Plasma modelling using FEniCS and FEDM

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FEniCS 2021
25 March 2021

Funded by the Deutsche Forschungsgemeinschaft - project number 407462159

FROM IDEA TO PROTOTYPE

Introduction

- Plasma is a gaseous state in which free electrons and ionised atoms or molecules exist.
- Non-thermal low-temperature plasmas considered here are usually produced by electric discharges.
- They are used for different applications, such as chemical and surface processing, or biomedical applications.
- In order to describe physical and chemical processes in plasma, experimental studies are often supplemented by numerical modelling.

Images obtained from https://www.inp-greifswald.de/

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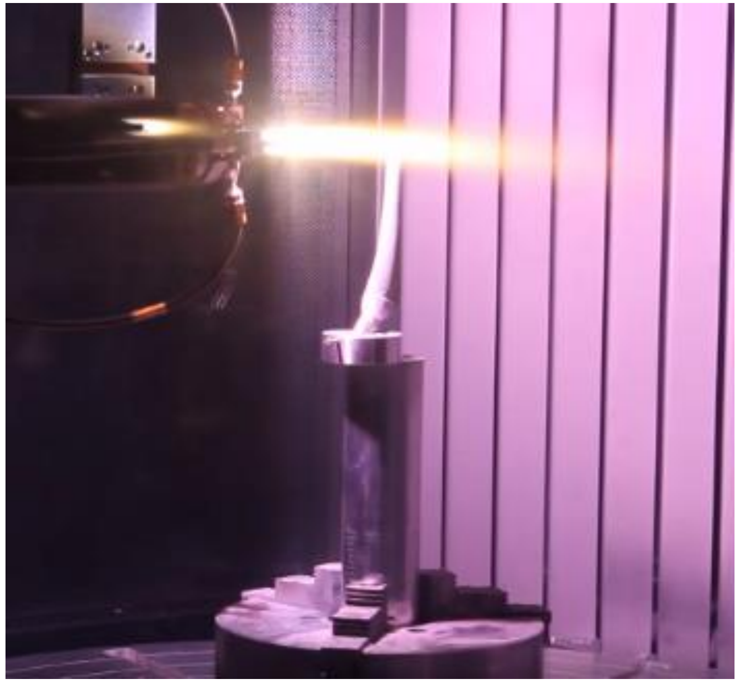

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Governing equations

- Poisson's equation for electric potential

$$-\varepsilon_0\varepsilon_\mathrm{r}\nabla^2\phi = \textstyle\sum_p q_p n_p$$

$$\mathbf{E} = -\nabla\phi$$

- Electron energy balance equation

$$\frac{\partial w_\mathrm{e}}{\partial t} + \nabla\cdot\mathbf{Q}_\mathrm{e} = -e_0\mathbf{E}\cdot\mathbf{\Gamma}_\mathrm{e} + \widetilde{S}_\mathrm{e}$$

$$\mathbf{Q}_\mathrm{e} = -\tfrac{5}{3}b_\mathrm{e}\mathbf{E}w_\mathrm{e} - \nabla(\tfrac{5}{3}D_\mathrm{e}w_\mathrm{e})$$

$$\widetilde{S}_\mathrm{e} = \sum_{j=1}^{N_r}\Delta\varepsilon_j R_j$$

- Continuity equation for particle densities

$$\frac{\partial n_p}{\partial t} + \nabla\cdot\mathbf{\Gamma}_p = S_p$$

$$\mathbf{\Gamma}_p = \mathrm{sgn}(q_p)b_p\mathbf{E}n_p - \nabla(D_p n_p)$$

$$S_p = \sum_{j=1}^{N_r}(G_{pj} - L_{pj})k_j\prod_{i=1}^{N_s} n_i^{\beta_{ij}}$$

- In order to solve the equations, appropriate set of boundary conditions is used:
  - Dirichlet and Robin boundary conditions for Poisson's equation
  - Robin boundary conditions for continuity equations, and electron energy balance equation.

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

INP FROM IDEA TO PROTOTYPE

Challenges in plasma modelling

- For appropriate description of the processes in plasma, lots of particles, and consequently, lots of processes need to be taken into account.

Table 1 Collision processes related to TMS included in the basic reaction kinetics model in addition to the argon model reported in [34]

Index	Reaction	Rate coefficient	References
Elastic electron collisions			
1	$(CH_3)_4Si + e \rightarrow (CH_3)_4Si + e$	$f(u_e)$	[45]
Electron impact excitation and dissociation			
2	$(CH_3)_4Si + e \rightarrow (CH_3)_4Si[v_1] + e$	$f(u_e)$	[45]
3	$(CH_3)_4Si + e \rightarrow (CH_3)_4Si[v_2] + e$	$f(u_e)$	[45]
4	$(CH_3)_4Si + e \rightarrow (CH_3)_3Si + CH_3 + e$	$f(u_e)$	[20, 45]
Electron impact ionization and detachment			
5	$(CH_3)_4Si + e \rightarrow (CH_3)_3Si^+ + CH_3 + 2e$	$f(u_e)$	[46]
6	$(CH_3)_3Si^- + e \rightarrow (CH_3)_3Si + 2e$	$f(u_e)$	[47–49]
Dissociative electron attachment			
7	$(CH_3)_4Si + e \rightarrow (CH_3)_3Si^- + CH_3$	$f(u_e)$	[45]
Ion-molecule reactions			
8	$Ar^+ + (CH_3)_4Si \rightarrow (CH_3)_3Si^+ + CH_3 + Ar[1p_0]$	1.5×10^{-15}	[36, 50]
9	$Ar_2^+ + (CH_3)_4Si \rightarrow (CH_3)_3Si^+ + CH_3 + 2\,Ar[1p_0]$	1.2×10^{-15}	[36, 50]
Quenching of excited argon species leading to Penning ionization			
10–16	$Ar^* + (CH_3)_4Si \rightarrow (CH_3)_3Si^+ + CH_3 + Ar[1p_0] + e$	k^{PI}_{M,Ar^*}	See text
Quenching of excited argon species leading to neutral products			
17–23	$Ar^* + (CH_3)_4Si \rightarrow (CH_3)_3Si + CH_3 + Ar[1p_0]$	k^{Q}_{M,Ar^*}	See text
24–27	$Ar_2^* + (CH_3)_4Si \rightarrow (CH_3)_3Si + CH_3 + 2\,Ar[1p_0]$	k_{M,Ar^*}	Analogous to Ar^* [51, 52]

