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New inflow boundary conditions for relativistic and Newtonian fluids

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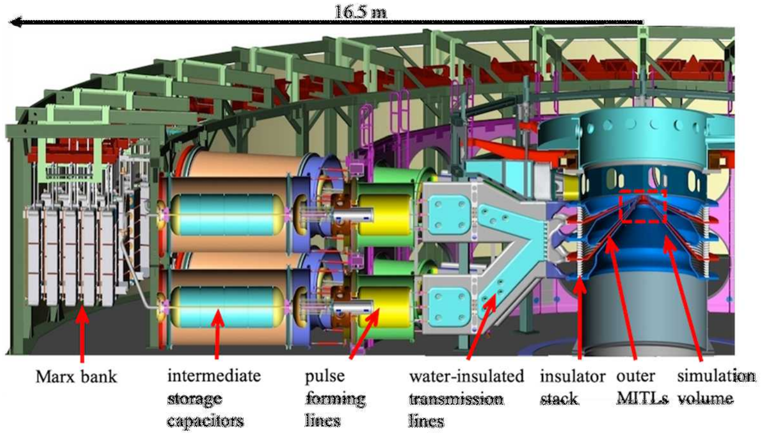
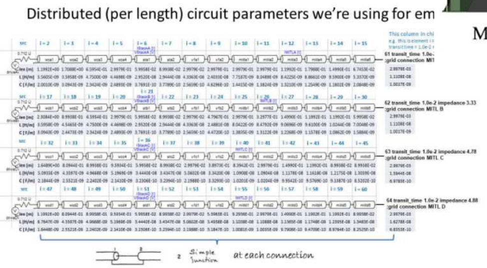
Progress in MITL modeling with EMPIRE

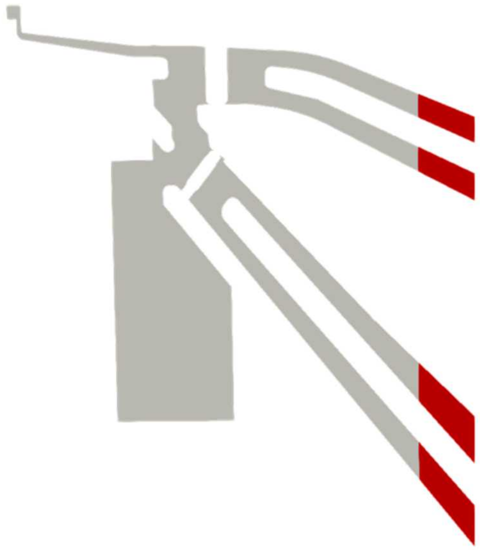
Accurate modeling of power flow from capacitors to load requires several different models

Over the lifetime of the GC-LDRD, EMPIRE has made great strides

- Transmission line models, bidirectional power flow to the inner section
- Wave launching and absorbing boundary conditions
- Current flows into the center section
- Space Charge Limited particle emission (SCL)
  - Large electron flux
- Surfaces heat up through ohmic heating and electron bombardment
  - Neutrals are created







MITL flow is traditionally modelled using particle-in-cell techniques, which can be costly due to need to resolve Debye length. Relativistic fluid models provide an alternative that offer reduced computational cost.

Overview

- Neumann boundary conditions in EMPIRE-Fluid
- Considerations for inflow boundary conditions

- Mass injection boundary
  - Injects a user-specified mass flux $\Gamma(t)$

- Thermal desorption boundary
  - Injects a temperature-dependent mass flux of substance
  - Can be used to model thermionic emissions

- Space charge limited (SCL) boundary
  - Injects a charged substance so that the electric field at the emitting surface relaxes to nearly zero

Neumann boundary conditions in EMPIRE-Fluid

The equations for an ideal fluid can written in conservation form,

$$\frac{\partial \vec{u}}{\partial t} + \nabla \cdot \vec{F}(\vec{u}) = 0$$

Where $\vec{u}$ are the conserved quantities and $\vec{F}$ is the *flux*.

For a 2D Newtonian fluid,

$u_1 = \rho$	(mass density)	$F_1 = \rho\vec{v} \cdot \hat{n}$	(mass flux)
$u_2 = \rho(\vec{v} \cdot \hat{e}_x)$	(momentum dens. x)	$F_2 = \rho\,(\vec{v} \cdot \hat{n})\,(v \cdot \hat{e}_x) + p(\hat{n} \cdot \hat{e}_x)$	(momentum flux x)
$u_3 = \rho\left(\vec{v} \cdot \hat{e}_y\right)$	(momentum dens. y)	$F_3 = \rho\,(\vec{v} \cdot \hat{n})\left(v \cdot \hat{e}_y\right) + p\left(\hat{n} \cdot \hat{e}_y\right)$	(momentum flux y)
$u_4 = \rho_E$	(energy density)	$F_4 = (\vec{v} \cdot \hat{n})\,(\rho_E + p)$	(energy flux)

