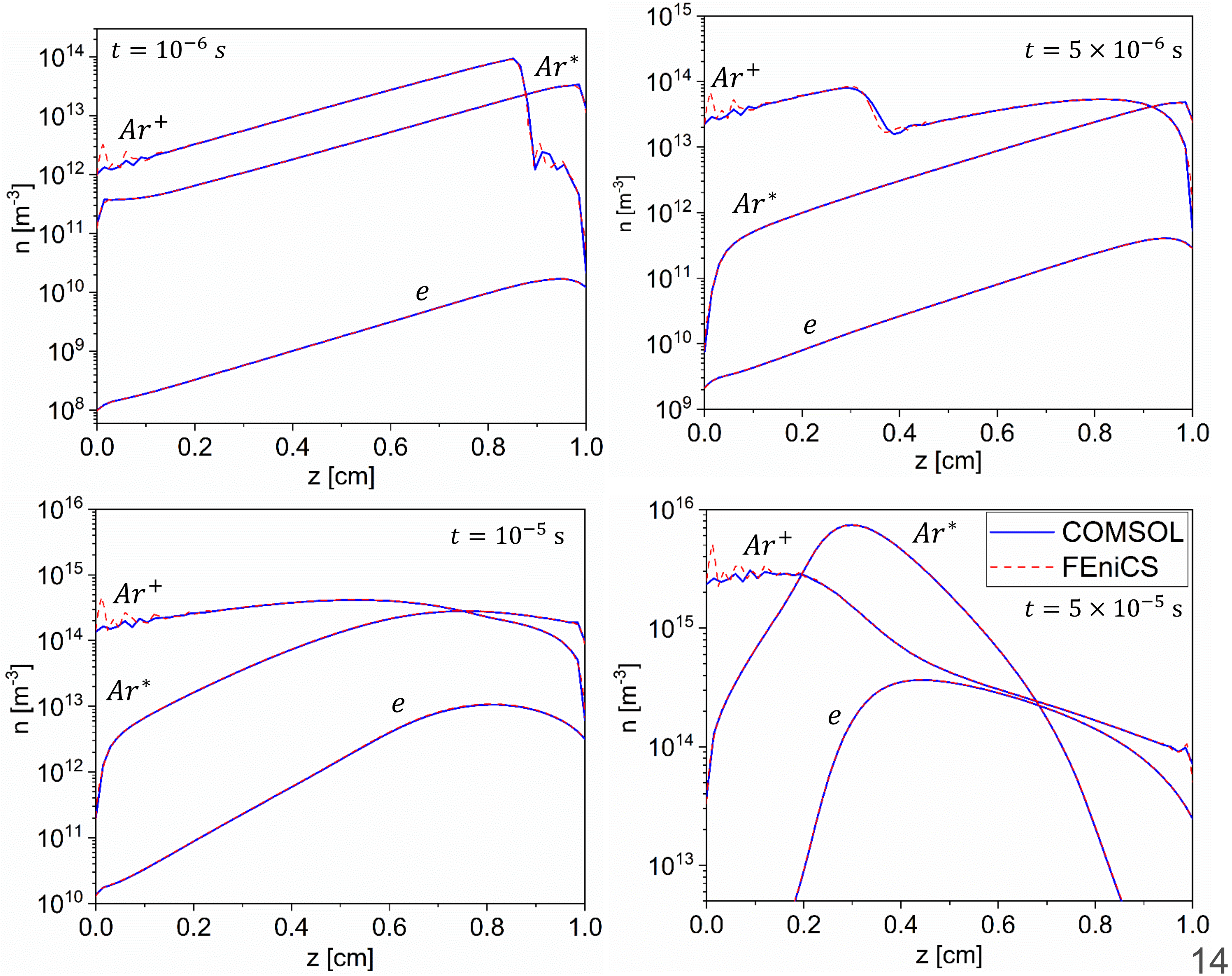
- Poisson particle balance equation and electron energy balance equation are solved

