Interface Boundary Conditions for Global Models of Multi-Chamber Negative Hydrogen Ion Sources

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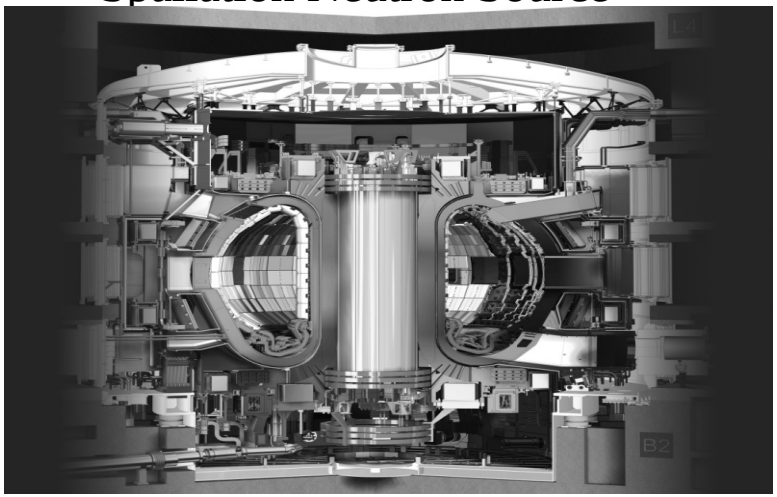
Applications of Negative Hydrogen Ion Sources (NHIS)

- Particle accelerators
  - Allow doubling of the beam energy compared to the proton beam (Alvarez, 1951)
- Fusion reactors
  - Heating of the tokomak plasma by neutral beam injection (NBI) (Bacal, 2012)
- Medical applications
  - Used in cyclotrons in order to produce short-lived isotopes for radionuclide imaging with positron emission tomography and single photon emission computer tomography (Muramatsu & Kitagawa, 2012)
- Space propulsion

Spallation Neutron Source*



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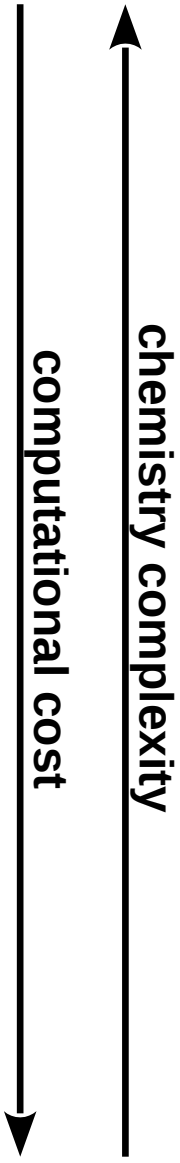
Simulation methods of NHIS

- 0D kinetic (global) models
  - Spanning from simple space uniform to advanced state-to-state volume averaged models including Boltzmann equation for EEDF
    - Gaboriau and Boeuf (2014)
    - Averkin et al (2015, 2017)
- Fluid models
  - Drift-diffusion models
    - Gao et al (2017)
  - Multi-fluid multi-temperature models
    - Hagelaar et al (2011), Boeuf et al (2011)
- Kinetic models
  - Particle-In-Cell (PIC)
    - Kolev et al. (2009)
  - Direct Simulation Monte Carlo (DSMC)
    - Taccogna et al. (2007)