These definitions have been generalized to the relativistic case. See for example *Mignone et al*. *"The piecewise parabolic method for multidimensional relativistic fluid dynamics." (2005)*

Neumann conditions in EMPIRE-Fluid prescribe a value for the flux $\vec{F}$ at the boundaries

Considerations for inflow boundary conditions

Given that one desires an inflow mass flux of $\Gamma(x,t)$

injection velocity v

injection temperature T

one might consider implementing an inflow boundary condition by simply prescribing $\vec{F}(\Gamma, v, T)$

- Unless the flow is supersonic, an ill-posed system results!
- $\vec{F}$ must account for the outgoing characteristics. We compute $\vec{F}$ with an approximate Riemann solver:

$$\vec{F} = \vec{F}_{RI}(\vec{\mathrm{u}}_V, \vec{\mathrm{u}}_I)$$

$\vec{\mathrm{u}}_V$ is a “virtual state” which we assign

$\vec{\mathrm{u}}_I$ is the interior state

- See *Mengaldo et al. "A guide to the implementation of boundary conditions in compact high-order methods for compressible aerodynamics." (2014)*

Mass injection boundary condition I (Newtonian fluid system)

The applications described later (especially the thermal desorption boundary) require precise injection of a time-dependent mass flux.

- As far as we know, existing inflow boundary condition algorithms do not offer precise control of total injected mass as a function of time
- The following algorithm is somewhat similar to the outflow boundary outlined in *Rodriguez et al., "Formulation and Implementation of Inflow/Outflow Boundary Conditions to Simulate Propulsive Effects." (2018)*

- The user prescribes for a boundary sideset,
  - Mass influx $\Gamma(t)$
  - Virtual state temperature T_V
  - A virtual state "desired" velocity $\vec{v}'_V$

- Given the current value of the interior state $\vec{\mathrm{u}}_I$, a virtual state $\vec{\mathrm{u}}_V$ is constructed so that,

$$F_1 = \rho\vec{v} \cdot \hat{n} = \Gamma(t)$$

Mass injection boundary condition 2 (Newtonian fluid system)

1. Virtual state velocity, $\vec{v}_V = \hat{n}\, v_V$, is constructed using a *heuristic* so that

$$\frac{v_V}{c_V} \approx \frac{v_I}{c_I}$$

where c_V and c_I are the speeds of sound in the virtual and interior states respectively

v_I is the normal flow speed in the interior state

2. Virtual state density is determined by considering the Riemann invariants,

$$\rho_V = \left(\frac{c_V^2 \left(\frac{\Gamma}{v_b}\right)^{\gamma-1}}{c_b^2} \right)^{\frac{1}{\gamma-1}}$$

$$c_b \equiv \frac{2\, c_I \,+\, 2\, c_V \,+\, (v_I \,-\, v_V)(\gamma - 1)}{4};\;\; v_b \equiv \frac{v_I \,+ v_V}{2} + \frac{c_I \,-\, c_V}{\gamma - 1};\;\; \gamma \equiv 5/3$$

Mass injection boundary condition 3 (Newtonian fluid system)

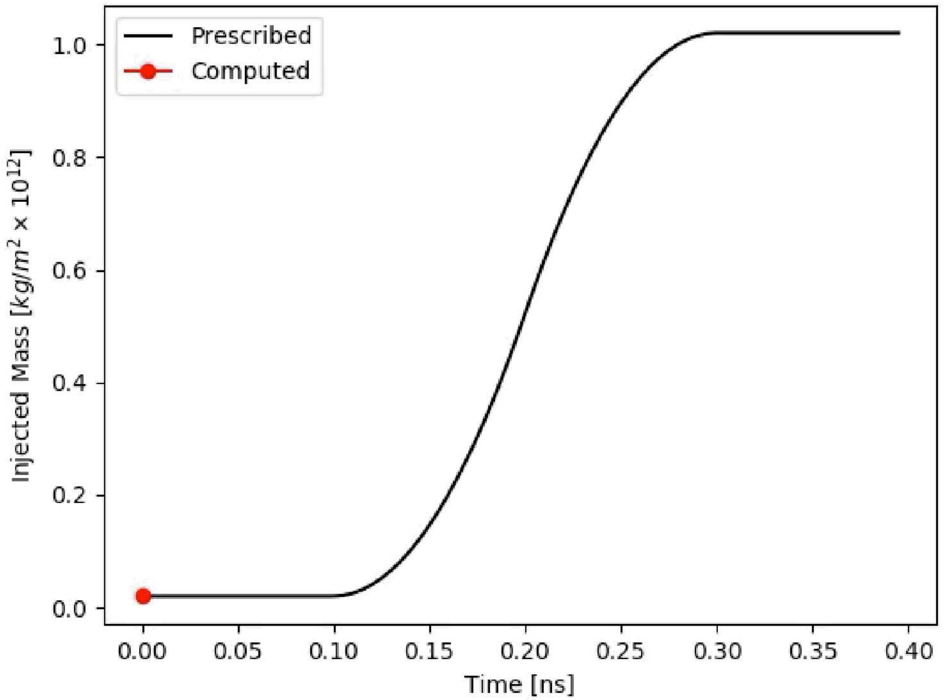
3. We then prescribe the numerical boundary flux,