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Table 2 (continued)

Index	Reaction	Rate coefficient	References
552	$CH_4 + C_2H \rightarrow C_2H_2 + CH_3$	2.3×10^{-18}	[130]
553	$CH_4 + C_2 \rightarrow C_2H + CH_3$	1.7×10^{-17}	[131]
554	$CH_4 + CH \rightarrow C_2H_4 + H$	9.0×10^{-17}	[132]
555	$C_2H_6 + C_2H \rightarrow C_2H_2 + C_2H_5$	3.5×10^{-17}	[133]
556	$C_2H_6 + C_2 \rightarrow C_2H + C_2H_5$	1.6×10^{-16}	[134]
557	$C_2H_6 + CH \rightarrow C_2H_4 + CH_3$	1.3×10^{-16}	[129]
558	$C_2H_6 + CH \rightarrow C_3H_6 + H$	3.0×10^{-17}	[129]
559	$C_2H_5 + C_2H_5\,(+M) \rightarrow C_4H_{10}\,(+M)$	1.9×10^{-17}	[126]
560	$C_2H_5 + C_2H_5 \rightarrow C_2H_6 + C_2H_4$	2.4×10^{-18}	[126]
561	$C_2H_5 + C_2H_3\,(+M) \rightarrow C_4H_8\,(+M)$	2.5×10^{-17}	[135]
562	$C_2H_5 + C_2H_3 \rightarrow 2C_2H_4$	8.0×10^{-19}	[135]
563	$C_2H_5 + C_2H_3 \rightarrow C_2H_6 + C_2H_2$	8.0×10^{-19}	[135]
564	$C_2H_5 + CH_2 \rightarrow CH_3 + C_2H_4$	3.0×10^{-17}	[135]
565	$C_2H_5 + H \rightarrow 2CH_3$	6.0×10^{-17}	[126]
566	$C_2H_4 + C_2H \rightarrow C_2H_2 + C_2H_3$	1.2×10^{-16}	[133]
567	$C_2H_4 + C_2 \rightarrow 2C_2H_2$	3.3×10^{-16}	[134]
568	$C_2H_4 + H\,(+M) \rightarrow C_2H_5\,(+M)$	1.1×10^{-18}	[126, 127]
569	$C_2H_3 + C_2H_3\,(+M) \rightarrow C_4H_6\,(+M)$	1.6×10^{-17}	[135]
570	$C_2H_3 + C_2H_3 \rightarrow C_2H_4 + C_2H_2$	1.6×10^{-18}	[135]
571	$C_2H_3 + CH_2 \rightarrow CH_3 + C_2H_2$	3.0×10^{-17}	[135]
572	$C_2H_3 + H \rightarrow C_2H_2 + H_2$	2.0×10^{-17}	[126]
573	$C_2H + CH_2 \rightarrow CH + C_2H_2$	3.0×10^{-17}	[135]
574	$C_2H + H\,(+M) \rightarrow C_2H_2\,(+M)$	3.0×10^{-16}	[135]
575	$C_2 + H_2 \rightarrow C_2H + H$	1.5×10^{-18}	[136]

