

- When re-running the 2D 1 Torr GEC case file, the simulation started to fail.
- Three main things were changed to get the simulation running:
  - Line search was set to 'none' (Note: none = basic)
  - The terms in the EconomouDielectricBC boundary condition was rearranged to reduce the residual norm by a magnitude.
  - A structured mesh was used, instead of the previous unstructured mesh
- A more detail summary is on the following slides.

- When trying to run the full 2D 1 Torr GEC Case, the simulation starts to diverge and fail.
  - This should be the same file for the results shown at 2019 GEC.
  - This is only a problem with the 1 Torr case, the 100mTorr case still runs the same as in last November.
- After looking at the output log and results, I believe the problem is with the 'EconomouDielectricBC' boundary condition.
- To test this, three version of the boundary condition were compared to each other.
  - The current form, noted as Default
  - A form with the terms rearranged, noted as Rearranged
  - A form where the flux terms were defined as the fluid flux, noted as FluidFlux

## Default

- The current EconomouDielectricBC is defined as:

$$e \frac{d_i}{\varepsilon_i} (\Gamma_+ - \Gamma_e) + \frac{d_i \varepsilon_0}{\varepsilon_i} \frac{\partial \nabla V}{\partial t} - \frac{\partial V}{\partial t} = 0$$

- Where the fluxes as defined as:

$$\Gamma_+ = \alpha \mu_+ n_+ (-\nabla V)$$

$$\text{Where } \alpha = \begin{cases} 1, & \text{if } -\nabla V \cdot n > 0 \\ 0, & \text{if else} \end{cases}$$

$$\Gamma_e = \frac{1}{4} \sqrt{\left( \frac{8eT_e}{\pi m_e} \right)} n_e - \gamma_{se} \Gamma_+$$

## Rearranged

- The rearranged version moves the permittivity and thickness of the dielectric, defined as:

$$e (\Gamma_+ - \Gamma_e) + \varepsilon_0 \frac{\partial \nabla V}{\partial t} - \frac{\varepsilon_i}{d_i} \frac{\partial V}{\partial t} = 0$$

- The flux terms are the same as before.

## FluidFlux

- The “fluid flux” version is in the same arrangement as the current BC, but redefines the flux terms as:

$$\Gamma_+ = \alpha \mu_+ n_+ (-\nabla V) - D_+ \nabla n_+$$

$$\text{Where } \alpha = \begin{cases} 1, & \text{if } -\nabla V \cdot n > 0 \\ 0, & \text{if else} \end{cases}$$

$$\Gamma_e = -\beta \mu_e n_e (-\nabla V) - D_e \nabla n_e$$

$$\text{Where } \beta = \begin{cases} 1, & \text{if } \nabla V \cdot n > 0 \\ 0, & \text{if else} \end{cases}$$

- Along with testing the three different version of the dielectric boundary condition, simulation run with/without Actions.
- All simulation ran with SMP as the preconditioner and the executioner options of:

`automatic_scaling = true`

`compute_scaling_once = false`

`solve_type = NEWTON`

`scheme = bdf2`

`dtmax = 1e-9`

`dtmin = 1e-14`

`line_search = none`

`petsc_options = '-snes_converged_reason -snes_linesearch_monitor'`

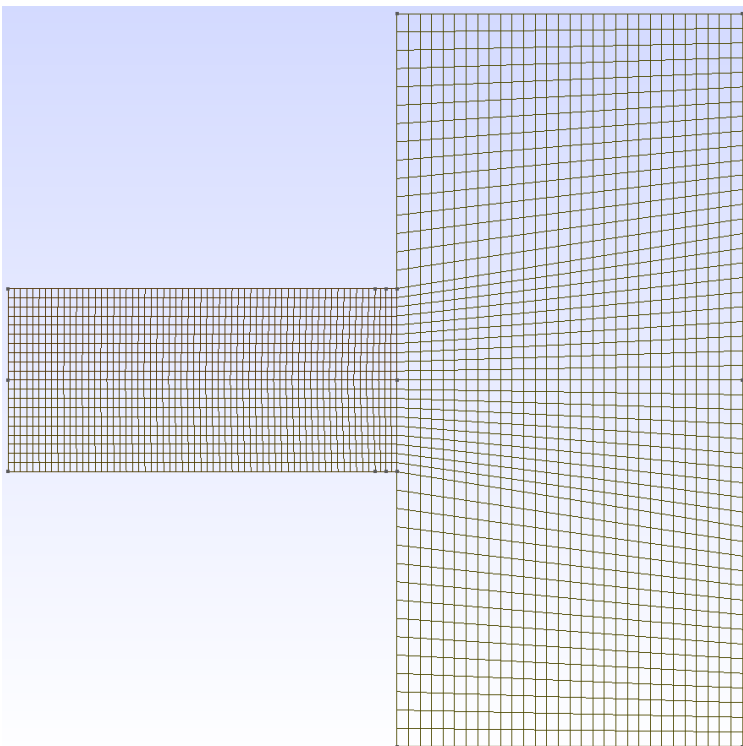
`petsc_options_iname = '-pc_type -pc_factor_shift_type -pc_factor_shift_amount -ksp_type -snes_linesearch_minlambda'`

`petsc_options_value = 'lu NONZERO 1.e-10 fgmres 1e-3'`

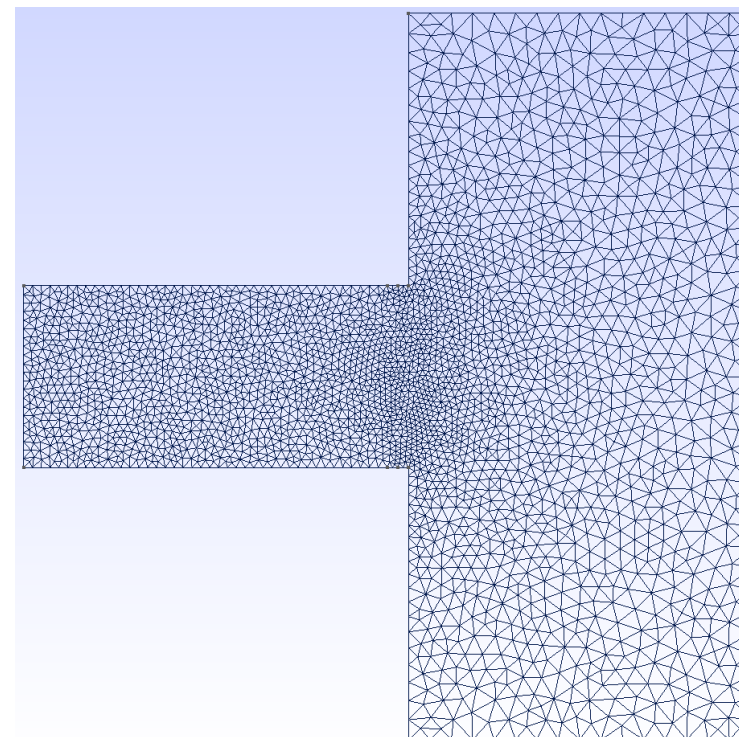
- For the first sets of results, only the FluidFlux BC ran for the allowed wall time (48 hours) for both the Action and non-Action runs.
- Both the Default and Rearranged BC failed.
  - The solution between the Default and Rearranged BC (both with and without the Actions) were all the same.
  - It should be noted that the Rearranged BC had significantly smaller residual norm than the Default BC by about a magnitude
    - 0 iteration  $|R| \approx 1e15$  for Default and 0 iteration  $|R| \approx 1e5$  for Rearranged during most of the run.
- Next set of runs involved along the Default and Rearranged BC, but without any position scaling (i.e. position\_units = 1.0).
  - These sets of simulations failed sooner, but showed similar behavior to the previous runs
    - With position scaling, failed at  $t = 2.83e-7$
    - Without position scaling, failed at  $t = 3.177e-8$

- Next step was to see if the simulation would converge with a coarser mesh, one structured and the other unstructured.
  - Both mesh had approximately 3000 nodes, with slight refinement in-between the electrodes and insulators.
- For these runs, only the Rearranged BC and Actions were tested, along with and without position scaling.

## Structured

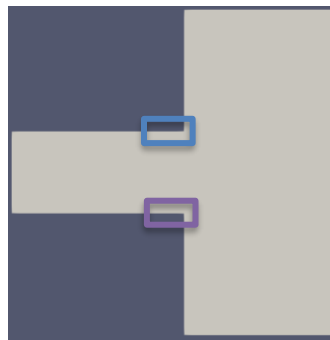


## Unstructured

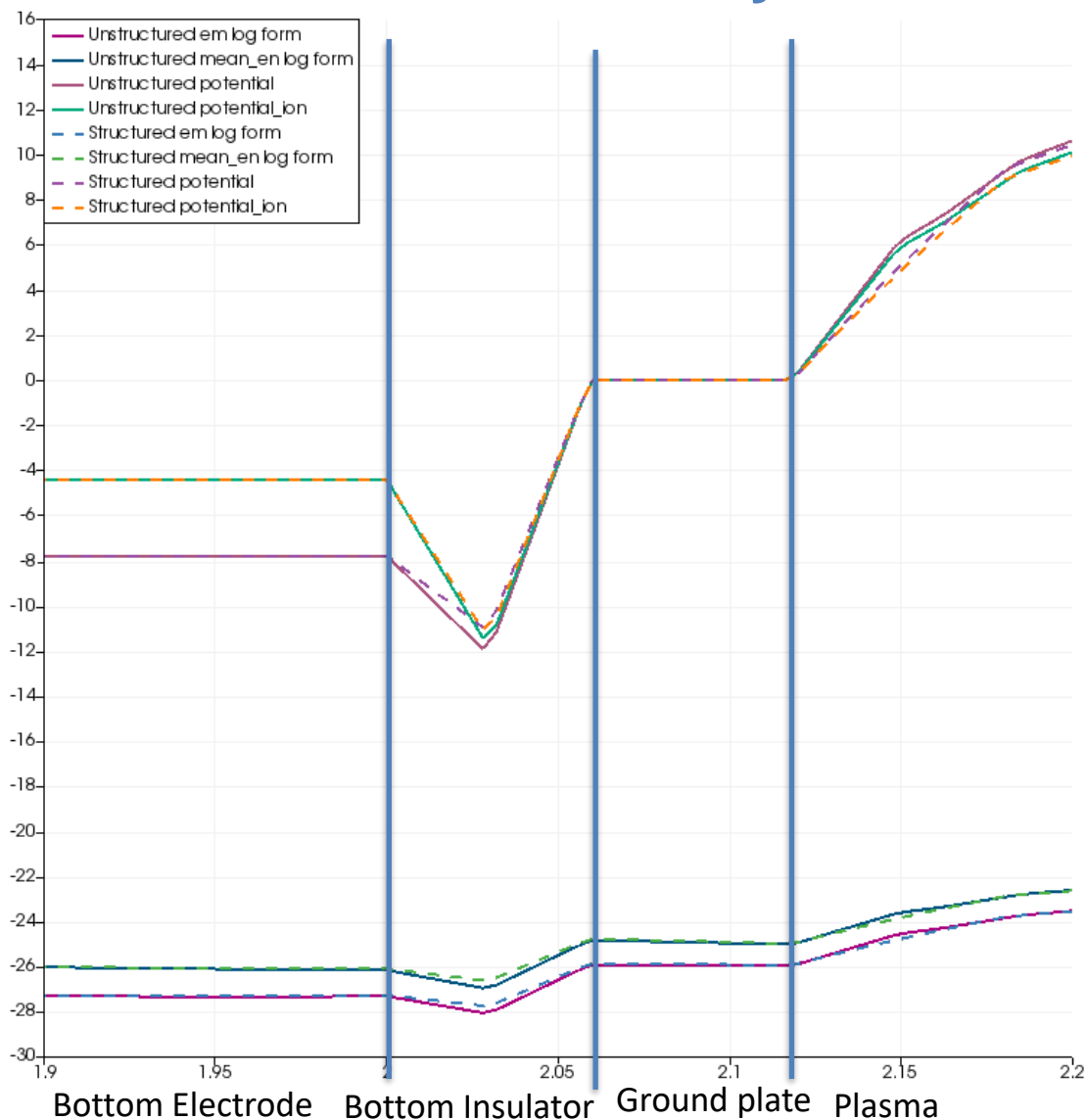


- For the unstructured mesh, the simulations failed both with and without position scaling.
  - The main cause of failure might be that using the dielectric boundary condition cause the argon ions to try to hit zero near the insulator's edges. Though, because Zapdos is cased in log form, the argons never hits zero and only reaches high negative values (e.g.  $\lim_{x \rightarrow 0^+} \ln x = -\infty$ ).
  - Zapdos does have the LogStabilizationMoles kernel for this reason but using it can cause artificial higher bulk densities.
- For the structured mesh, the simulations ran to completion (500 rf cycles), both with and without position scaling.
  - Similar to the unstructured mesh, the ion density is low at the insulator's edges early in the simulation, but the ions recover and grow later on.