$$\nabla^2\phi = -\sum_i \frac{q_i n_i}{\varepsilon}$$

$$\frac{\partial n_i}{\partial t} + \nabla \cdot \boldsymbol{\Gamma}_i = S_i$$

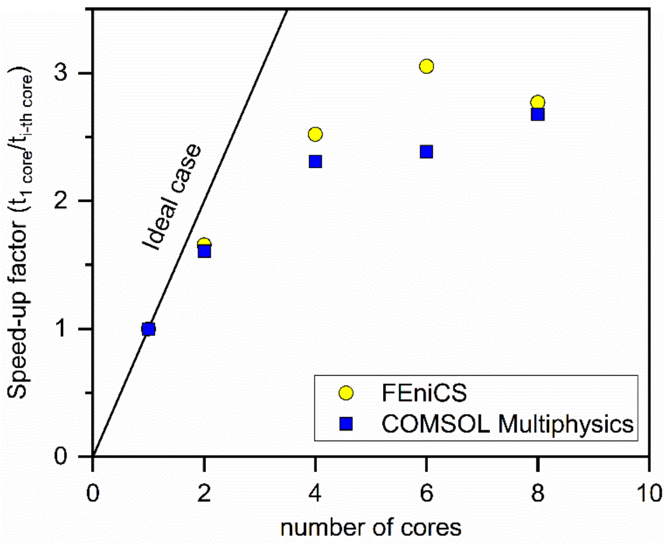
$$\frac{\partial w_e}{\partial t} + \nabla \cdot \boldsymbol{Q}_e = \tilde{S}_e$$

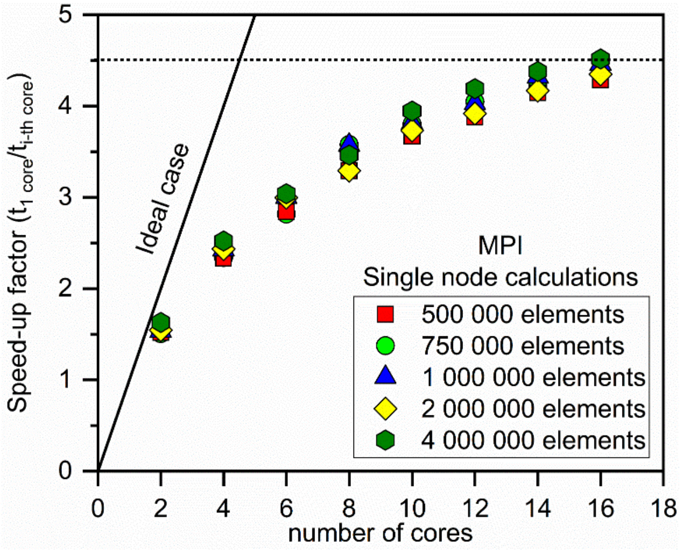
- Numerical model takes into account four particle species: Ar, Ar^*, Ar^+ and electrons
- Approx. 20 000 elements were used
- Adaptive time step was used ($\Delta t_{max} = 10^{-8}$ s)