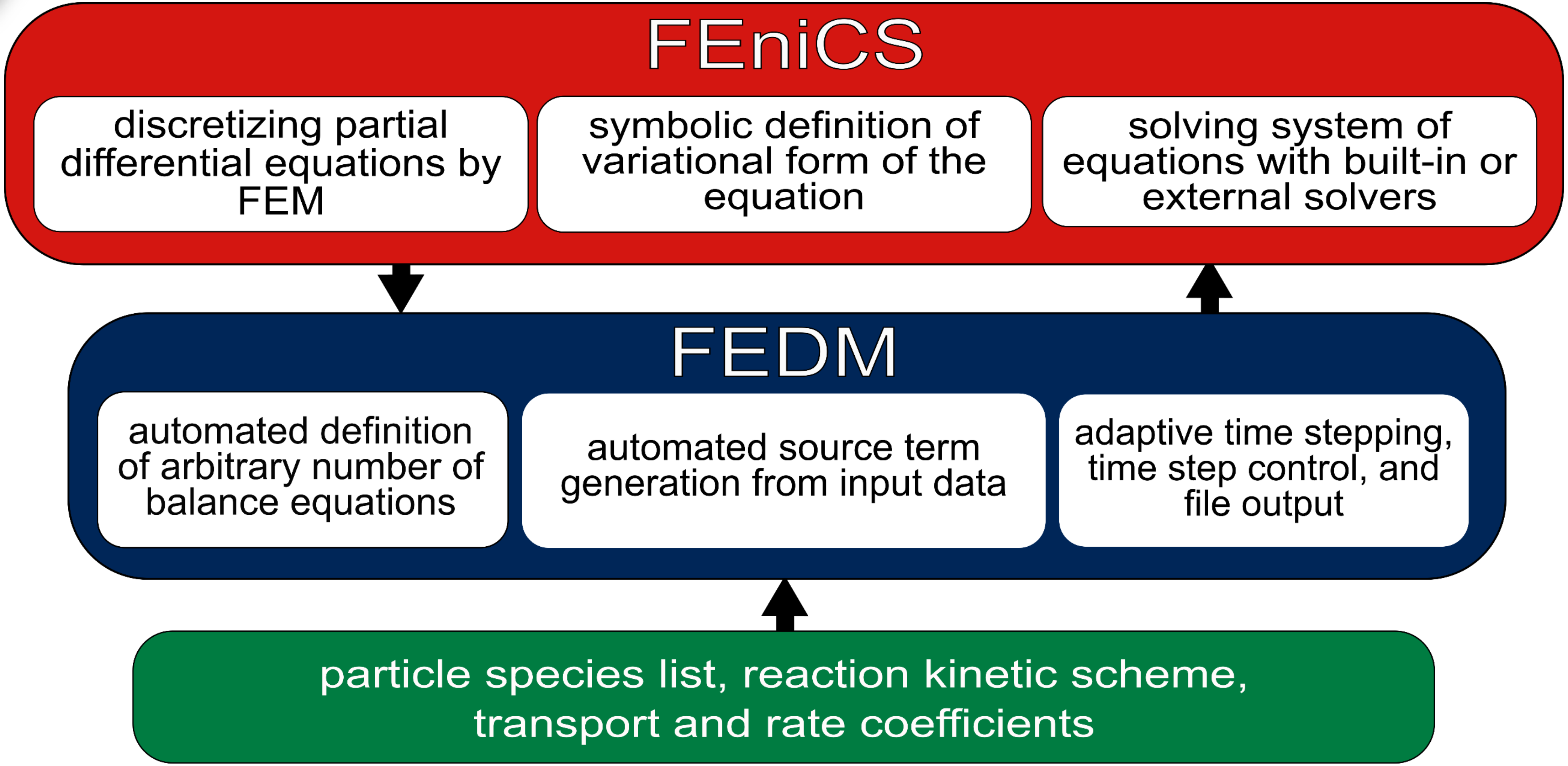
310 Plasma Chemistry and Plasma Processing (2021) 41:289–334

D. Loffhagen et al., Plasma Chem. Plasma Process. **41** (2021) 289

- Chemical reactions in plasma model usually lead to stiff system of equations.

- Time scale of the problem spans from picoseconds to tens of seconds.

FEDM (Finite Element Discharge Modelling) code



FEDM (Finite Element Discharge Modelling) code

- Transport and reaction rate coefficients are imported into model in form of functions or look-up tables.
- Source term definition is automated based on the reaction kinetic scheme.
- Time discretization is done using backward differentiation formula.

$$y_{n+2} - \frac{(1+\omega_{n+1})^2}{1+2\omega_{n+1}} y_{n+1} + \frac{\omega_{n+1}^2}{1+2\omega_{n+1}} y_n = \Delta t_{n+2} \frac{1+\omega_{n+1}}{1+2\omega_{n+1}} f_{n+2}$$

- Time stepping control is done using either *H*211*b* or PI.3.4 controllers.

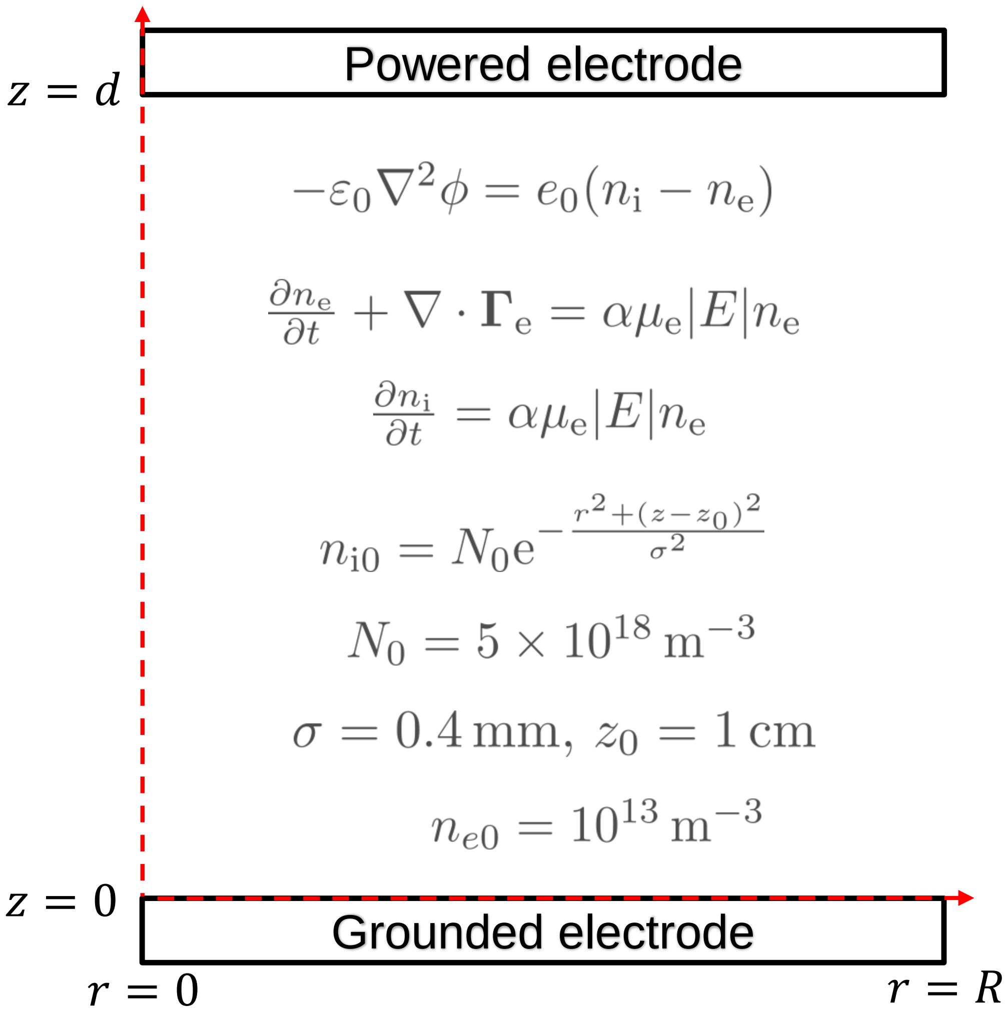
$$\Delta t_{n+1} = \left(\frac{0.8TOL}{\hat{r}_{n+1}}\right)^{0.3/k} \left(\frac{\hat{r}_n}{\hat{r}_{n+1}}\right)^{0.4/k} \Delta t_n$$