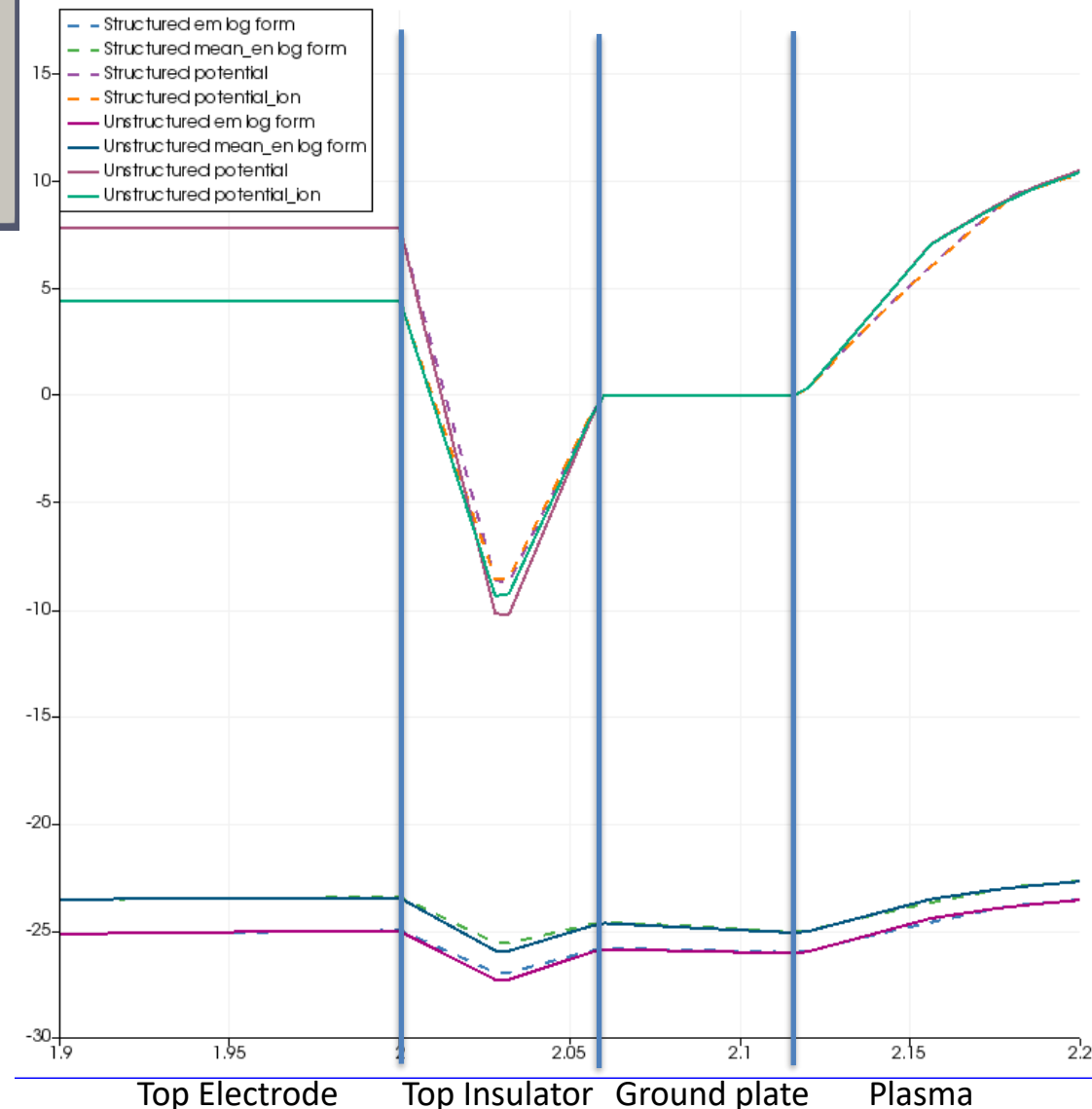
$t = 8.45e-7s$



## Bottom Boundary

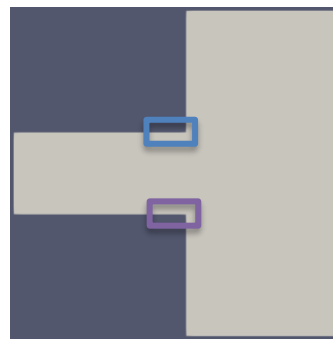


## Top Boundary

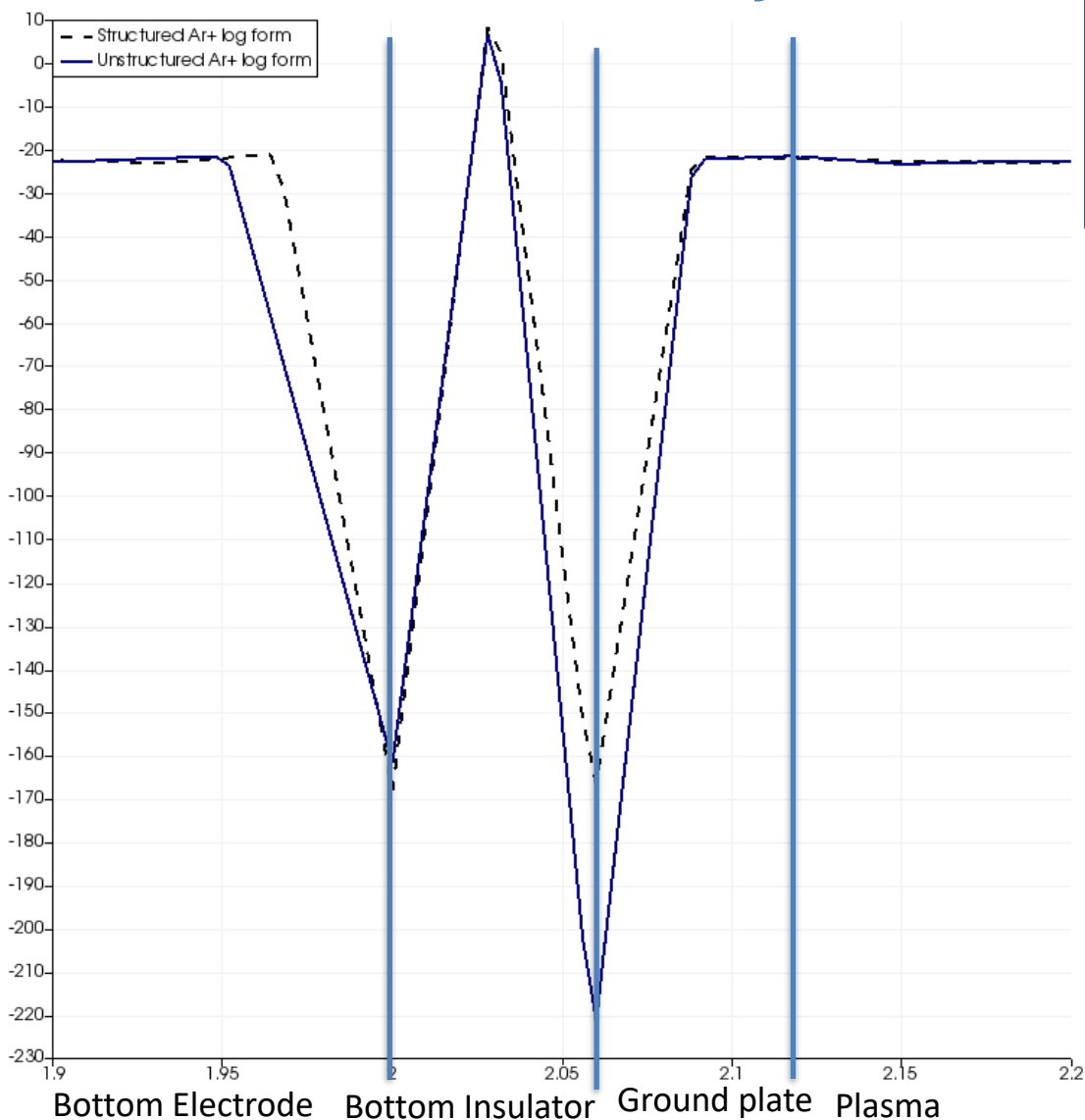




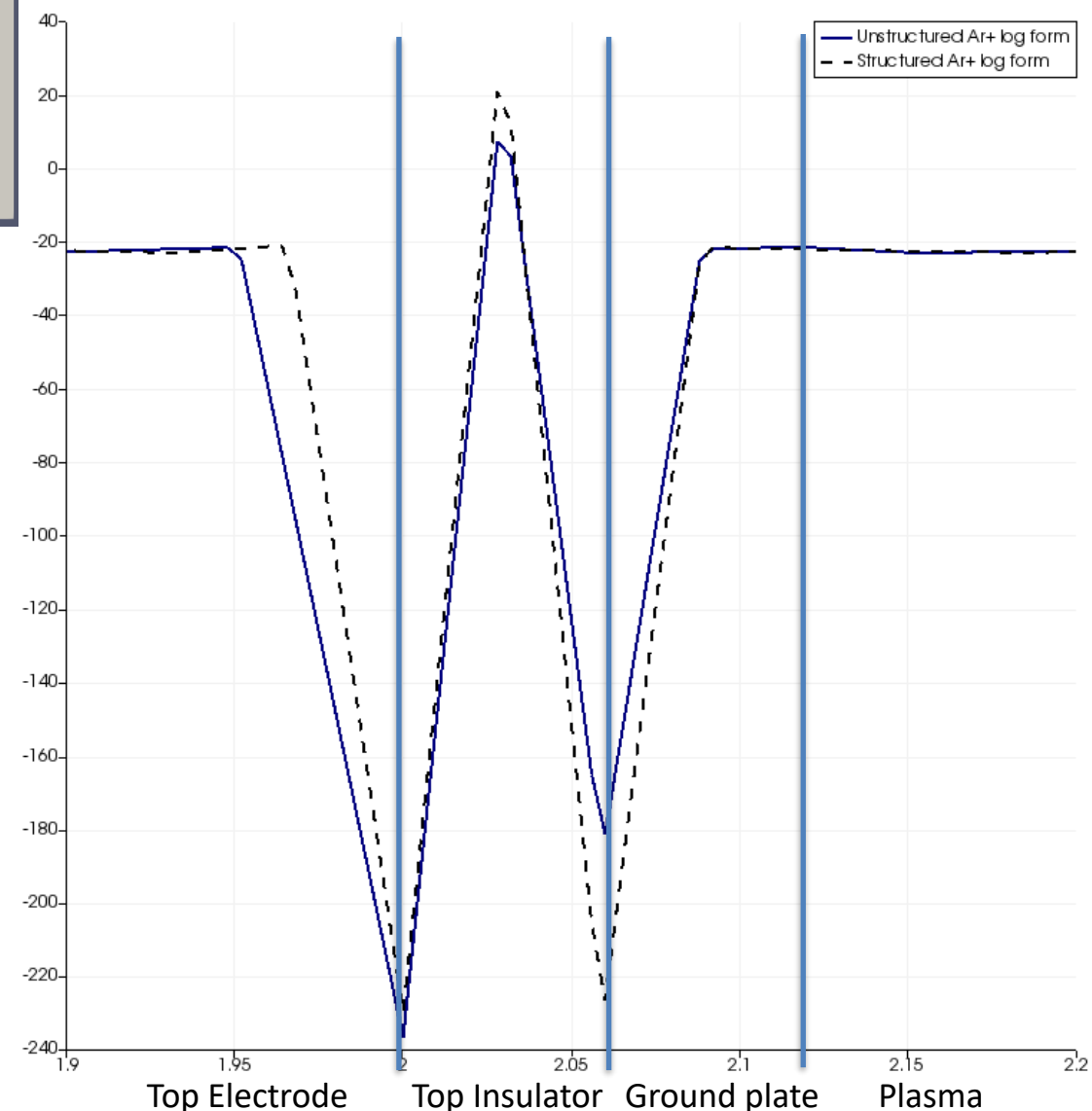
$t = 8.45e-7s$



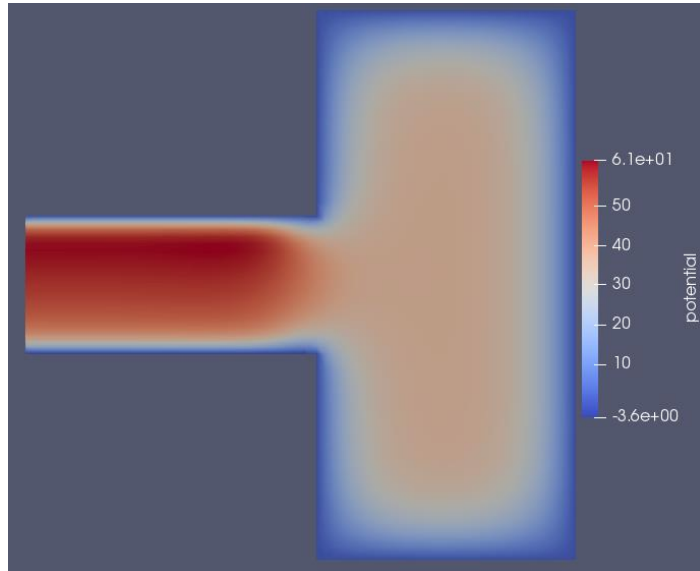
## Bottom Boundary



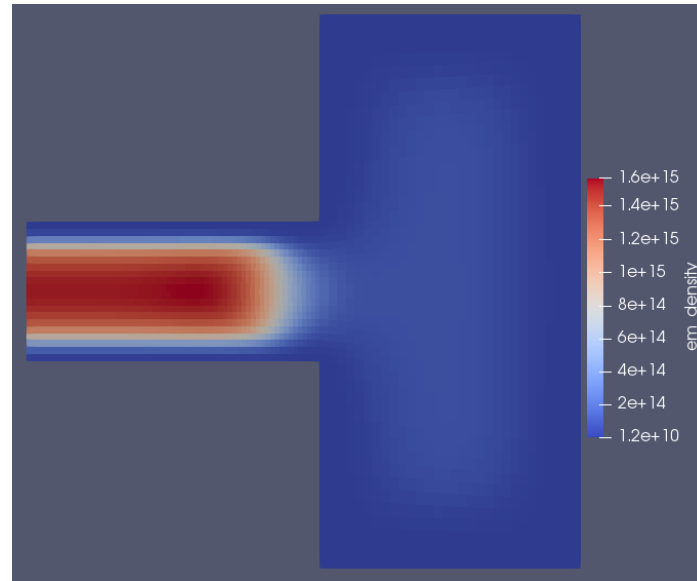