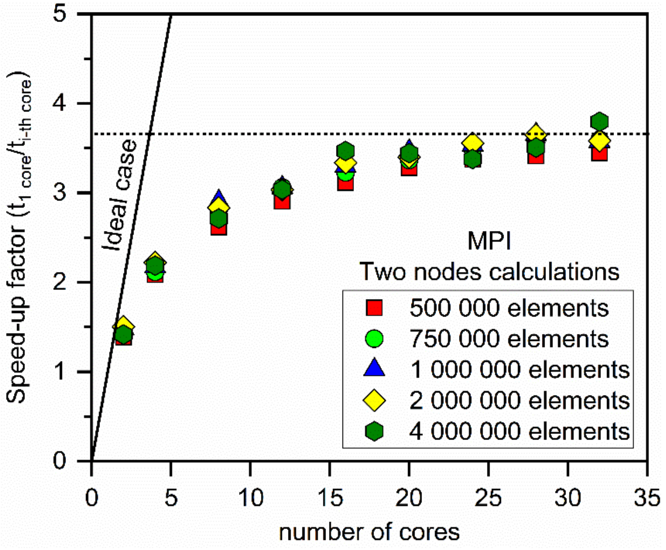


Performance testing

- Speed-up factor is calculated by running streamer benchmark code on a different number of cores
- In all the cases MPI was used, since OMP did not have any influence on the performance
- Single-node calculations: similar speed-up as in parallel performance comparison.
- Two-node calculations: speed-up is worse than for single-node case due to limited speed of data transfer between the nodes (1Gbit/s-Ethernet).
- Better multi-node performance is expected with InfiniBand connection between compute nodes (to be tested).