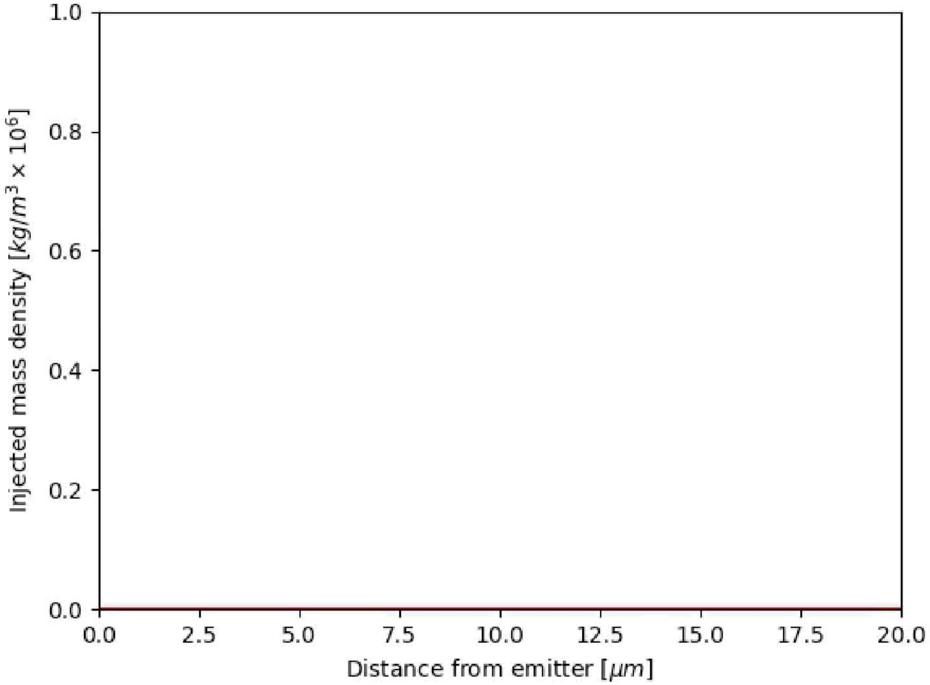
$$\vec{F} = \vec{F}(\vec{u}_b)$$

   where $\vec{u}_b$ are the conserved quantities "on the boundary"

- $\vec{u}_b$ can be computed using the quantities c_b, ρ_b and v_b shown on the previous slide.

Mass injection boundary condition 4 (Newtonian fluid system)





This simple test problem demonstrates the injection of a “tent function” flux that is “on” between t=0.1 and 0.3 ns. The total mass in the system closely tracks the required total mass (as determined by the specified injection flux).

Mass injection boundary condition I (relativistic fluid system)

The user prescribes for a boundary sideset,

- Mass influx $\Gamma(t)$
- Virtual state temperature T_V
- Virtual state velocity $\vec{v}_V$