## Top Boundary



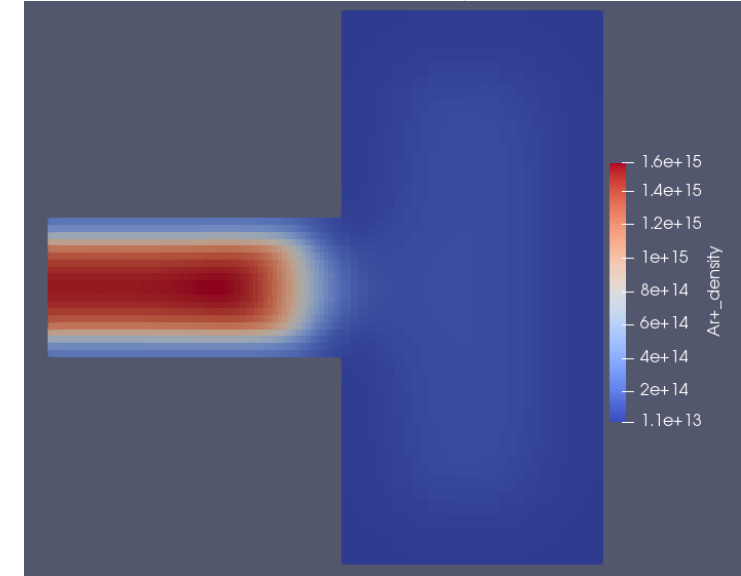
Potential [V]



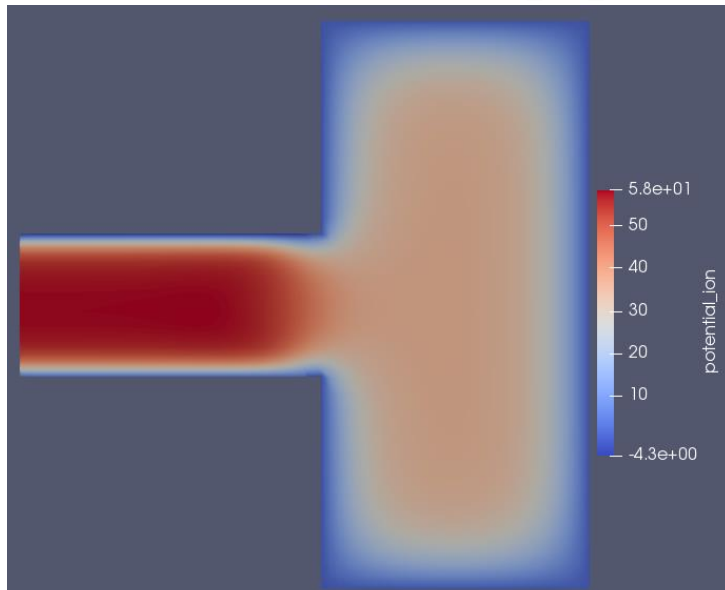
Electron Density [ $m^3$ ]



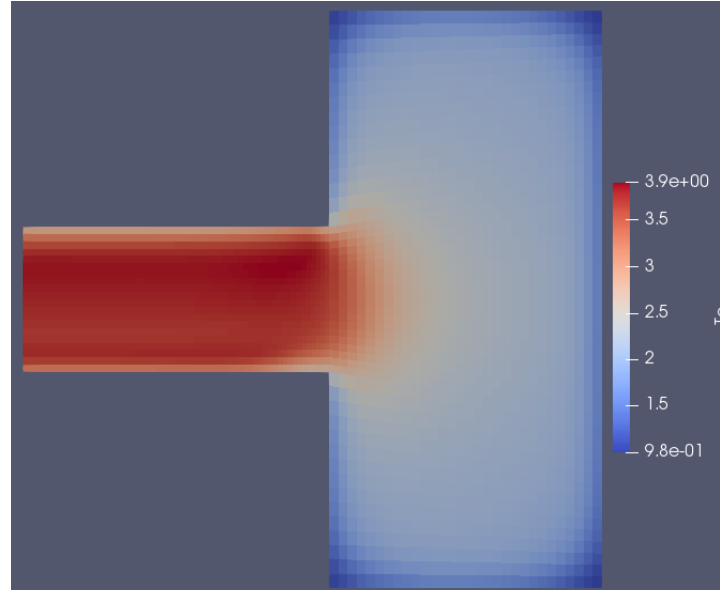
Ion Density [ $m^3$ ]



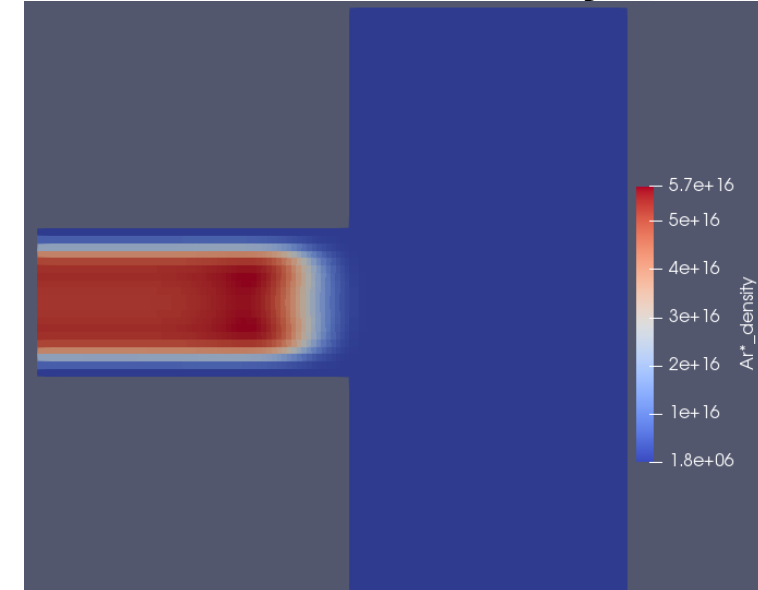
Ion Potential [V]



Electron Temp. [V]



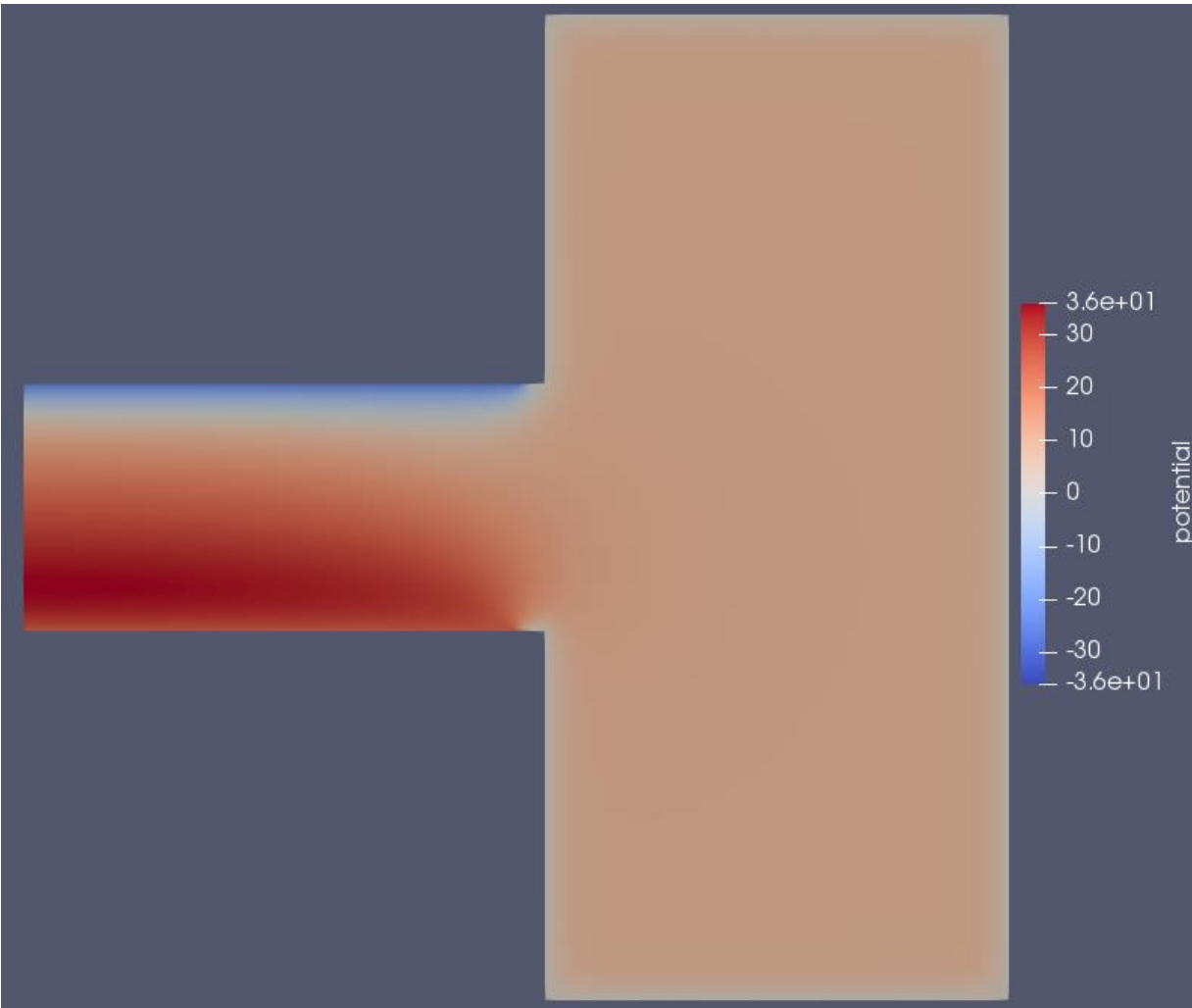
Metastable Density [ $m^3$ ]