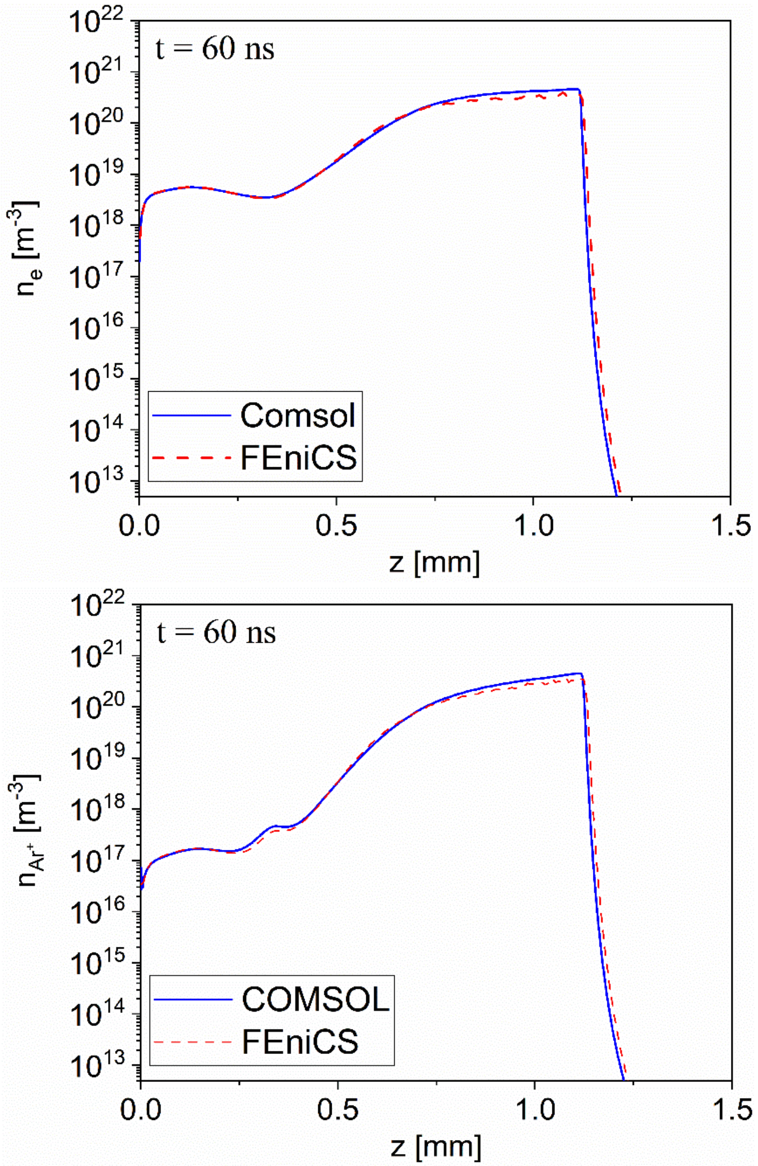


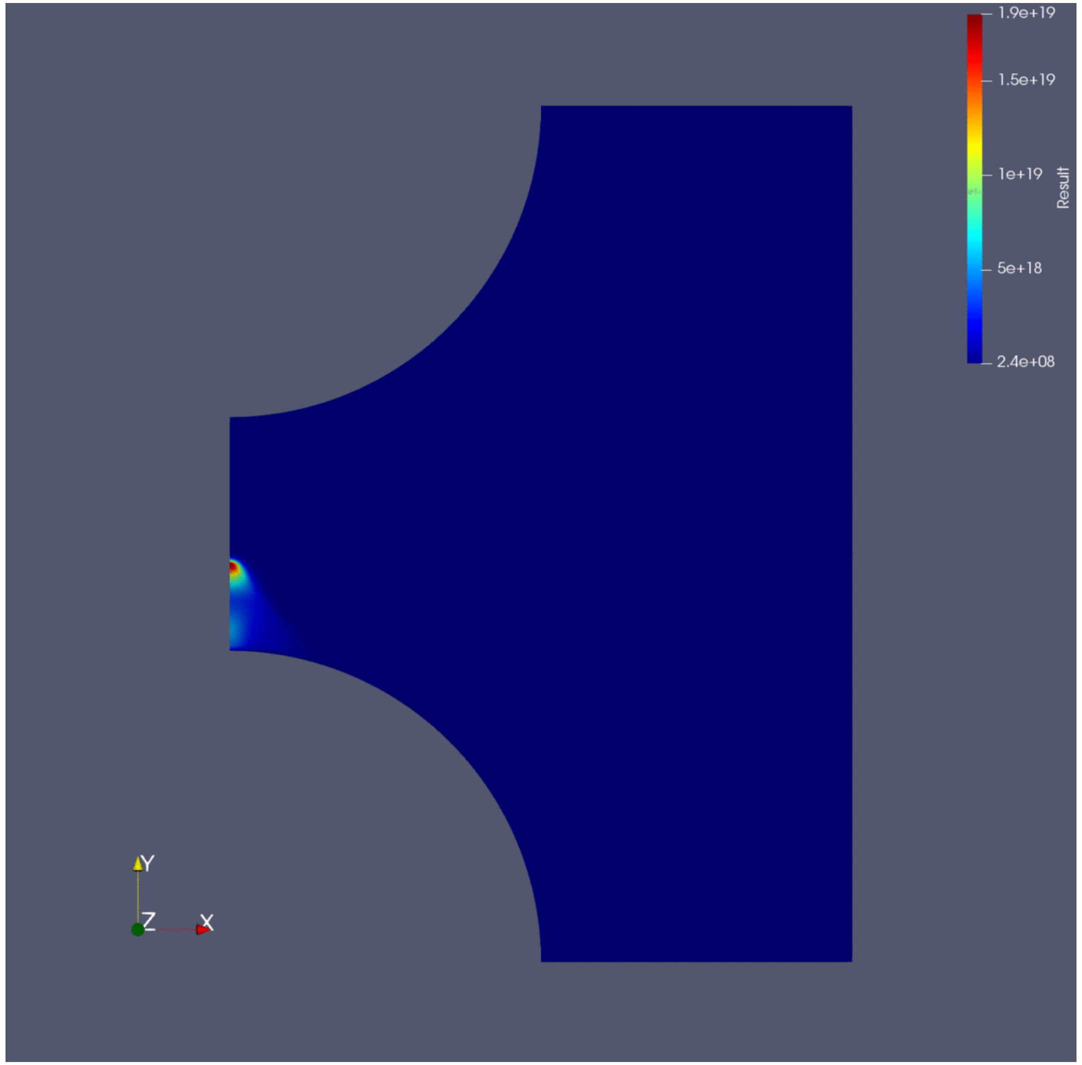
Conclusion

- Code for electrical discharge modeling at various conditions is developed in FEniCS
- The code is verified using method of exact solutions and benchmarking
- Performance was tested by running the streamer benchmark code in parallel on a computer cluster
- Relatively good speed-up is observed on a single node, comparable to COMSOL Multiphysics performance
- Speed-up obtained by using two cluster nodes is not satisfying due to connection speed between nodes, but can be improved using InfiniBand

Outlook

- Modeling single filament dielectric barrier discharge at atmospheric pressure
- Adapt the model for two or more subdomains
- Adapt model for arbitrary number of particle species