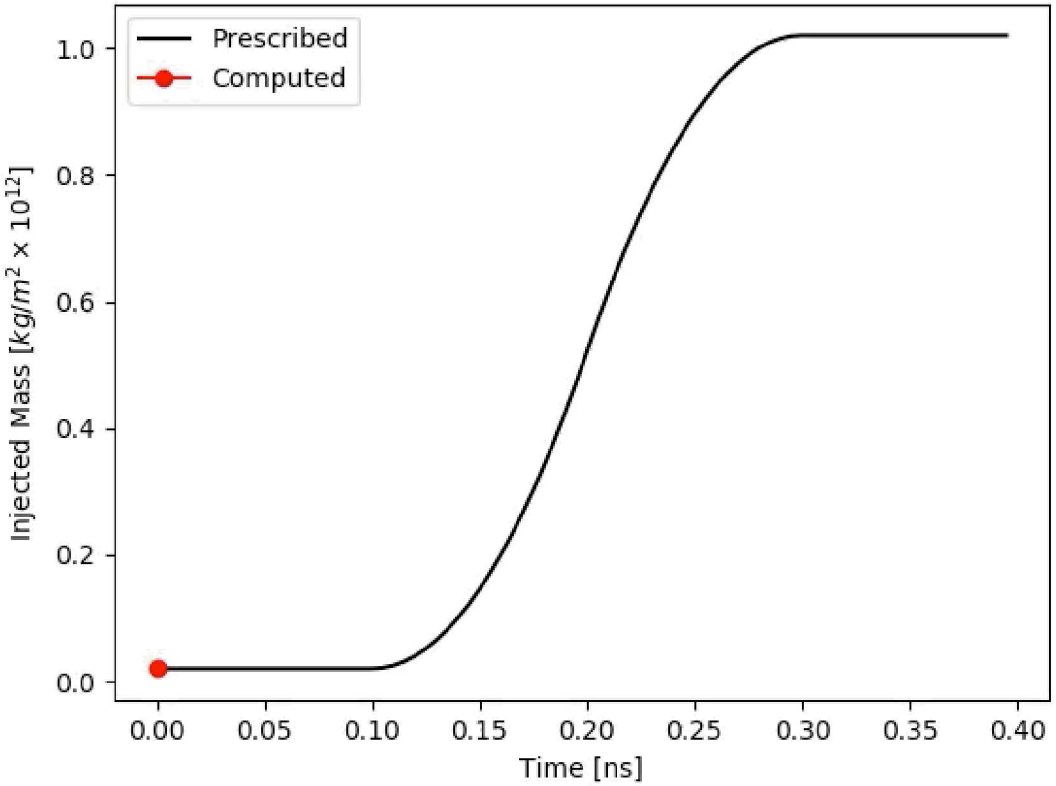
Then for each boundary mesh face,

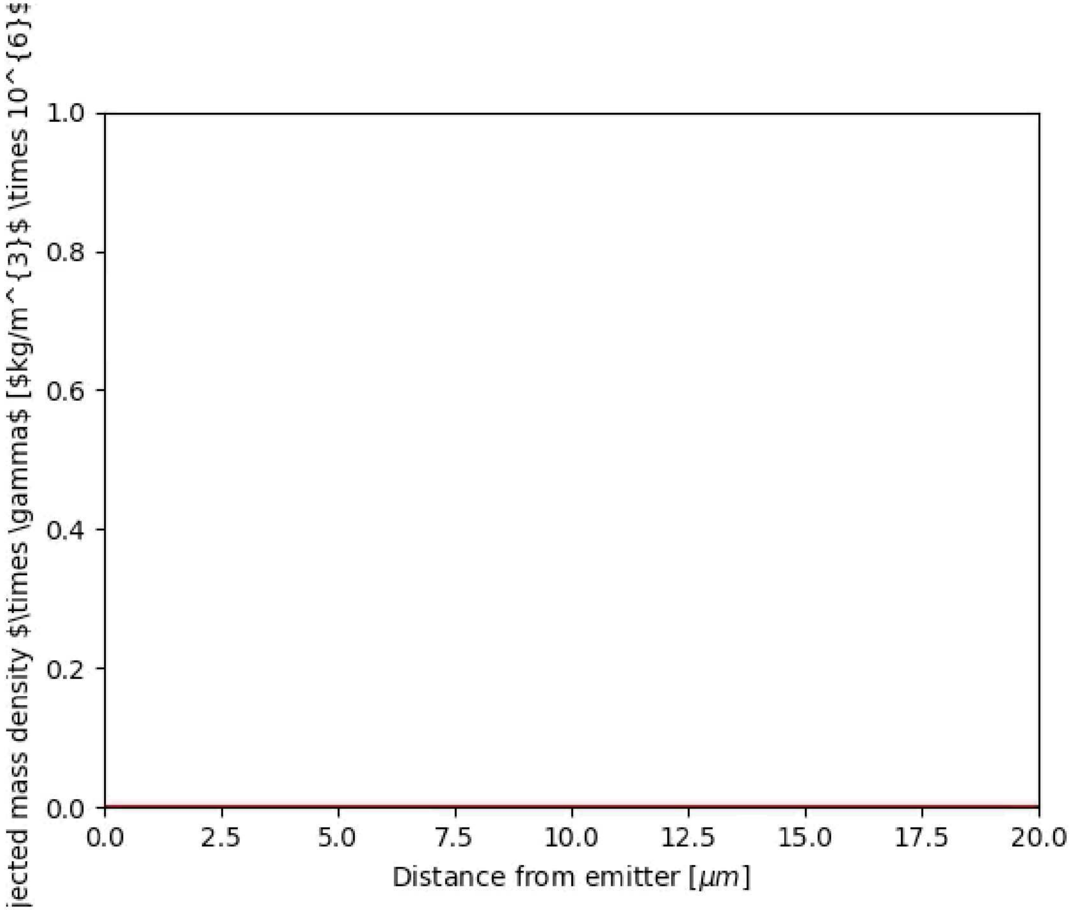
1. A virtual state density ρ_V is then computed by using the Brent method so that the relativistic HLL mass flux at the interior boundary is,

$$F_{HLL,1}(\vec{\mathrm{u}}_V, \vec{\mathrm{u}}_I) = \Gamma(t)$$

2. $\vec{F}_{HLL}(\vec{\mathrm{u}}_V, \vec{\mathrm{u}}_I)$ is then assigned as the boundary flux on that mesh face