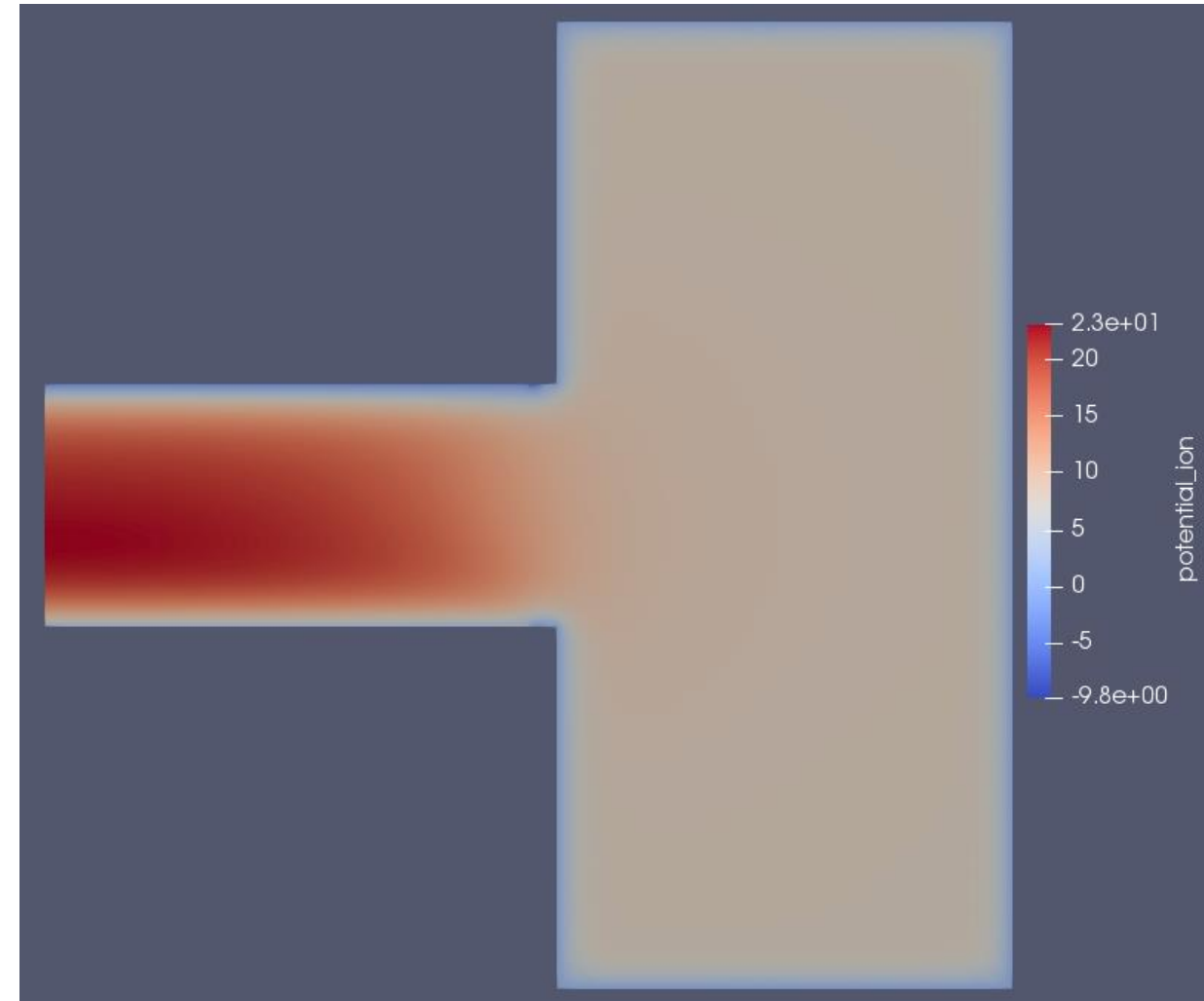
**The Following Slides are Results of the Failed Simulations**

# Results for Default BC / Actions / Standard Mesh

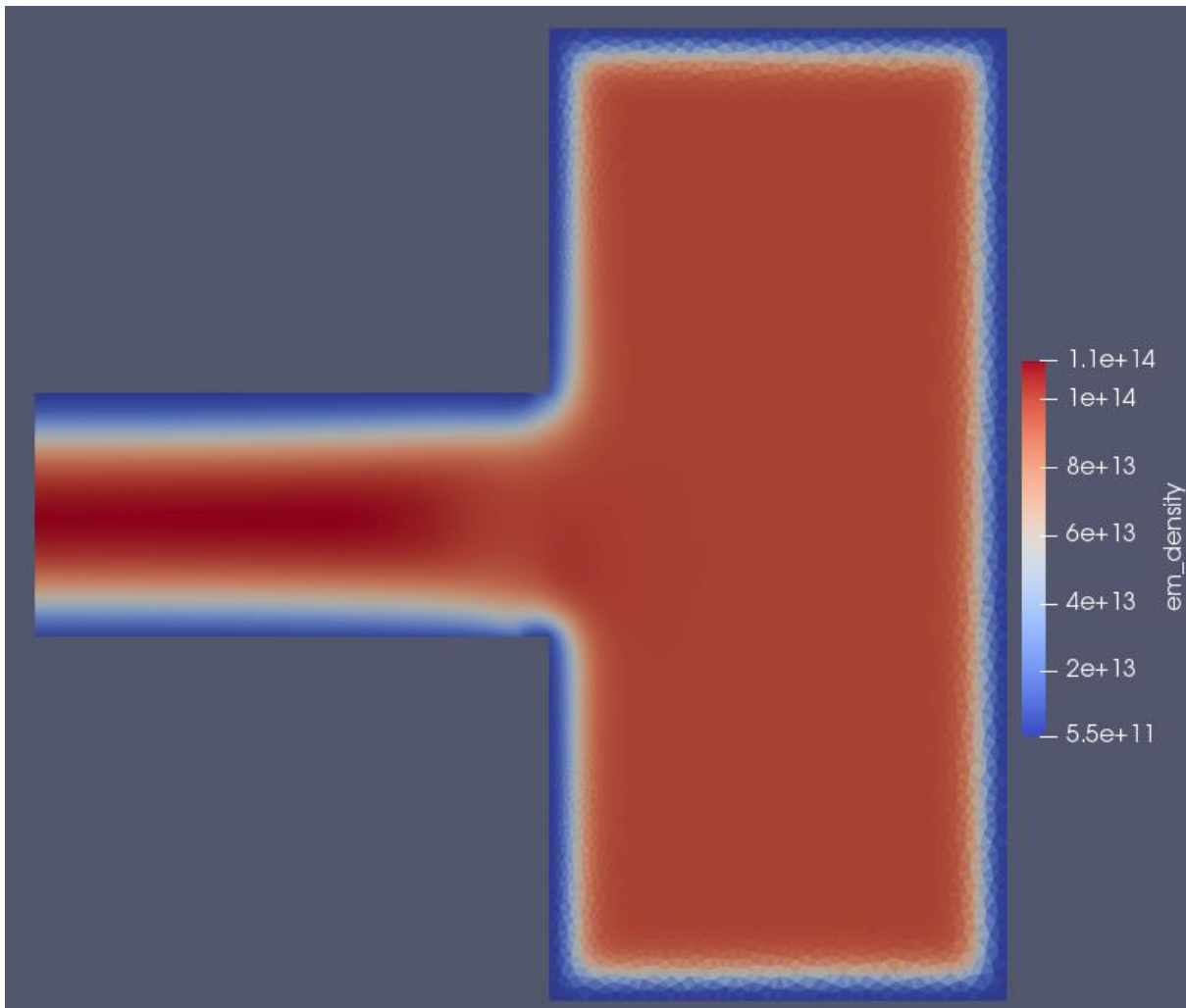
Potential [V]



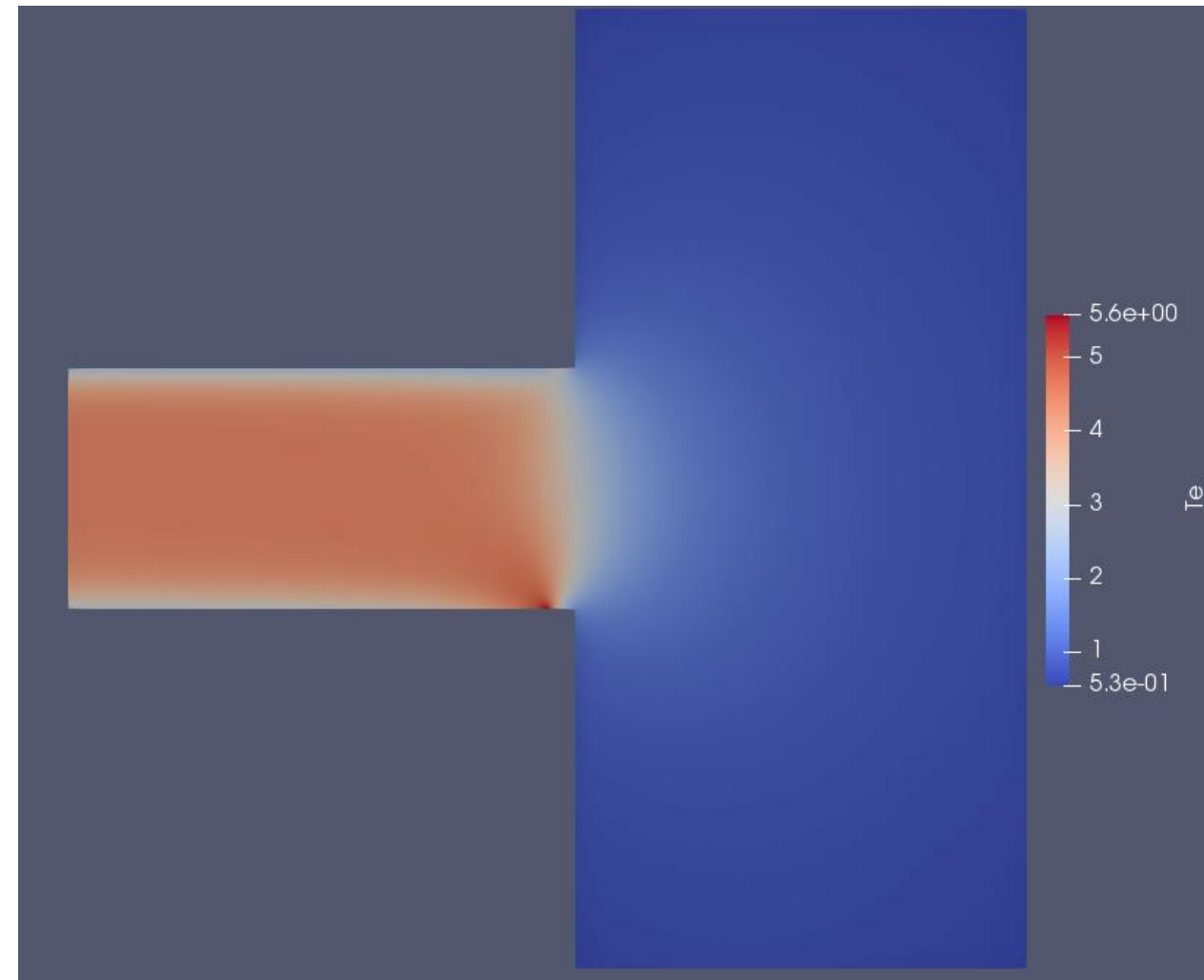
Ion Potential [V]