$$\Delta t_{n+1} = \left(\frac{0.8TOL}{\hat{r}_n}\right)^{0.25/k} \left(\frac{0.8TOL}{\hat{r}_{n-1}}\right)^{0.25/k} \left(\frac{\Delta t^n}{\Delta t^{n-1}}\right)^{-0.25} \Delta t^n$$

E. Alberdi Celaya et al., Procedia Comput. Sci., ***29****, 1014–1026 (2014)*
G. Söderlind and L. Wang, J. Comput. Appl. Math., ***185,*** *225–243 (2006)*
G. Söderlind, Numer. Algorithms, ***31****, 281–310 (2002)*

Code verification by benchmarking

- Axisymmetric positive streamer in air at atmospheric pressure and 300 K is modelled using 2D FEDM code.
- Square domain has radius and gap distance of 1.25 cm.
- Background electric field is 15 kV/cm.
- Gaussian seed near the powered electrode is introduced to locally enhance the field and initiate the streamer.
- Mesh is refined towards the axis and streamer region (approx. 500000 elements).
- Linear Lagrange elements are used for all the equations.
- Time-step size is constant: Δt = 5 ps.
- Temporal evolution is followed up to 12 ns (2400 time steps).



$$-\varepsilon_0 \nabla^2 \phi = e_0 (n_\mathrm{i} - n_\mathrm{e})$$

$$\frac{\partial n_\mathrm{e}}{\partial t} + \nabla \cdot \mathbf{\Gamma}_\mathrm{e} = \alpha \mu_\mathrm{e} |E| n_\mathrm{e}$$

$$\frac{\partial n_\mathrm{i}}{\partial t} = \alpha \mu_\mathrm{e} |E| n_\mathrm{e}$$

$$n_{\mathrm{i}0} = N_0 \mathrm{e}^{-\frac{r^2 + (z - z_0)^2}{\sigma^2}}$$

$$N_0 = 5 \times 10^{18}\,\mathrm{m}^{-3}$$

$$\sigma = 0.4\,\mathrm{mm},\ z_0 = 1\,\mathrm{cm}$$

$$n_{\mathrm{e}0} = 10^{13}\,\mathrm{m}^{-3}$$

B. Bagheri et al., *Plasma Sources Sci. Technol.* ***27*** *(2018) 095002*

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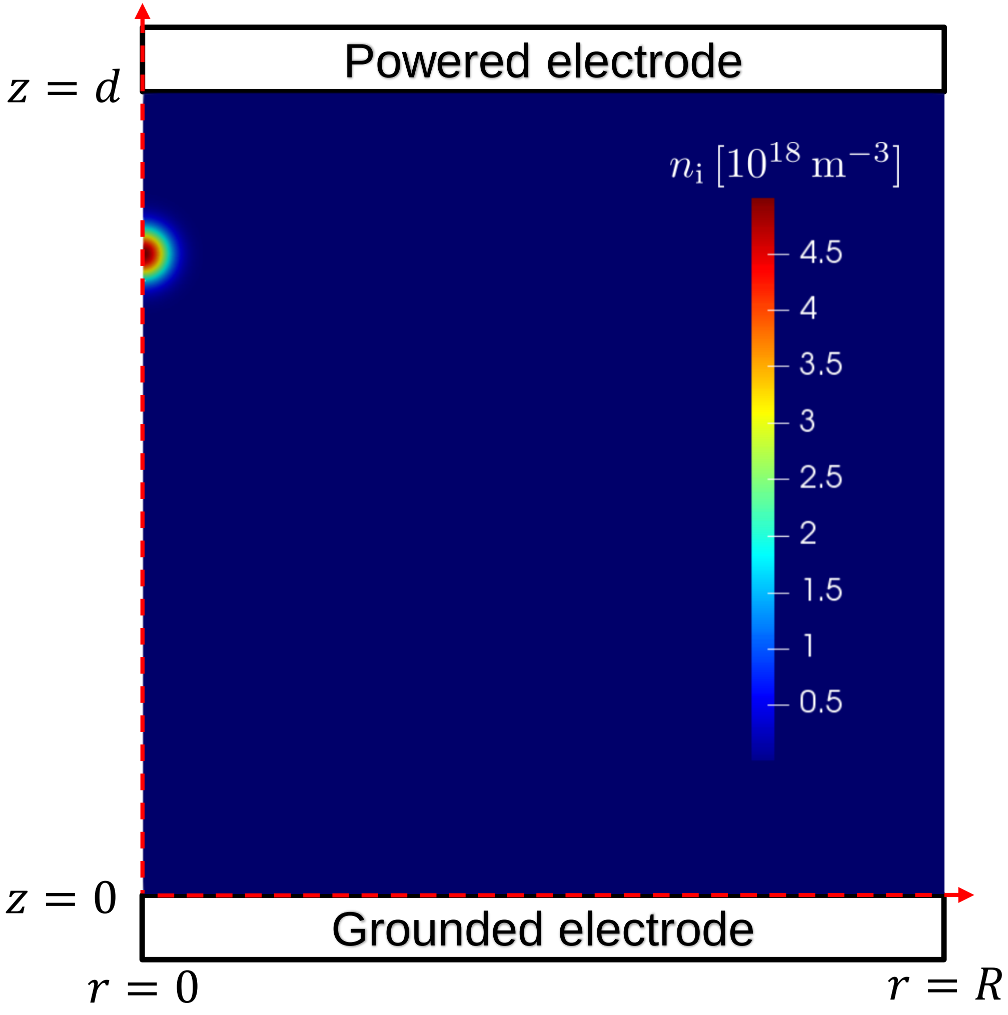