Mass injection boundary condition 2 (relativistic fluid system)





- We converted the test case, considered for the Newtonian boundary condition above, to demonstrate relativistic mass injection
- The correct amount of mass is injected (less than 1% relative error)
- The relativistic solution differs from the Newtonian solution, probably because of the difference in the virtual state velocity determination

Mass injection boundary condition, discussion

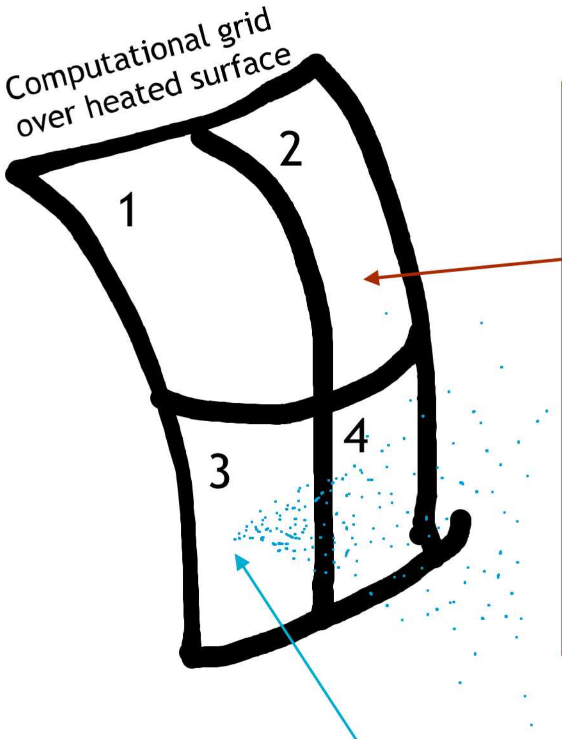
- The Newtonian and relativistic mass injection boundary conditions take different approaches to accomplish highly accurate injection of mass flux into the domain from a boundary
  - The difference in these approaches is orthogonal to any special considerations for relativistic fluids
- In practice, we found that the approach taken for relativistic fluids resulted in a more robust boundary condition
  - Larger timesteps can be taken with the relativistic fluid mass injection algorithm
- The undesirable "heuristic" virtual state velocity assignment in the Newtonian mass injection algorithm appears to be required for numerical stability

Thermal desorption / thermionic emission boundary condition

- Uses the “mass injection” BC framework to inject a by-mesh-face temperature dependent flux

- Emission flux model is consistent with,
  - Thermal desorption (Temkin, Polanyi-Wigner fluxes)
  - Thermionic emission (Richardson-Dushman flux) – additional work would be needed to prevent over-injection of thermionic electrons

- 1D heating model applied to each surface mesh face
  - Heating source term $Q(x,t)$ accounts for eddy current heating (consistent with magnetic field evolution)



Heating model

$$\frac{\partial u}{\partial t} = Q(x,t) - \frac{\partial q}{\partial x}$$

$$q = -k\,\frac{\partial T}{\partial x}$$

$$T(u) = \int_0^u \frac{du'}{c(u')}$$

$$q(x=0) = 0$$

$$u(x, t=0) = u_0$$

$$\lim_{x\to\infty} u(x,t) = u_0$$

Emission flux model

$$\Gamma = \nu\, T^{\alpha}\, \theta^{n} \exp\left(-\frac{E_a}{k_B\, T}\right)$$

$$\dot{\theta} = -\Gamma$$

SCL boundary condition

The SCL boundary condition injects a mass flux of charged substance as a function of the electric field,

$$\Gamma(t) = \Gamma_{SCL}\big(E(t)\big)$$

We are currently considering the following model (to be improved upon later if needed),

$$\Gamma_{SCL}\big(E(t)\big) = \gamma_0\left(\vec{E}(t)\cdot\hat{n}\right) + \gamma_1 \frac{\partial\left(\vec{E}(t)\cdot\hat{n}\right)}{\partial t}$$

The SCL boundary, with appropriate choice of parameters γ_0 and γ_1 will,

- **Cause $\vec{E}(t)\cdot\hat{n}$ to relax to zero**
- Adjust the injection flux $\Gamma(t)$ as the solution evolves to maintain $\vec{E}(t)\cdot\hat{n}\approx 0$