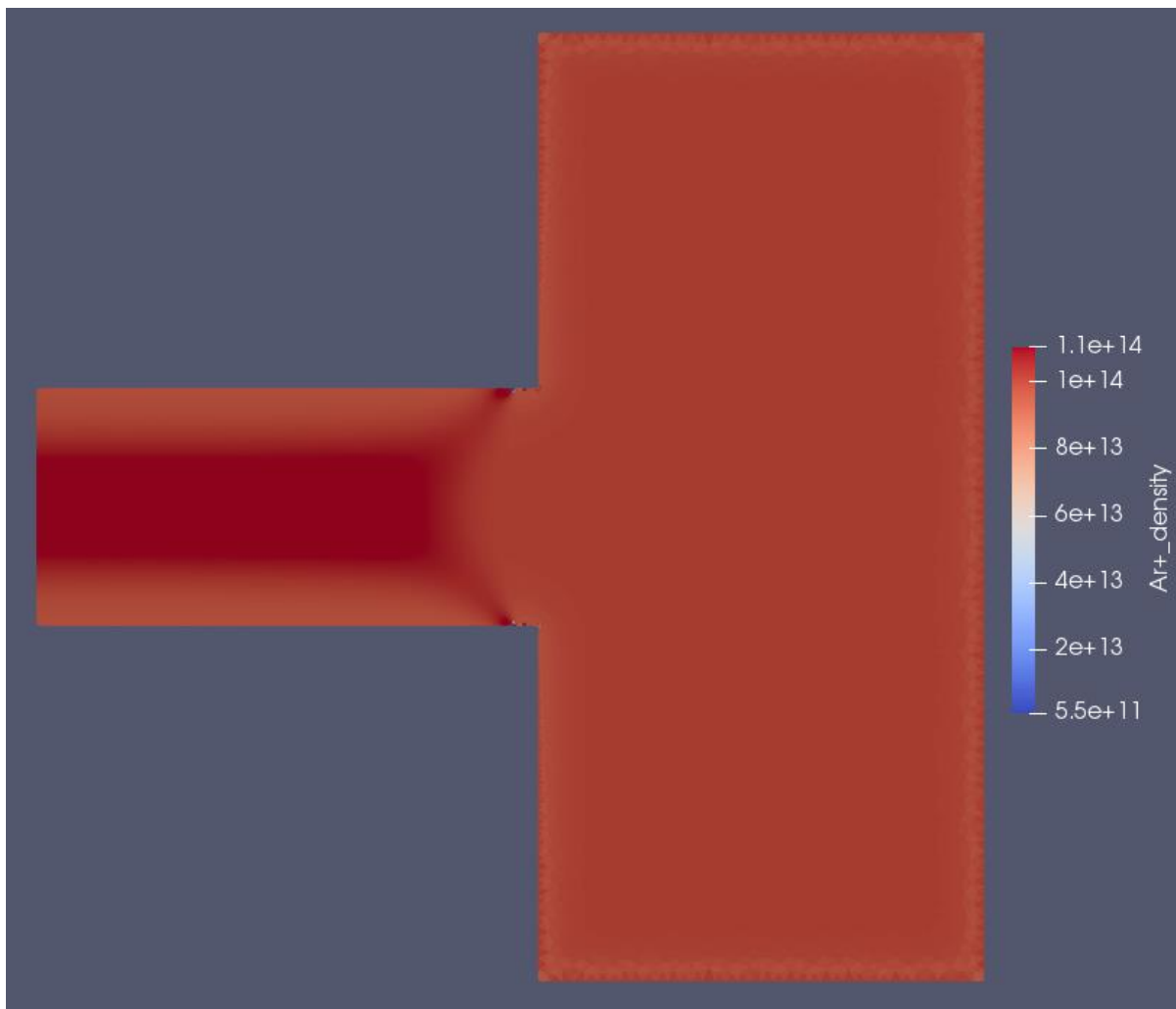
Electron Density [ $\text{m}^3$ ]



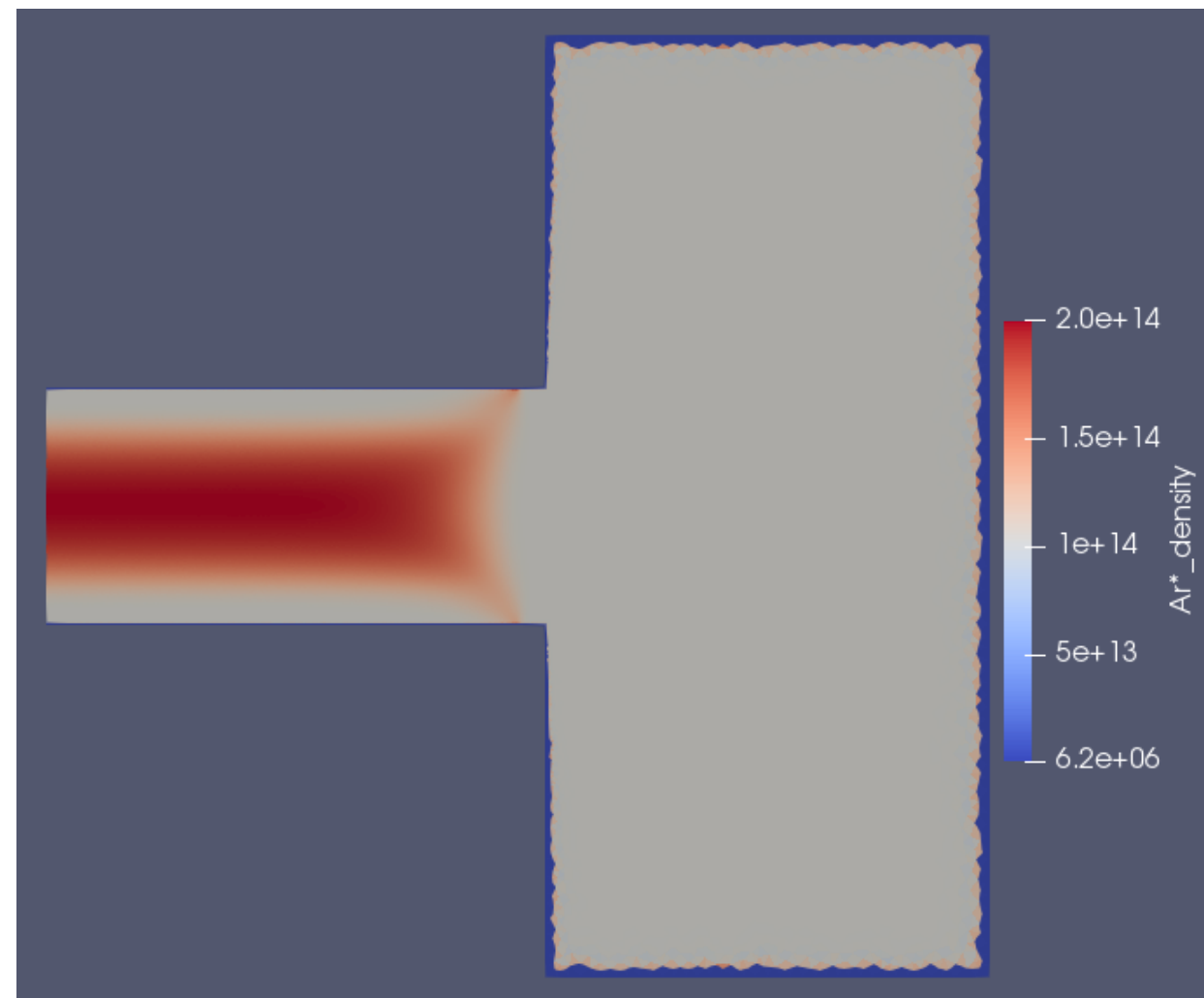
Electron Temperature [V]



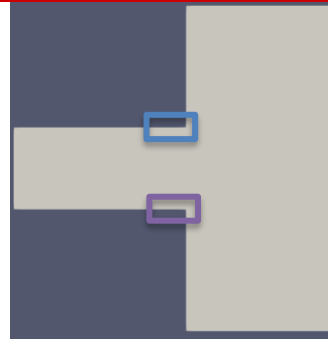
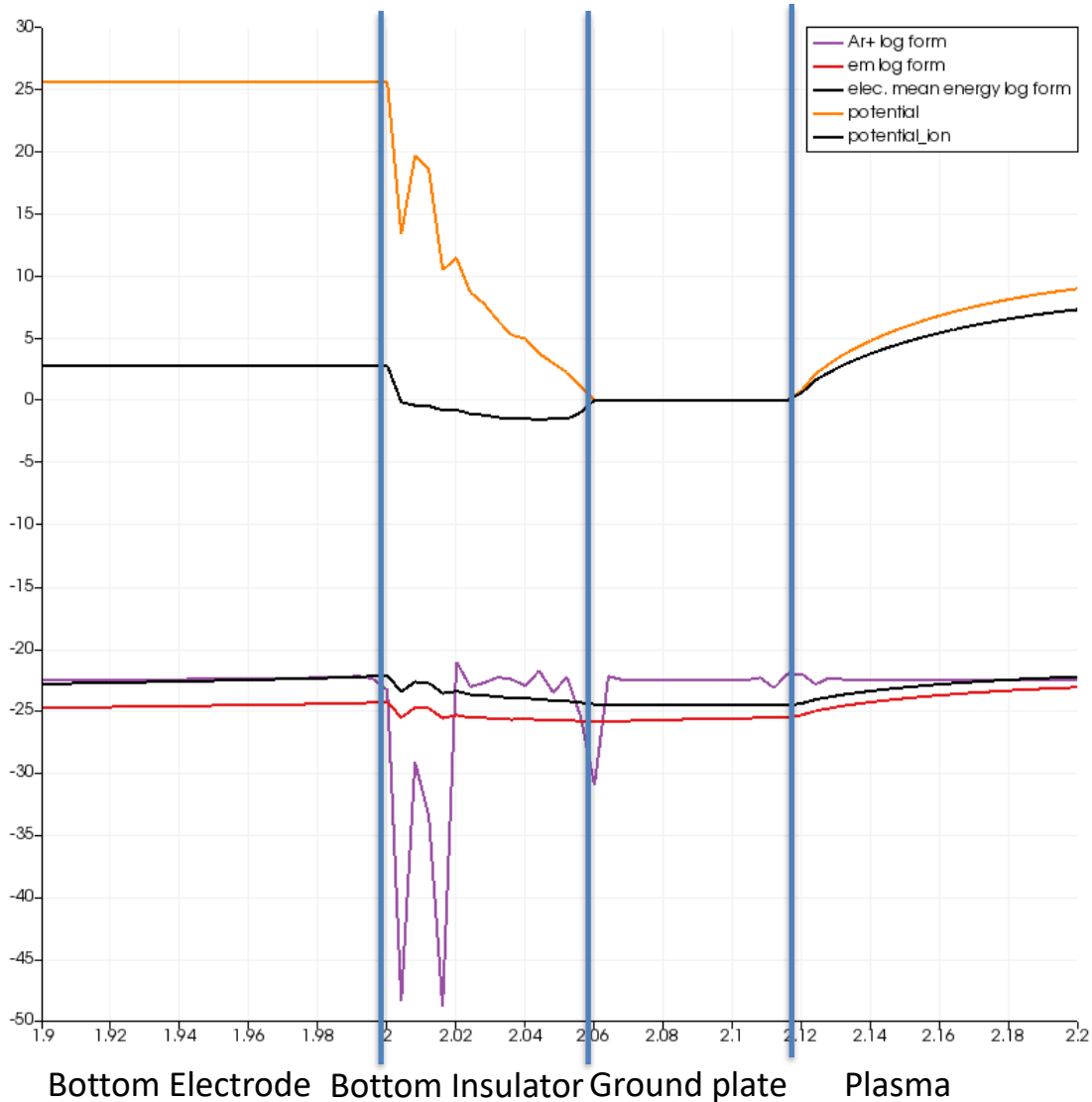
**Ion Density [m<sup>3</sup>]**