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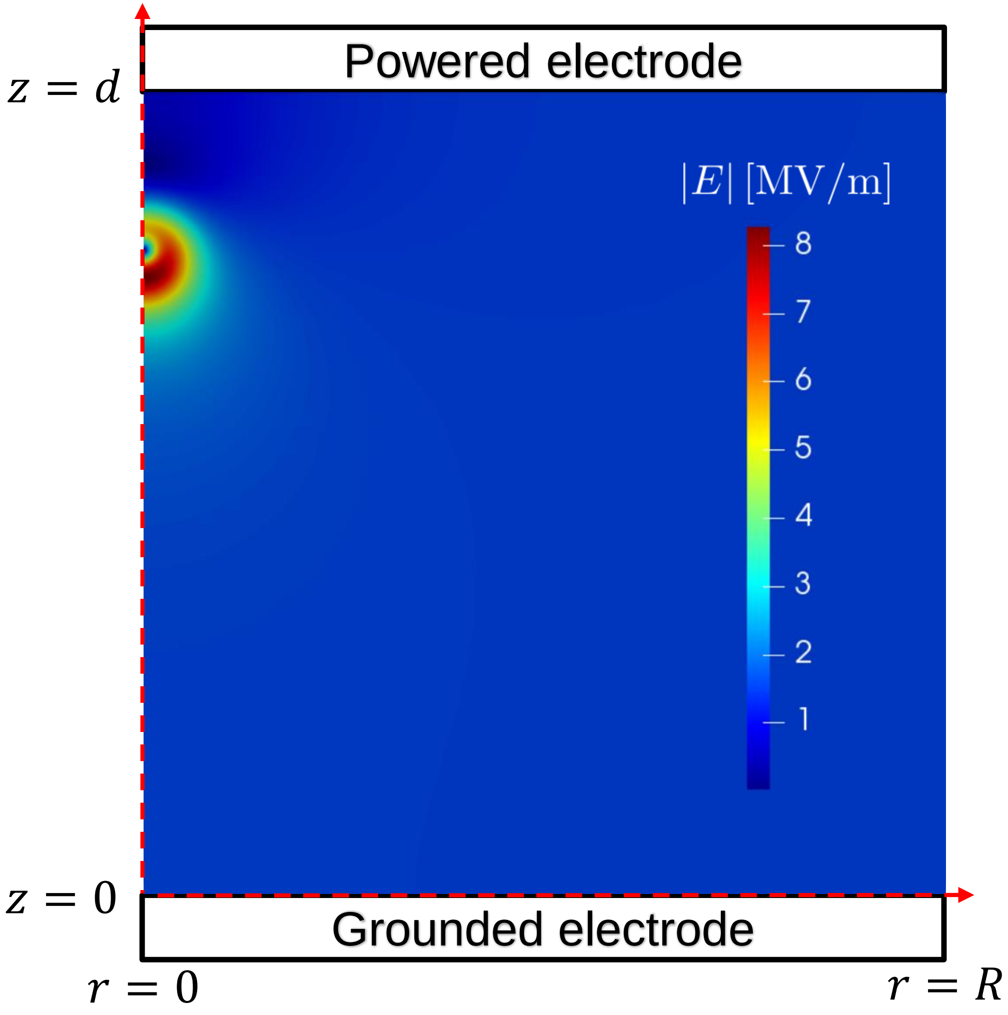