Motivation

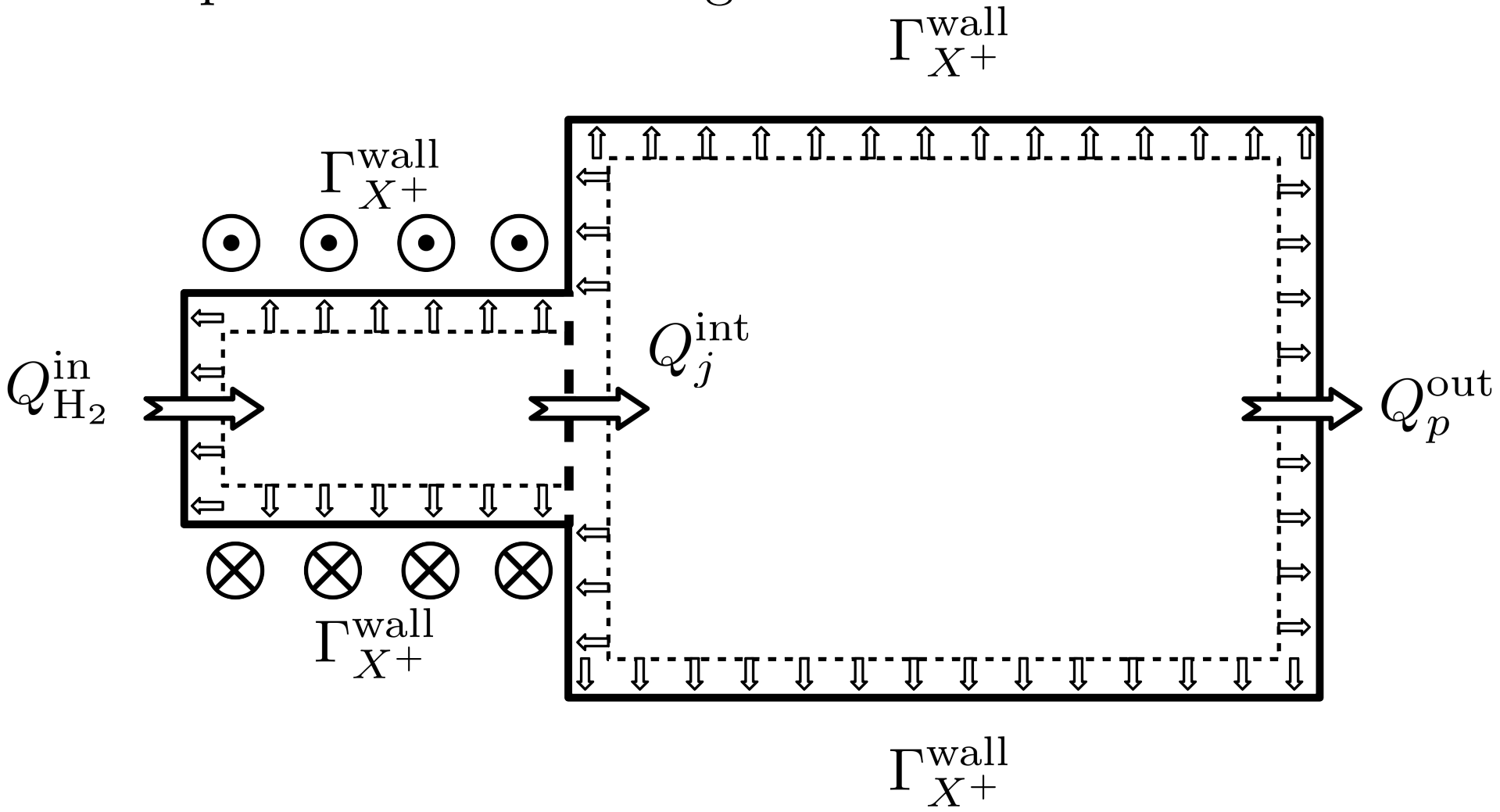
- Tech-X Corporation develops fluid software (USim) for accurate modeling of NHIS devices for long time scales, and to optimize NHIS designs over a wide range of parameters.
- Hydrogen plasma includes several species: excited molecules $H_2(v,r)$ and atoms $H(n)$, multiple positive ions H^+, H_2^+, H_3^+, H_5^+,... and their excited states, negative ions H^- , electrons.
- We present an extension of our global model work to multi-chamber NHIS simulations. This model is used in determination of the relevant reactive plasma species and chemistry channels for the USim fluid simulation model.
- The main challenge is how to impose interface boundary conditions

Global Enhanced Vibrational Kinetic Model

- Global Enhanced Vibrational Kinetic Model (GEVKM) was first developed to simulate high pressure RF inductive discharge of the High Current Negative hydrogen Ion source developed by Busek Co Inc and Worcester Polytechnic Institute.
- This model is based on the solution of volume averaged steady-state conservation laws (global model) of hydrogen plasma
- We are in the process of extending the GEVKM for multi-chamber NHIS by considering separate global models for each chamber and using interface boundary conditions to couple the systems of equations.
- In this work we present a simplified formulation that allows to get interface boundary conditions for multi-chamber NHIS