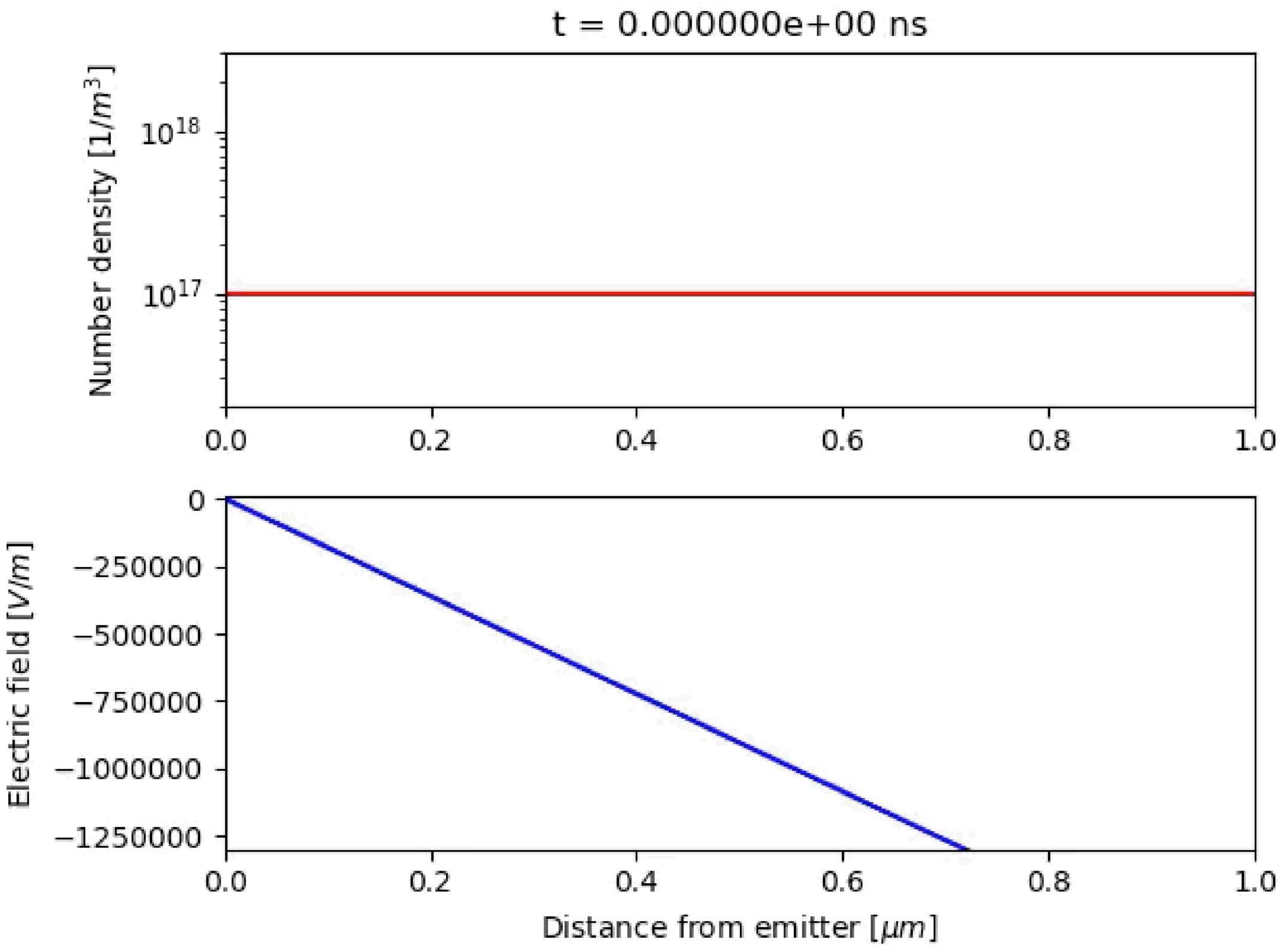
Note: Presently SCL uses a simpler, less accurate mass injection algorithm compared to the one described above

SCL boundary condition, demonstration (Newtonian fluid system)

- A simple 1D diode problem demonstrates the effectiveness of the boundary condition to adjust Γ so that the electric field at the cathode remains nearly zero