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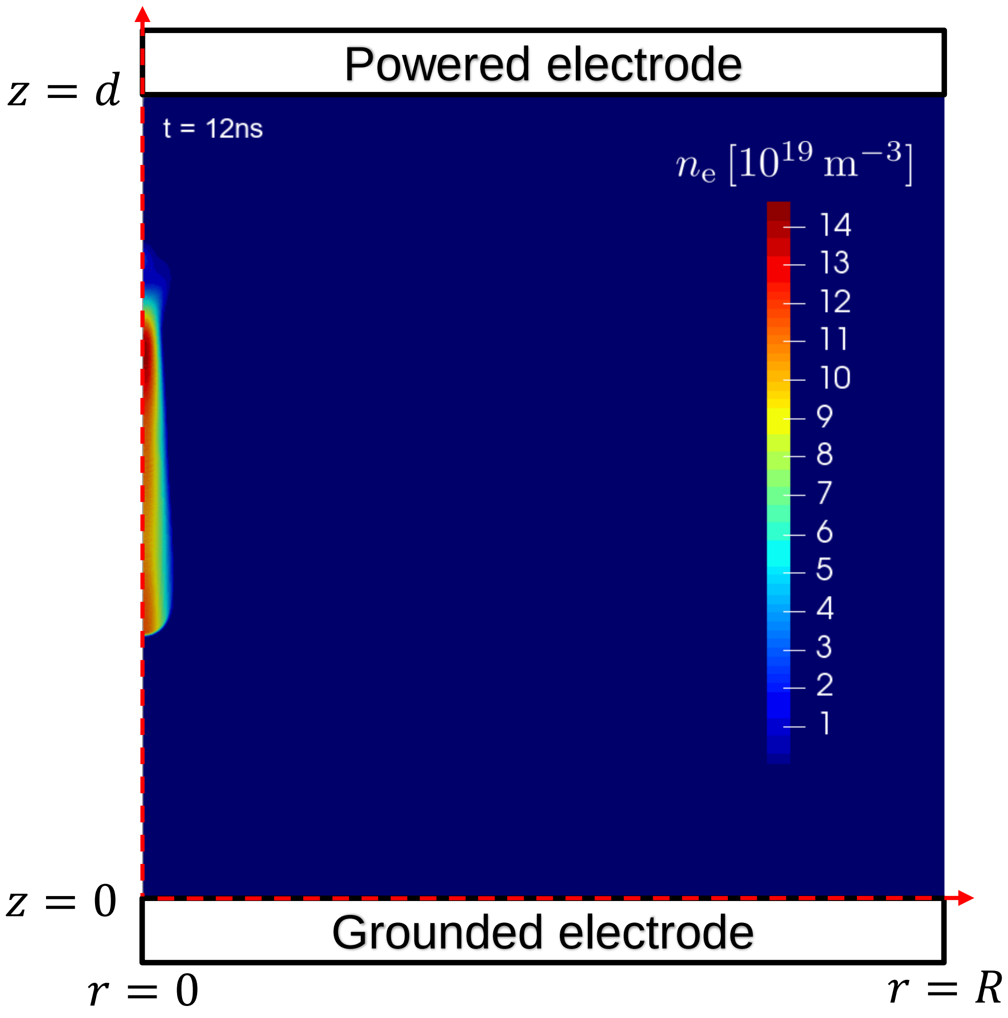

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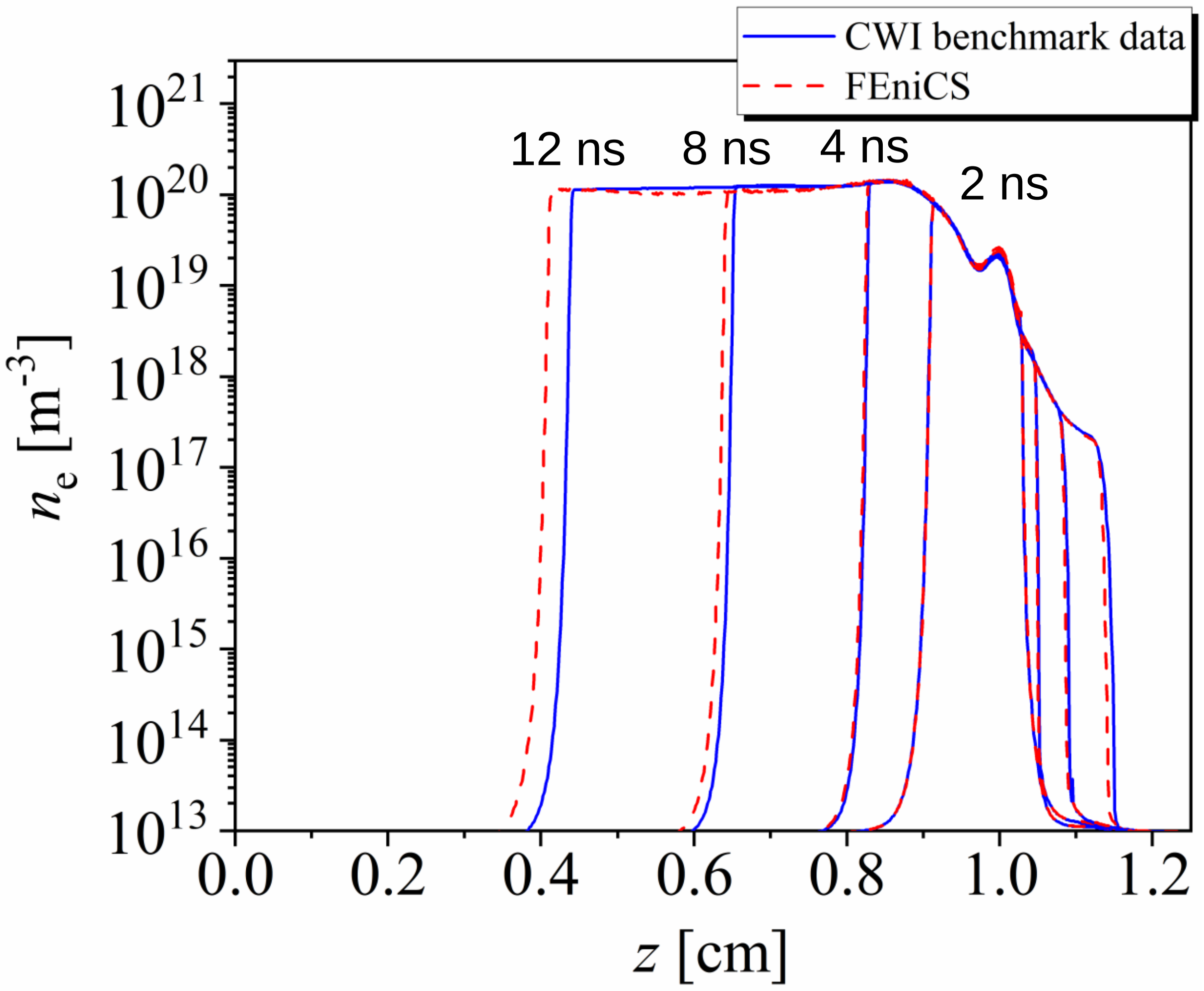