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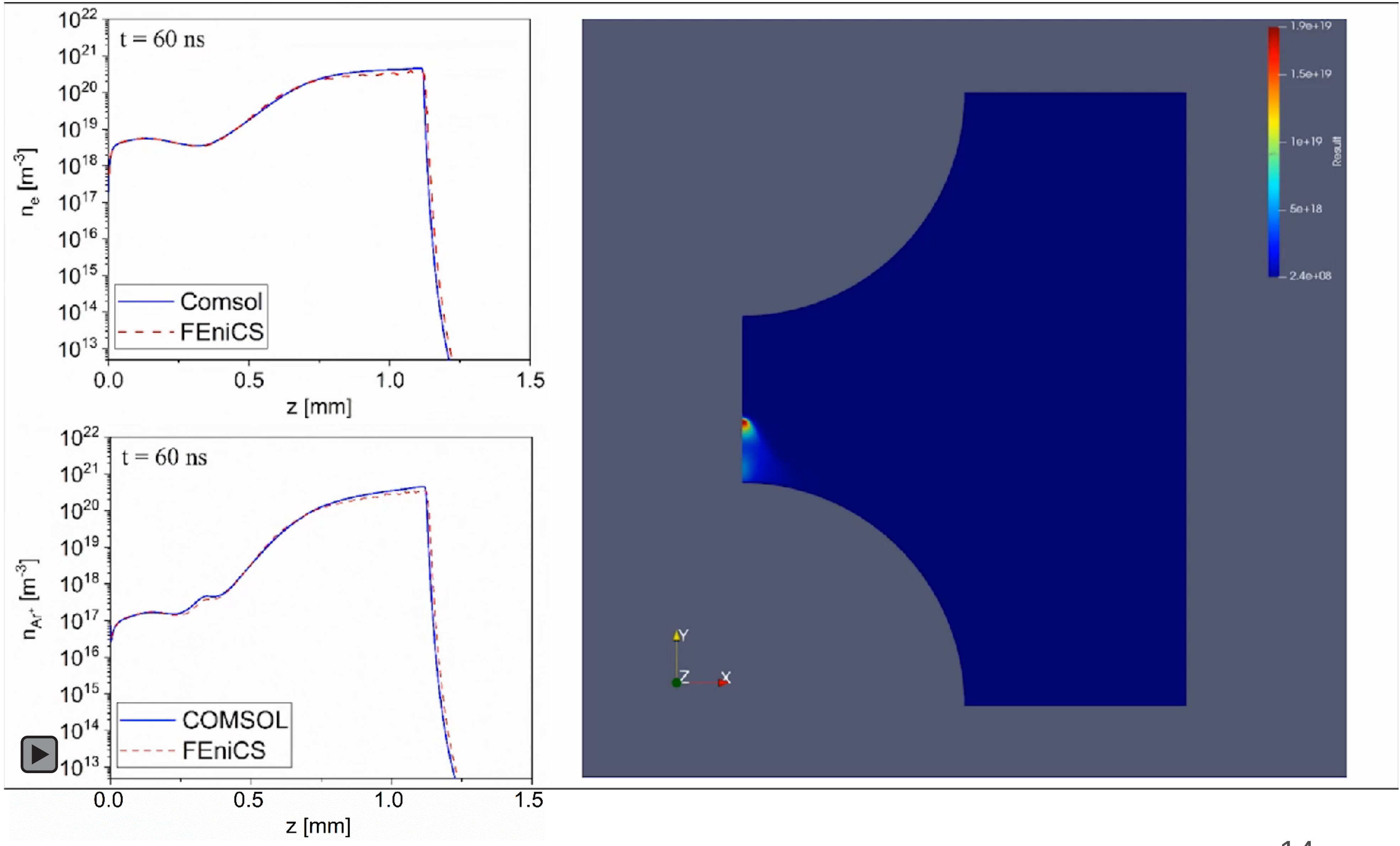

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