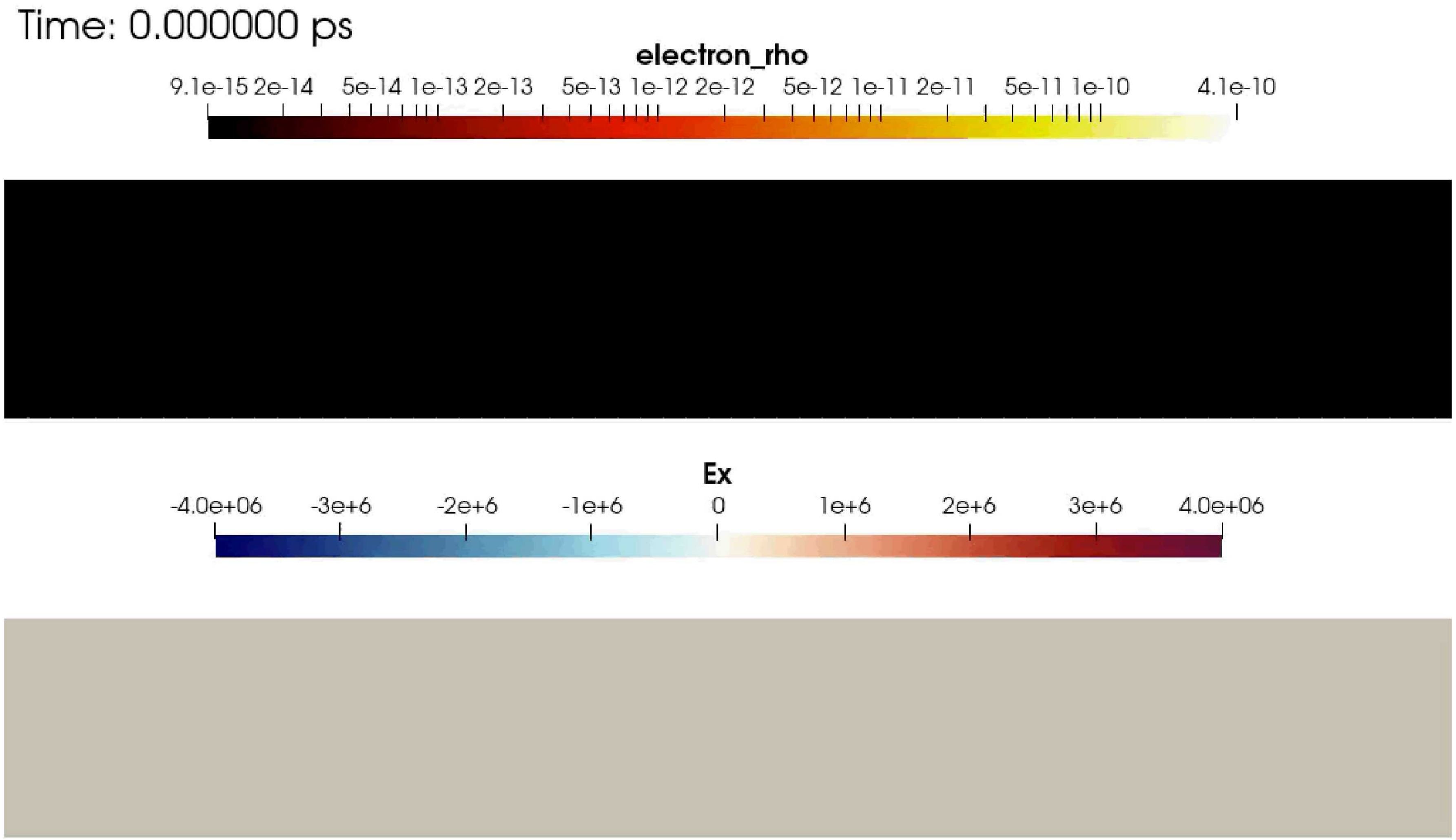
- The electric field is initially zero at the cathode so that the initial transient is less violent

- Less well behaved problems, with a larger initial transient, have not been observed to cause an issue with the boundary condition

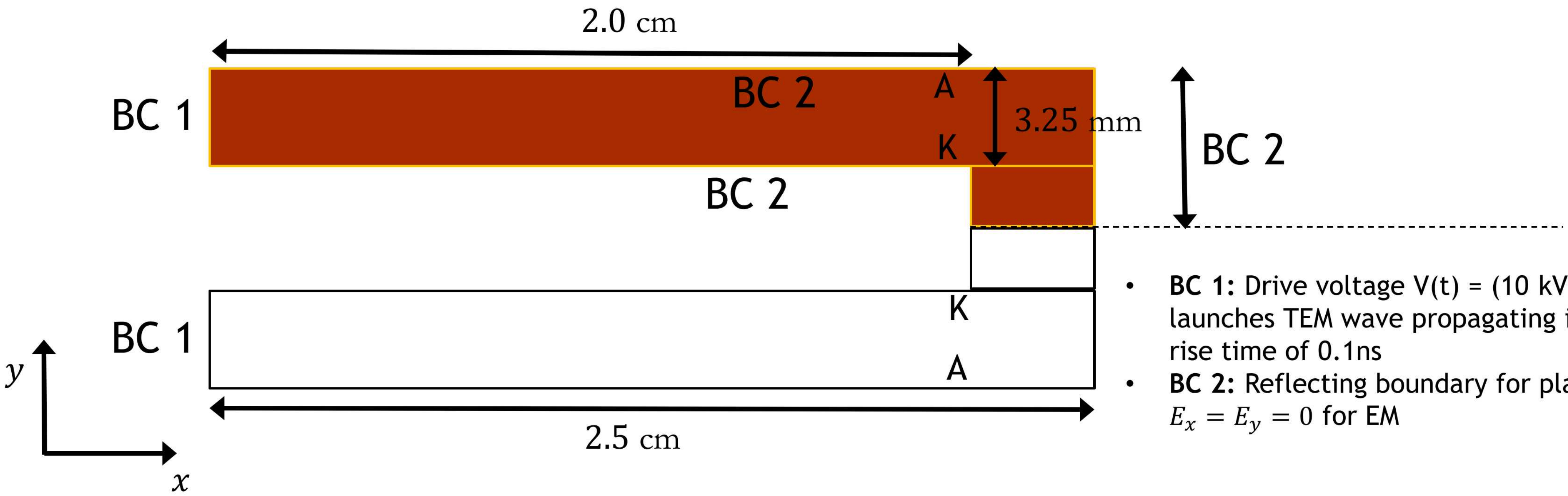


SCL boundary condition, simple demonstration problem (Relativistic fluid system)