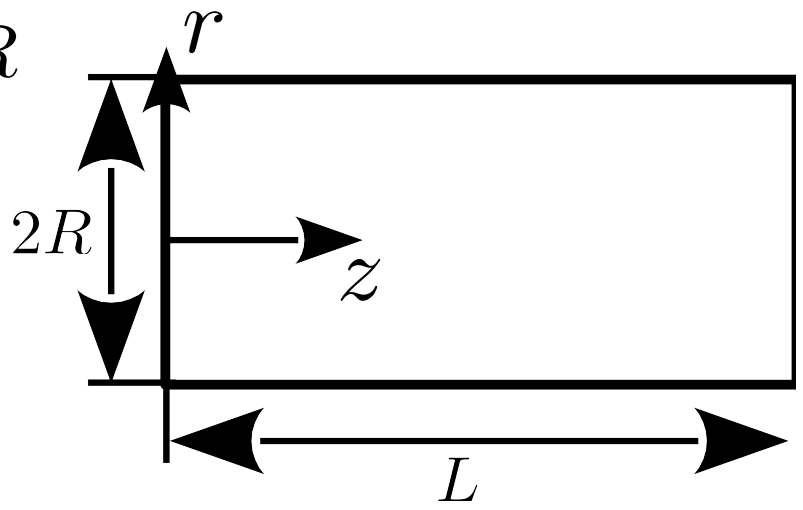
Simulation Geometry

- We consider double-chamber NHIS similar to the one developed at IPP Garching



Recap: Ambipolar transport in cylindrical discharges

- Cylindrical domain with radius R and length L
- Electron temperature is uniform
- Plasma consists of one sort of positive ions, electrons and background gas
- There are two reactions: volumetric ionization and surface recombination
- Ambipolar diffusion (high pressures)
- Steady state
- Under these conditions the diffusion equation has a form of Helmholtz equation (Lieberman & Lichtenberg, 2005)



$$\nabla^2 n + \frac{\nu_{\mathrm{iz}}}{D_a} n = 0,$$

$$n|_{\partial\Omega} = 0.$$

Recap: Ambipolar solution

- The solution of Helmholtz equation with everywhere positive number density corresponds to the lowest order eigenfunction

$$n(r,z) = n_0 J_0\left(\frac{\chi_{01} r}{R}\right) \sin\left(\frac{\pi z}{L}\right)$$

- Corresponding eigenvalue allows to determine electron temperature

$$\frac{\nu_{\mathrm{iz}}(T_e)}{D_a(T_e)} = \frac{\chi_{01}^2}{R^2} + \frac{\pi^2}{L^2}$$

- Central number density n_0 is determined from the electron energy equation

Ambipolar transport in two-chamber discharge

- Let's consider three distinct regions with their own electron temperatures that are uniform inside each region

$$\frac{\partial^2 n}{\partial r^2} + \frac{1}{r}\frac{\partial n}{\partial r} + \frac{\partial^2 n}{\partial z^2} = \frac{G_i}{D_{ai}} n,$$