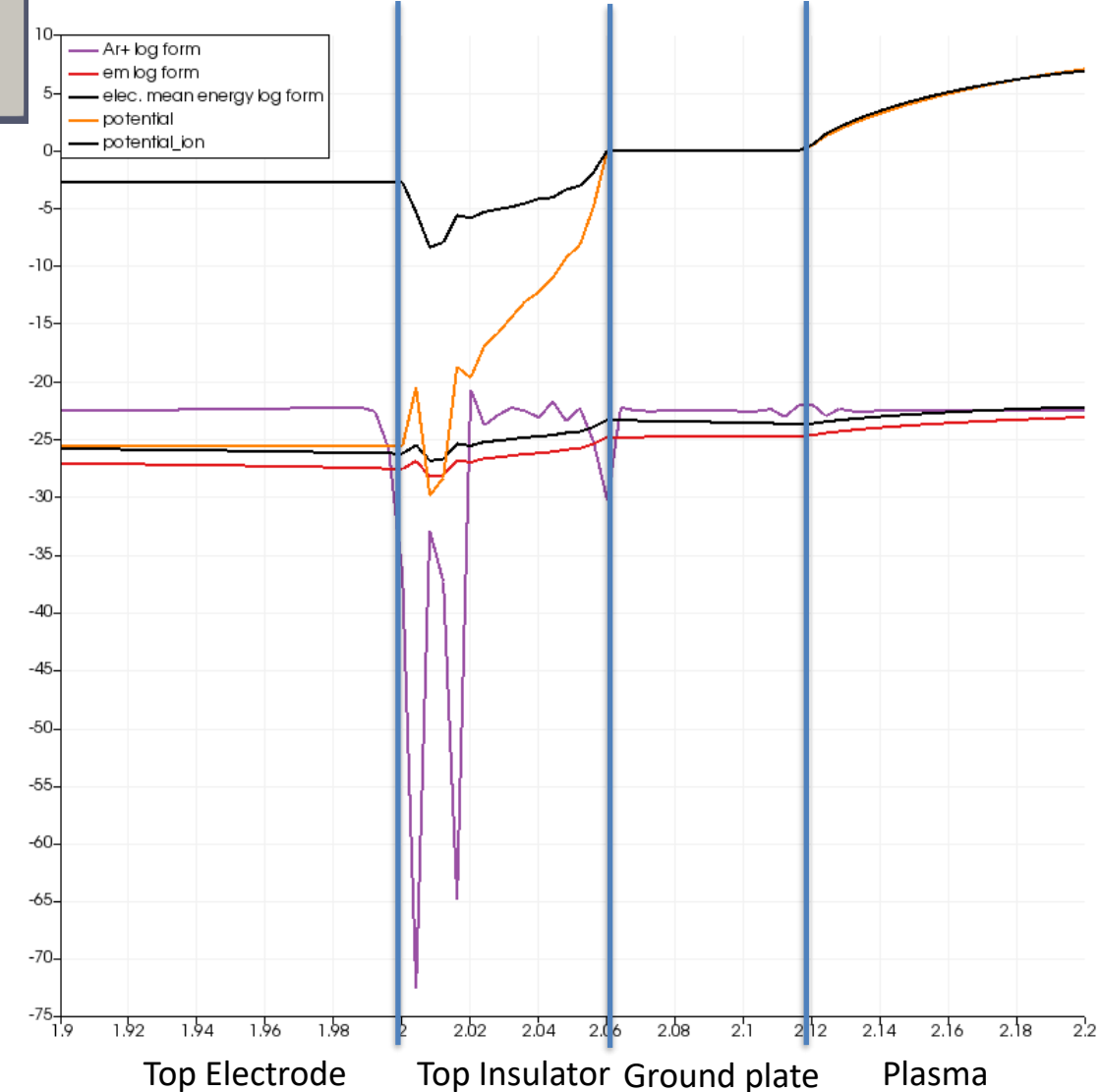
**Metastable Density [m<sup>3</sup>]**



## Bottom Boundary



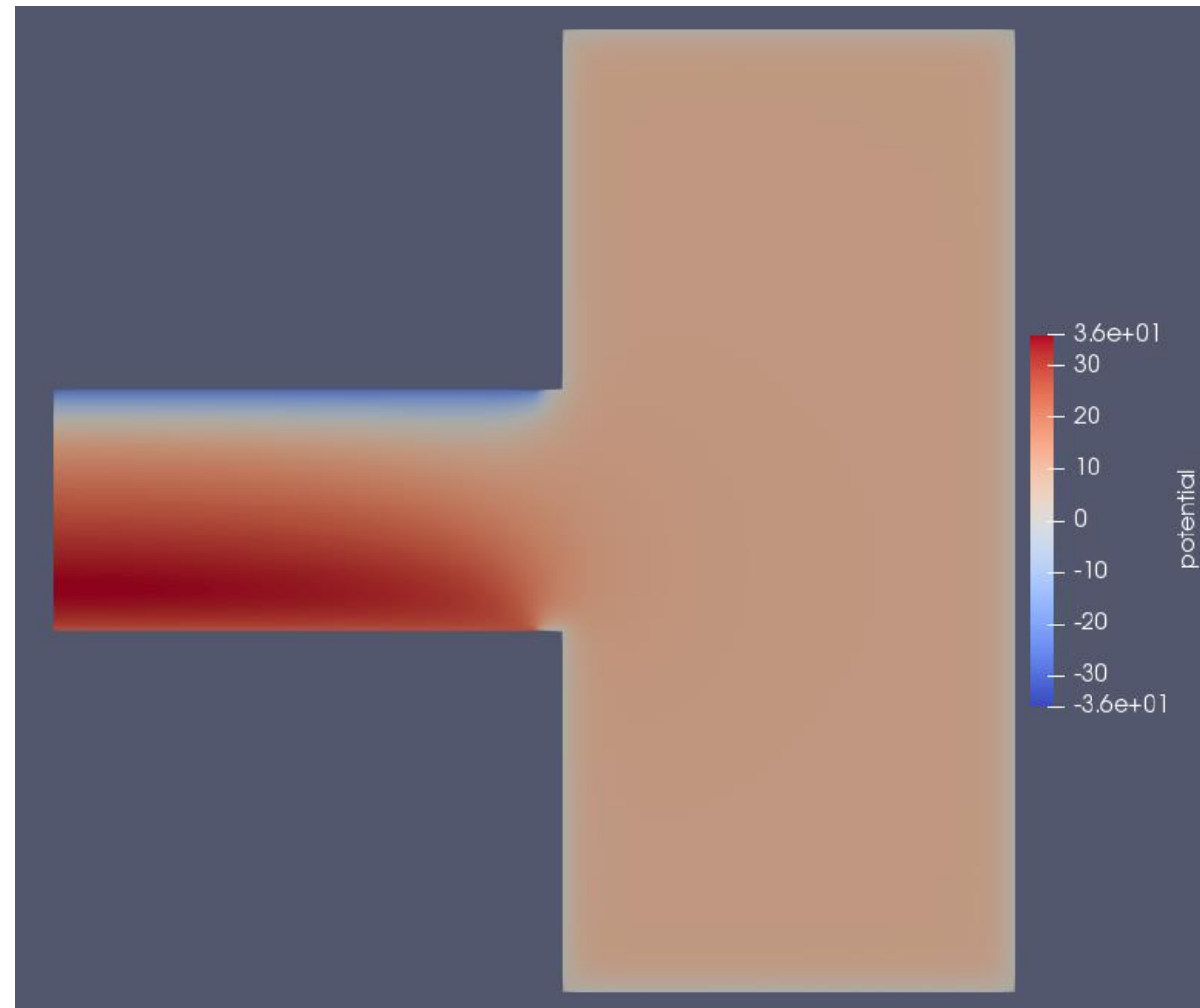
## Top Boundary



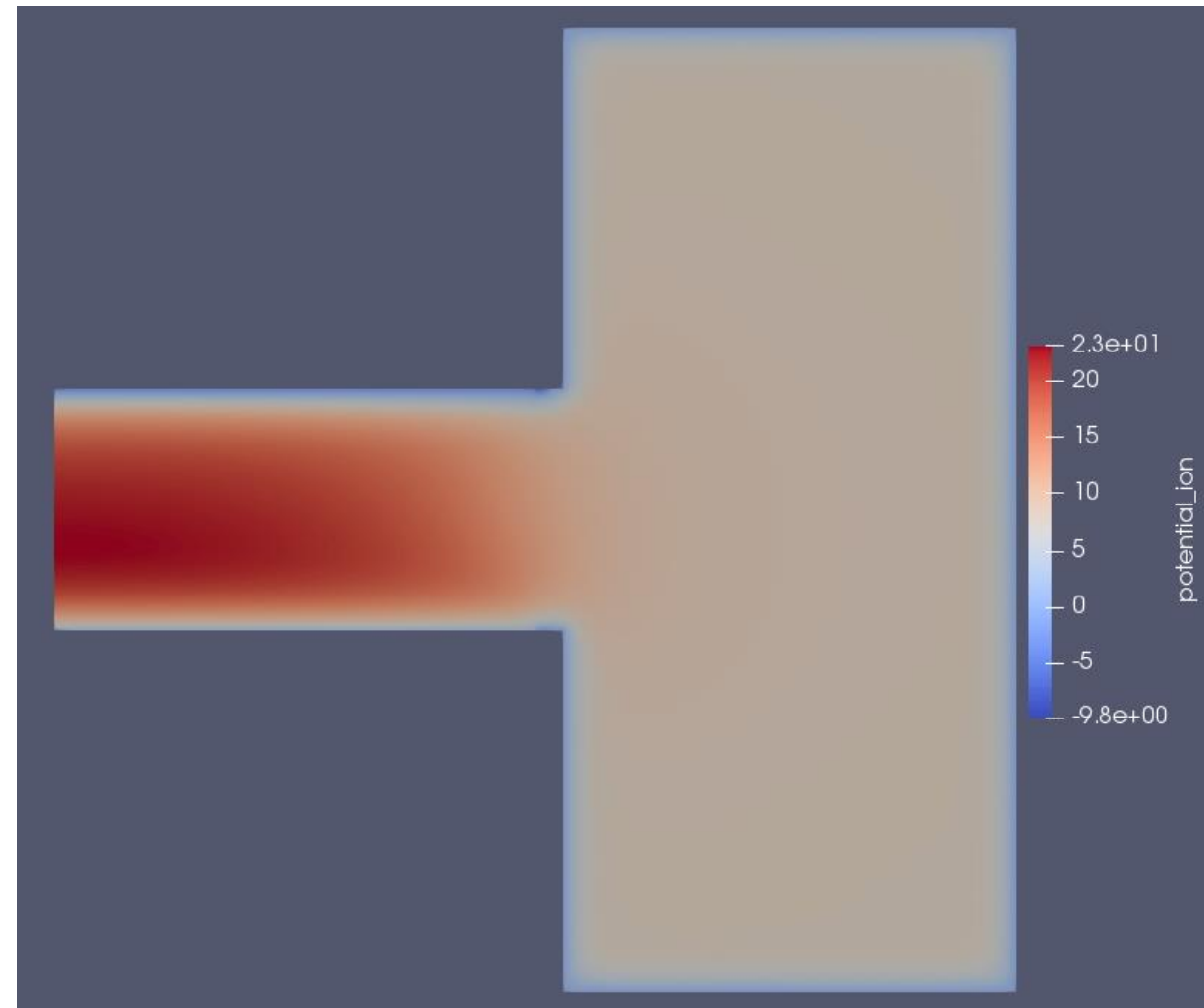