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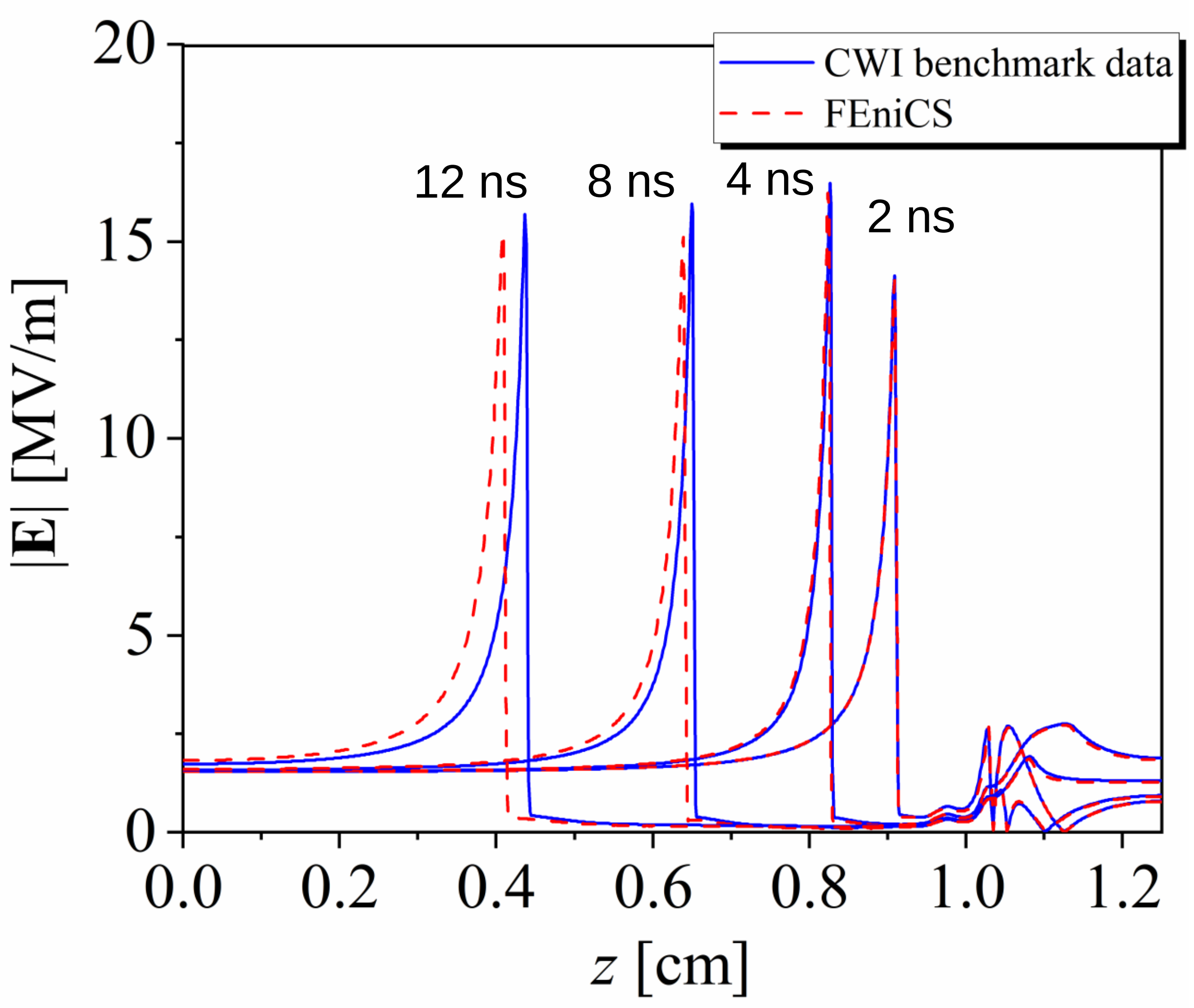