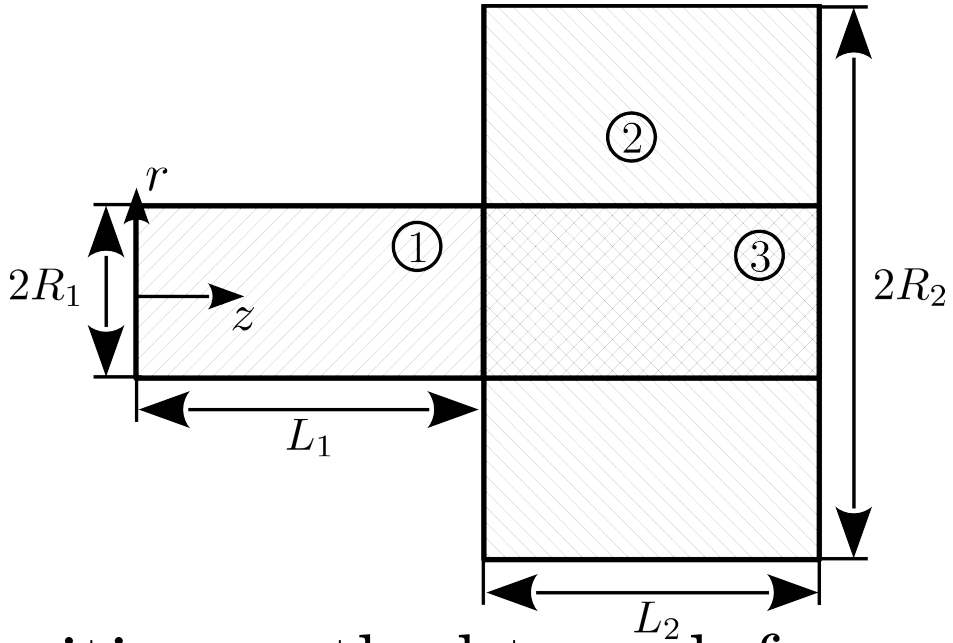
$$n(r,0) = 0, 0 \le r \le R_1,$$

$$n(R_1,z) = 0, 0 \le z \le L_1,$$

$$n(r,L_1) = 0, R_1 \le r \le R_2,$$

$$n(R_2,z) = 0, L_1 \le z \le L_2,$$

$$n(r,L_2) = 0, 0 \le r \le R_2.$$



- We use domain decomposition method to seek for solutions in each region
- Even though this system of equations results in discontinuities at each interface, we impose conservation of total fluxes and equate average number densities at each interface to couple separate equations

Equations and BCs for each interface

- Driver chamber (region 1)

$$N''_{r1}(r) + \frac{1}{r} N'_{r1}(r) = F_1 N_{r1}(r),$$
$$N_{r1}(R_1) = 0,$$
$$N''_{z1}(z) + \left(F_1 - \frac{G_1}{D_{a1}} \right) N_{z1}(z) = 0,$$
$$N_{z1}(0) = 0.$$

- Expansion chamber (region 2)

$$N''_{r2}(r) + \frac{1}{r} N'_{r2}(r) = F_2 N_{r2}(r),$$
$$N''_{z2}(z) + \left(F_2 - \frac{G_2}{D_{a2}} \right) N_{z2}(z) = 0,$$
$$N_{z2}(L_1 + L_2) = 0.$$

- Expansion chamber (region 3)

$$N''_{r3}(r) + \frac{1}{r} N'_{r3}(r) = F_3 N_{r3}(r),$$
$$N_{r3}(R_2) = 0,$$
$$N''_{z3}(z) + \left(F_3 - \frac{G_3}{D_{a3}} \right) N_{z3}(z) = 0,$$
$$N_{z3}(L_1) = 0,$$
$$N_{z3}(L_1 + L_2) = 0.$$

Coupling conditions at each interface

- Fluxes conservation through interfaces

$$D_{a1}N'_{z1}(L_1)\int_0^{R_1} N_{r1}(r)rdr = D_{a2}N'_{z2}(L_1)\int_0^{R_1} N_{r2}(r)rdr,$$

$$D_{a2}N'_{r2}(R_1)\int_{L_1}^{L_1+L_2} N_{z2}(z)dz = D_{a3}N'_{r3}(R_1)\int_{L_1}^{L_1+L_2} N_{z3}(z)dz.$$

- Average number densities at both sides of interfaces are equal

$$N_{z1}(L_1)\int_0^{R_1} N_{r1}(r)rdr = N_{z2}(L_1)\int_0^{R_1} N_{r2}(r)rdr,$$

$$N_{r2}(R_1)\int_{L_1}^{L_1+L_2} N_{z2}(z)dz = N_{r3}(R_1)\int_{L_1}^{L_1+L_2} N_{z3}(z)dz.$$

Number densities solutions

- Number densities inside each region

$$n_1(r,z) = n_{01} J_0\left(\frac{\chi_{01}}{R_1} r\right) \sin\left(z\sqrt{\frac{G_1}{D_{a1}} - \frac{\chi_{01}^2}{R_1^2}}\right),$$

$$n_2(r,z) = n_{02} J_0\left(\sqrt{F_2} r\right) \frac{\sin\left((L_1 + L_2 - z)\sqrt{\frac{G_2}{D_{a2}} - F_2}\right)}{\sin\left((L_1 + L_2)\sqrt{\frac{G_2}{D_{a2}} - F_2}\right)},$$

$$n_3(r,z) = n_{03}\left[J_0\left(r\sqrt{\frac{G_3}{D_{a3}} - \frac{\pi^2}{L_2^2}}\right) - Y_0\left(r\sqrt{\frac{G_3}{D_{a3}} - \frac{\pi^2}{L_2^2}}\right) \frac{J_0\left(R_2\sqrt{\frac{G_3}{D_{a3}} - \frac{\pi^2}{L_2^2}}\right)}{Y_0\left(R_2\sqrt{\frac{G_3}{D_{a3}} - \frac{\pi^2}{L_2^2}}\right)}\right] \frac{\sin\left((z - L_1)\frac{\pi}{L_2}\right)}{\cos\left(L_1\frac{\pi}{L_2}\right)}.$$