# **Results for Default BC / No Actions / Standard Mesh**

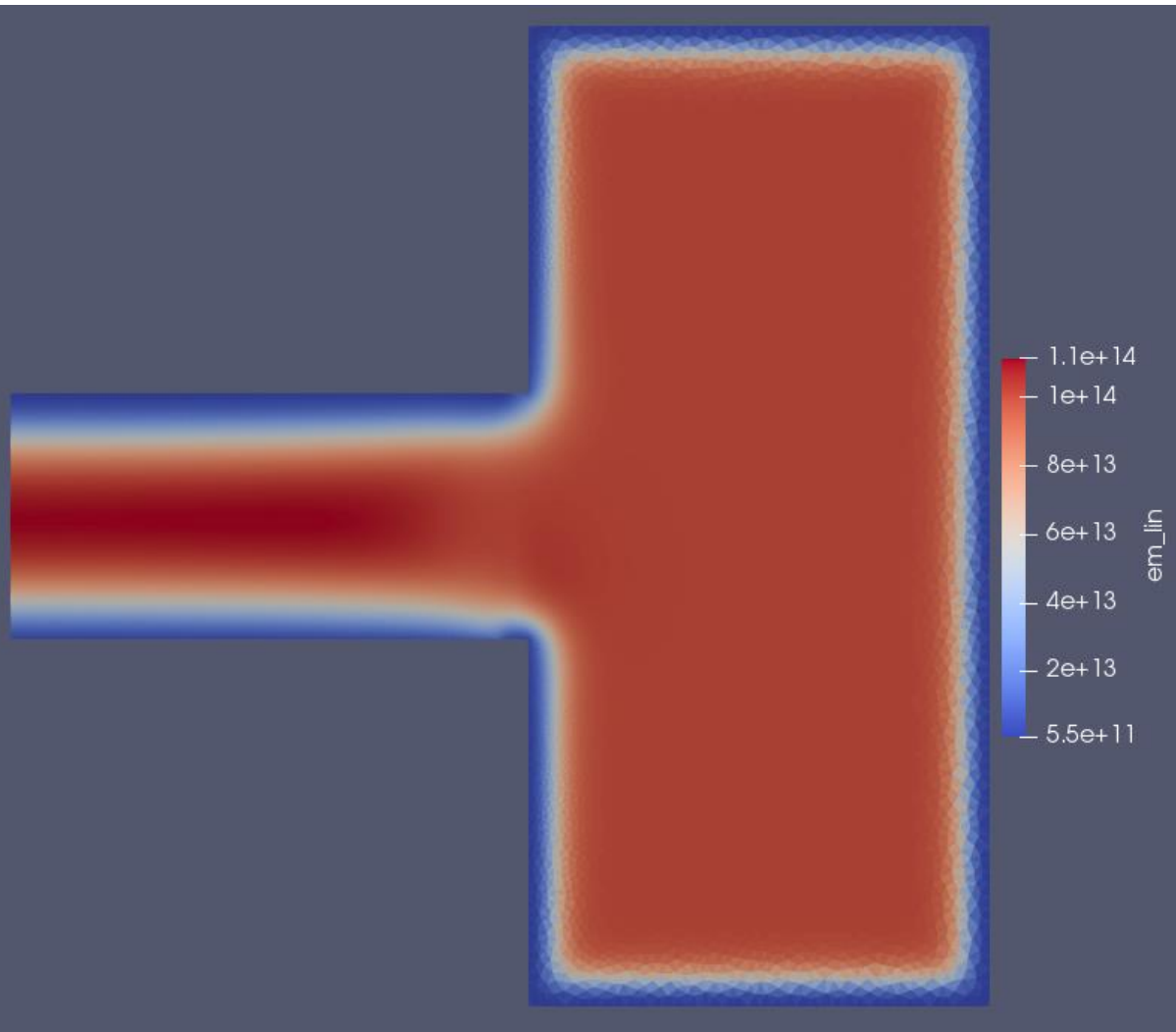
Potential [V]



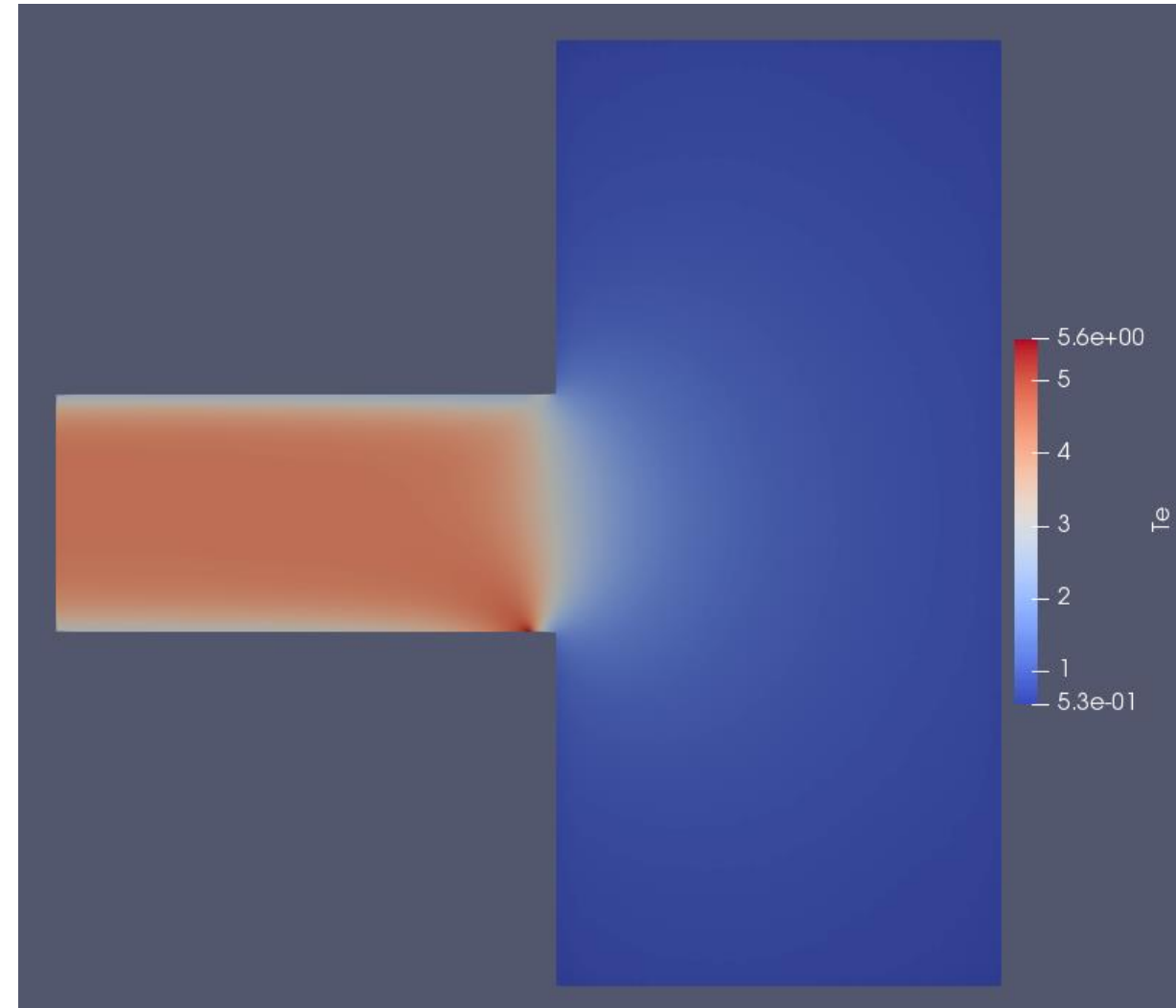
Ion Potential [V]



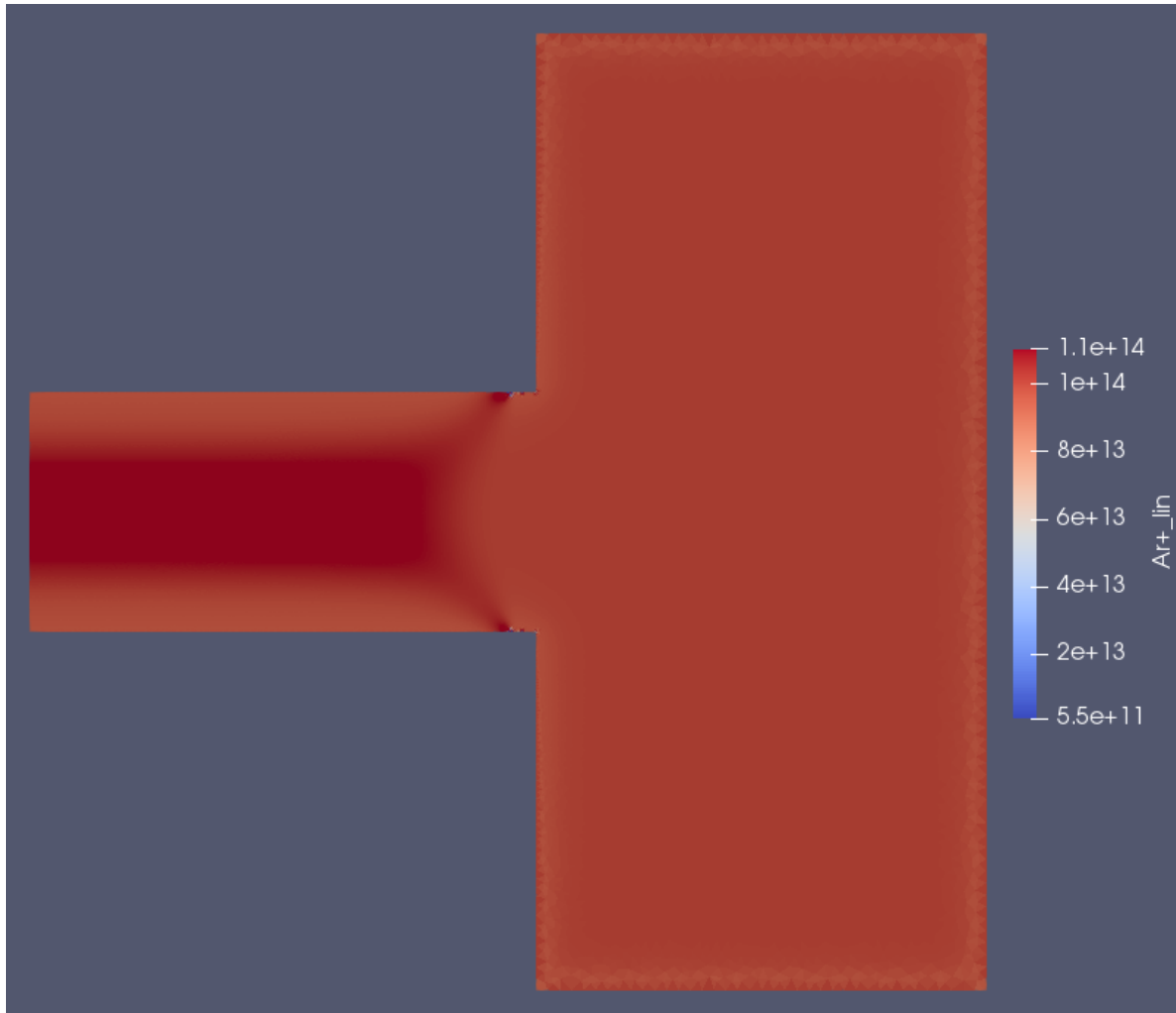
Electron Density [ $m^3$ ]