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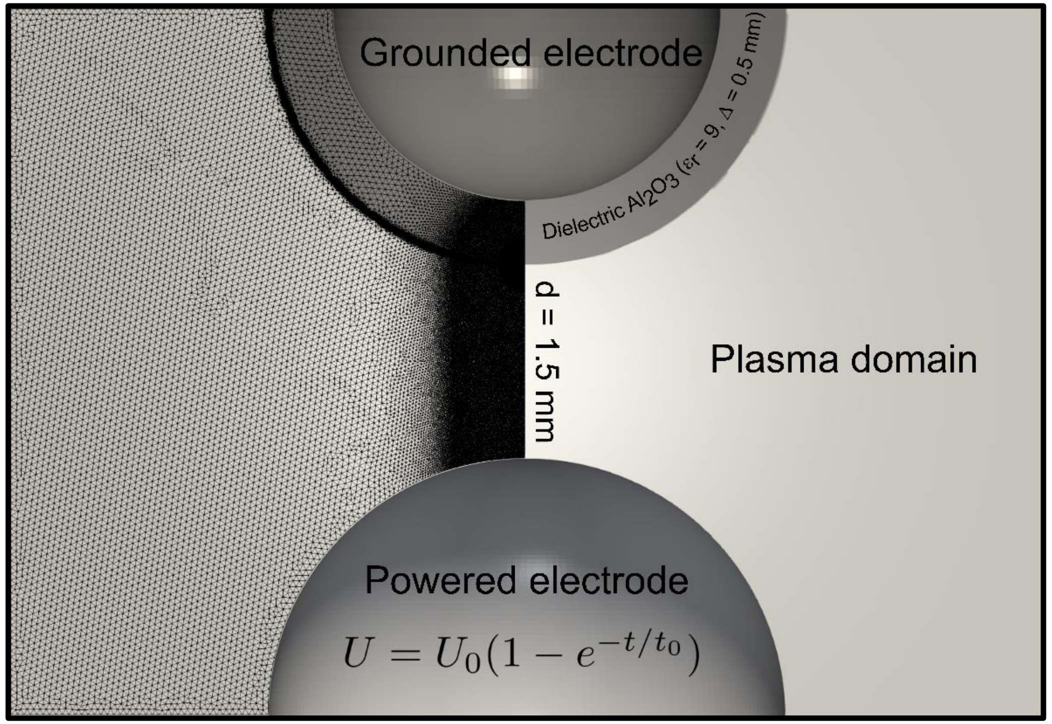
Dielectric barrier discharge (DBD) modelling

- Atmospheric-pressure DBD in argon in asymmetric configuration is modelled using 2D FEDM code.
- Electrodes of radius 2 mm are set 1.5 mm apart.
- Grounded electrode (top) is covered by 0.5 mm thick dielectric.
- Pulsed voltage is applied to powered electrode (bottom).
- Gaussian seed near the powered electrode is introduced to locally enhance the field and initiate the streamer.
- Mesh is refined near the streamer region and along the dielectric (approx. 350000 elements).
- Linear Lagrange elements are used for all the equations.
- Adaptive time stepping is used (1 ps < Δt < 100 ps).
- Temporal evolution is followed up to about 43 ns.



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$$\frac{\partial\sigma}{\partial t} = \sum_p q_p\mathbf{\Gamma}_p\cdot\boldsymbol{\nu}$$

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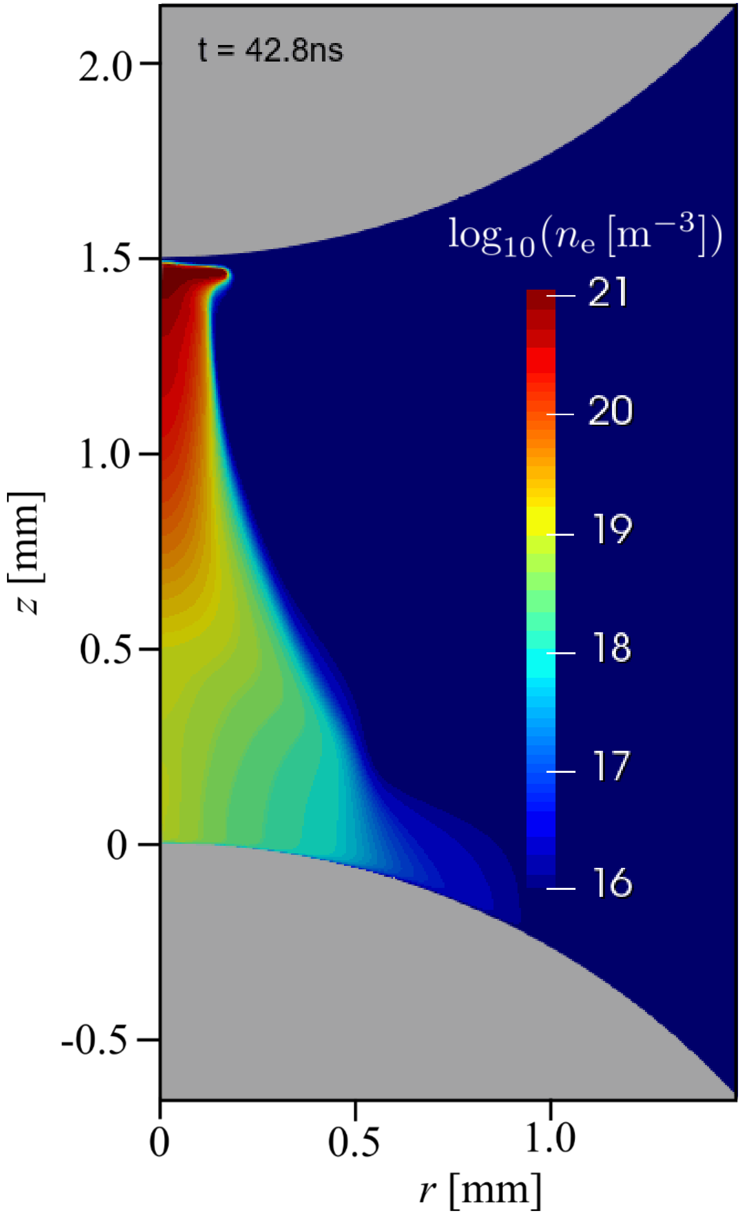

Conclusion and outlook

- FEDM code for automated set-up of the equations is developed.
- The code is verified using benchmarking.
- The challenges in cases where the problem is defined on several subdomains, such as DBDs, could possibly be resolved using mixed-dimensional formulation.
- Handling of electron-energy-dependent and electric-field-dependent coefficients should be further addressed because they can lead to small time-step sizes.

Contact

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