- There are 7 unknowns: n_{01}, n_{02}, n_{03}, T_{e1}, T_{e2}, T_{e3}, F_2
- Conditions on fluxes and average number densities give 4 conditions
- Remaining conditions are given by 3 electron energy equations for each region
- Unlike simple cylindrical discharge we cannot find electron temperatures separately. We have to solve a system of non-linear equations.

Volume averaged electron energy equations

- Region 1

$$\frac{5}{2}eT_{e1}Q_{e1\to 2,\mathrm{out}} + \Gamma_{\mathrm{wall},1}(2eT_{e1} + eV_{p1} + eV_{\mathrm{sh},1})$$
$$= \left[(k_B T_{g1} - eT_{e1})3\frac{m_e}{m_g}k_{g,\mathrm{el}}(T_{e1}) + E_{\mathrm{iz}}k_{\mathrm{iz}}(T_{e1})\right] n_{g1}\bar{n}_{e1}V_1 + P_{\mathrm{abs}},$$

- Region 2

$$\frac{5}{2}eT_{e2}Q_{e2\to 3,\mathrm{out}} - \frac{5}{2}eT_{e1,\mathrm{in}}Q_{e1\to 2,\mathrm{in}} + \Gamma_{\mathrm{wall},2}(2eT_{e2} + eV_{p2} + eV_{\mathrm{sh},2})$$
$$= \left[(k_B T_{g2} - eT_{e2})3\frac{m_e}{m_g}k_{g,\mathrm{el}}(T_{e2}) + E_{\mathrm{iz}}k_{\mathrm{iz}}(T_{e2})\right] n_{g2}\bar{n}_{e2}V_2,$$

- Region 3

$$-\frac{5}{2}eT_{e2,\mathrm{in}}Q_{e2\to 3,\mathrm{in}} + \Gamma_{\mathrm{wall},3}(2eT_{e3} + eV_{p3} + eV_{\mathrm{sh},3})$$
$$= \left[(k_B T_{g3} - eT_{e3})3\frac{m_e}{m_g}k_{g,\mathrm{el}}(T_{e3}) + E_{\mathrm{iz}}k_{\mathrm{iz}}(T_{e3})\right] n_{g3}\bar{n}_{e3}V_3$$

Gas densities estimates

- We assume that gas number densities are uniform in each region
- We assume the same gas number densities in regions 2 and 3 in the expansion chamber
- We consider gas heating in the driver chamber and disregard any heat fluxes to the walls