- This early demonstration problem considers SCL electron emission from a surface due to a DC transverse electromagnetic wave
- SCL emission drives the electric field to nearly zero at the emission surface

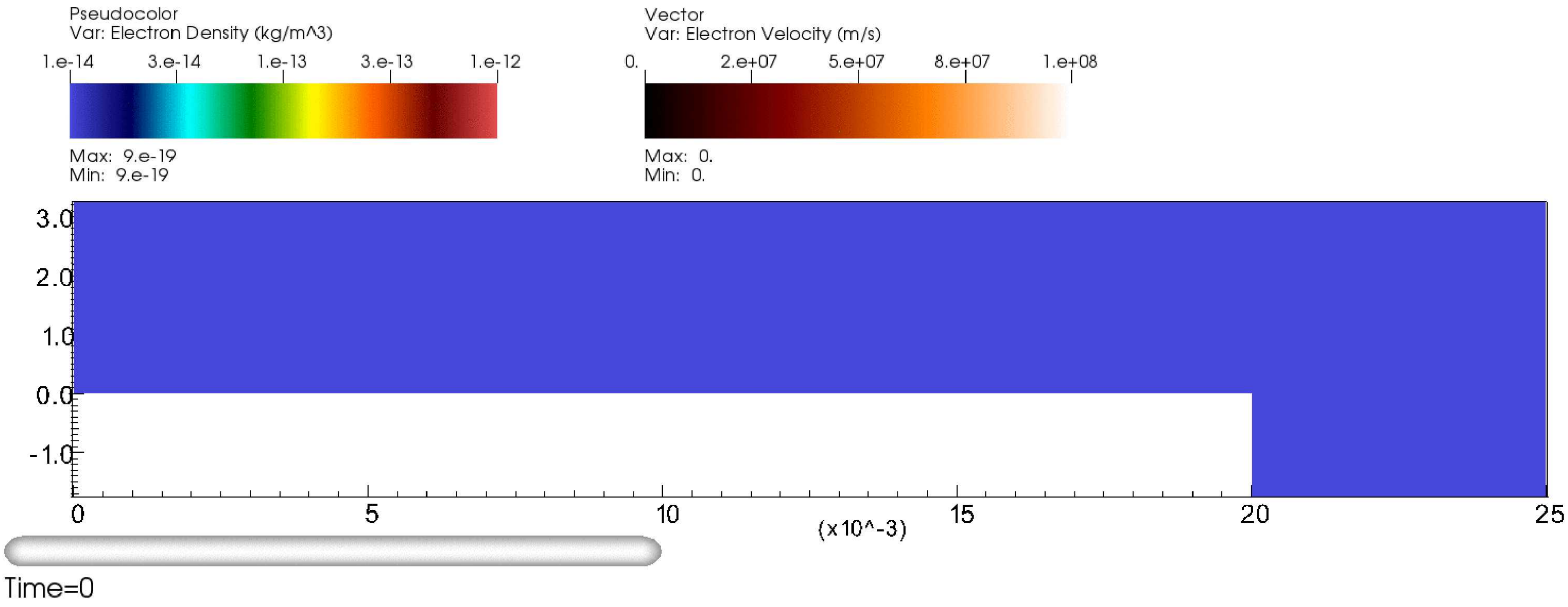


SCL boundary condition, simple MITL problem (Relativistic fluid system)



- **BC 1:** Drive voltage V(t) = (10 kV)*time/(0.1 ns), which launches TEM wave propagating in x-direction, with a rise time of 0.1ns
- **BC 2:** Reflecting boundary for plasma; $E_x = E_y = 0$ for EM

SCL boundary condition, simple MITL problem (Relativistic fluid system)



Summary

The Newtonian & relativistic mass injection boundary conditions offer precise control over the amount of substance injected into the computational domain.

The thermal desorption and SCL BCs are built upon these mass injection BCs:

- Thermal desorption
  - These boundary conditions self-consistently compute the surface temperature according to Ohmic heating
  - A flux of substance is injected at a rate that is determined by the surface temperature
- Newtonian & relativistic SCL
  - These boundary conditions inject charged substance at a rate so that the electric field at the emitting surface is reduced to nearly zero

Extra Slides: Mass injection test problem injection flux

Top: The mass injection flux Γ (in $kg\ m^{-2}s^{-1}$, versus time in s) for the simple test problem

Bottom: The cumulative injected mass (in kg/m^2, versus time in s)