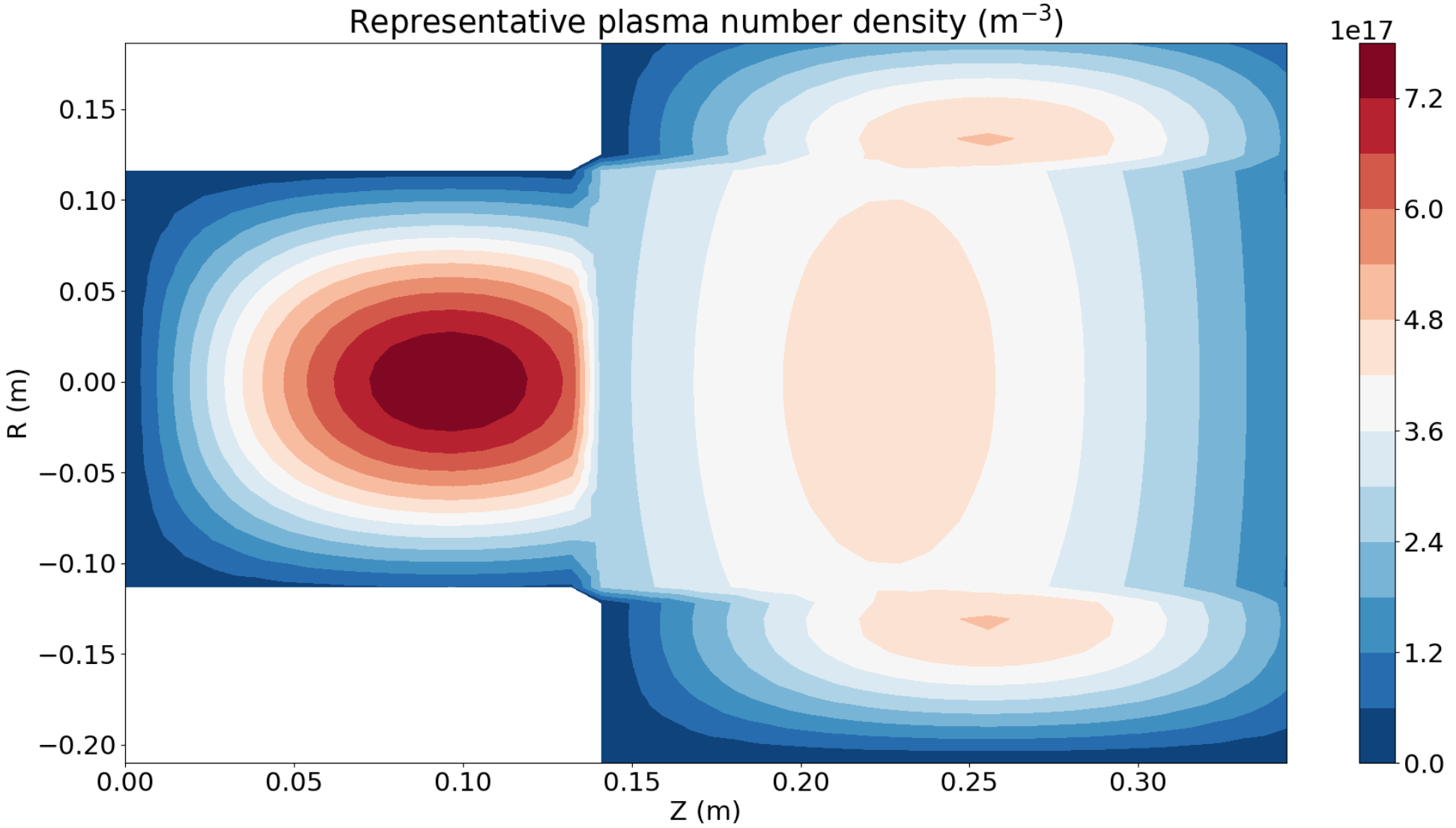
$$
\begin{aligned}
& m_0 Q_{\text{in}} = \rho_1 u_1 A_1, \\
& \rho_1 u_1 A_1 = \rho_2 u_2 A_2, \\
& \rho_2 u_2 A_2 = m_0 n_2 \frac{1}{4} \sqrt{\frac{8 k_B T_2}{\pi m_0}} A_{\text{out}}, \\
& p_1 A_1 + \rho_1 u_1^2 A_1 = p_2 A_2 + \rho_2 u_2^2 A_2, \\
& Q_{\text{in}} H_{\text{in}} + P_{\text{abs,gas}} = Q_{\text{in}} \left(H_1(T_1) + \frac{1}{2} m_0 u_1^2 \right), \\
& H_1(T_1) + \frac{1}{2} m_0 u_1^2 = H_2(T_2) + \frac{1}{2} m_0 u_2^2.
\end{aligned}
$$

- After solving the system of equations we get approximate gas number densities in each chamber

Solution procedure

- All terms in electron energy equations can be analytically integrated based on the number densities profiles
- We have a system of 7 non-linear algebraic equations. By eliminating central number densities in the first and the third region we reduce this system to 5 equations
- After solving the system of equations we get number density profiles in each region as well as electron temperatures

Example


Representative plasma number density (m^{-3})
1e17
7.2
6.0
4.8
3.6
2.4
1.2
0.0
R (m)
0.15
0.10
0.05
0.00
−0.05
−0.10
−0.15
−0.20
0.00
0.05
0.10
0.15
0.20
0.25
0.30
Z (m)

Conclusions

- We derived an approximate solution of diffusion equation for double-chamber geometry using a combination of domain decomposition method and separation of variables techniques
- We're still working on implementation of the numerical solution of resulting algebraic equations for getting center number densities and electron temperatures in each zone
- Next step is to add low-pressure corrections similar to conventional global models to extend validity of the model
- Final goal is to add new interface boundary conditions to the GEVKM to simulate full hydrogen chemistry