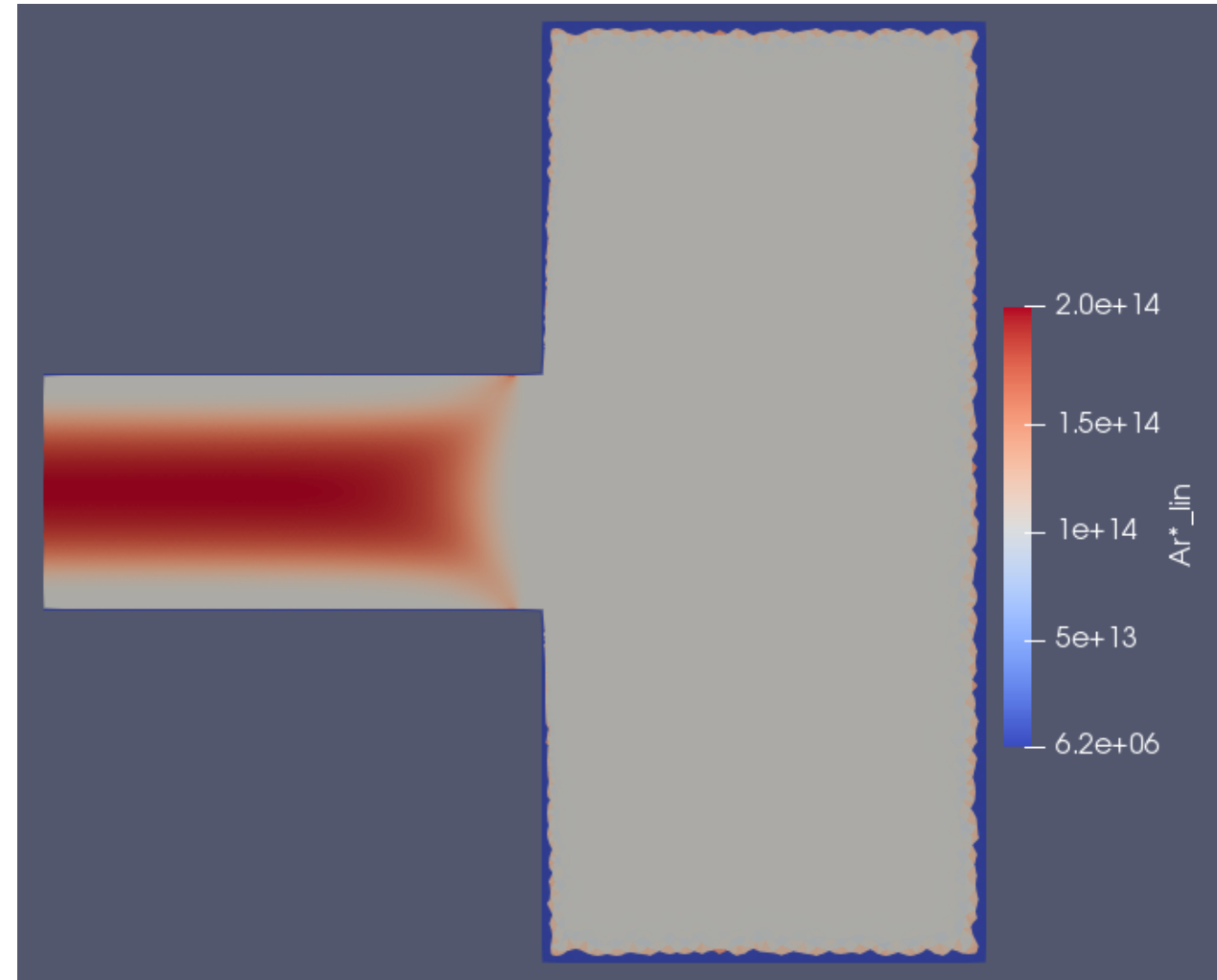
Electron Temperature [V]



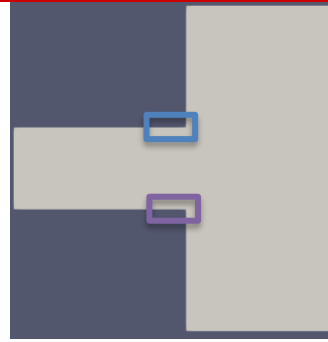
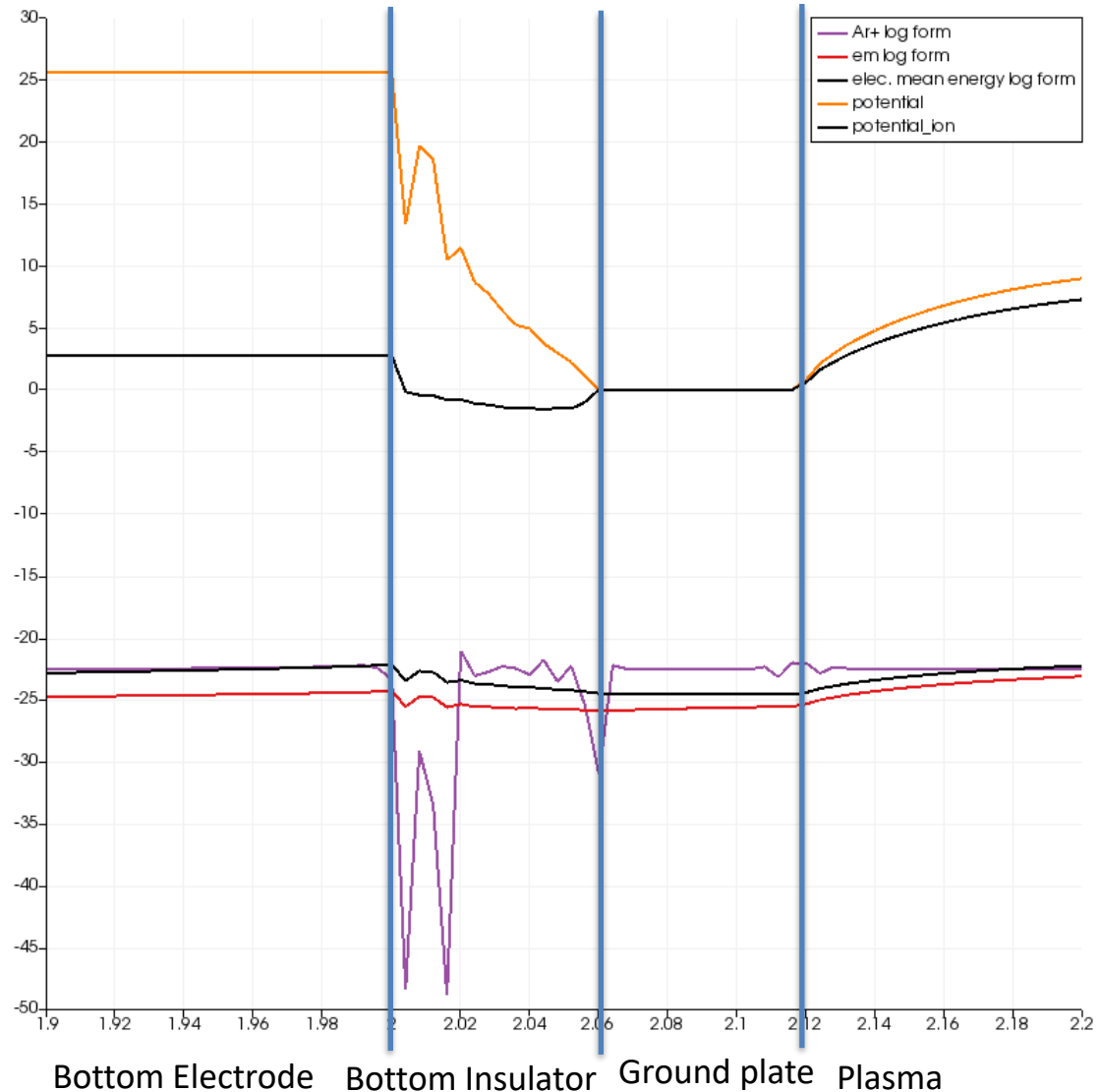
**Ion Density [ $m^3$ ]**



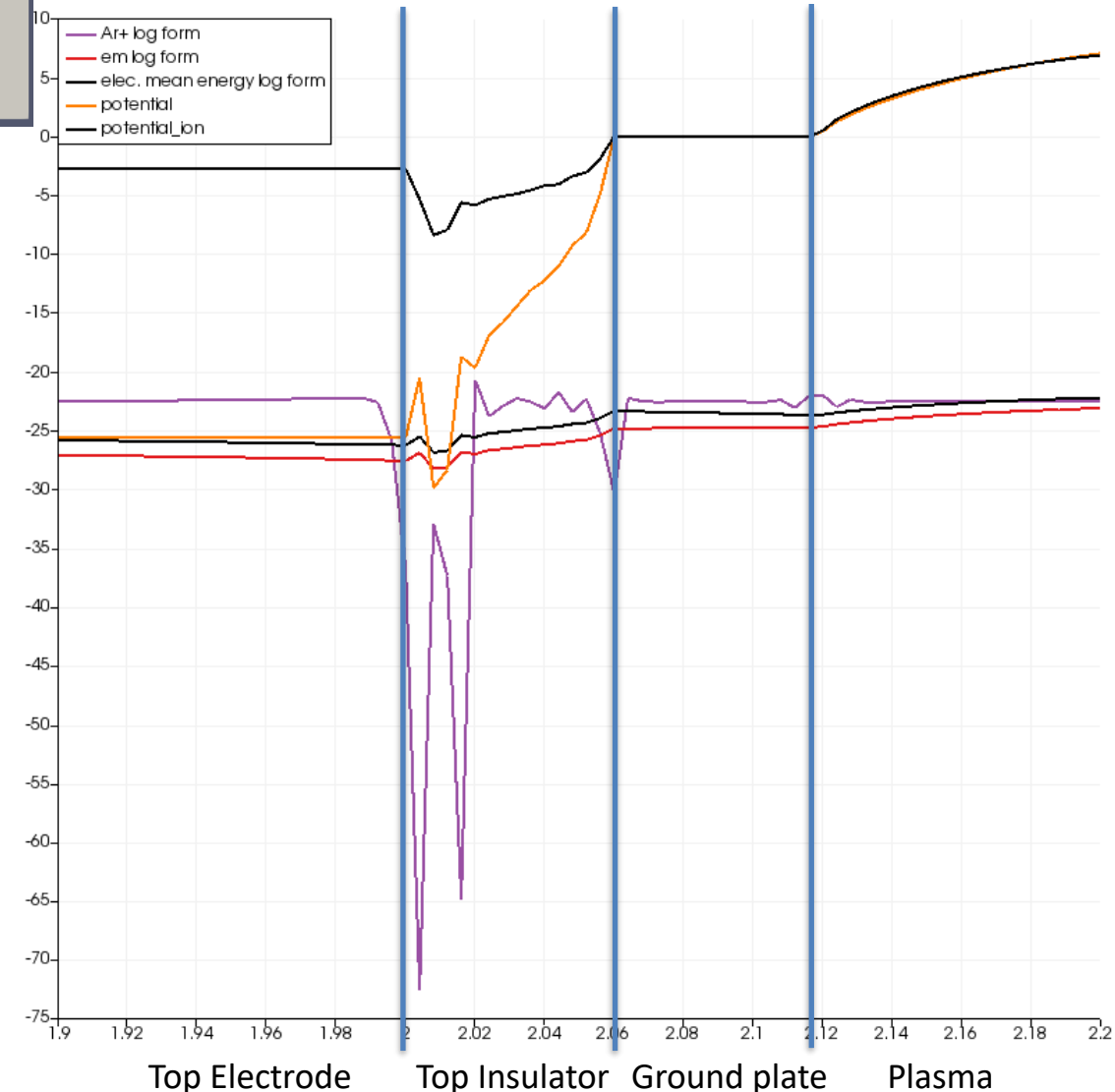
**Metastable Density [ $m^3$ ]**



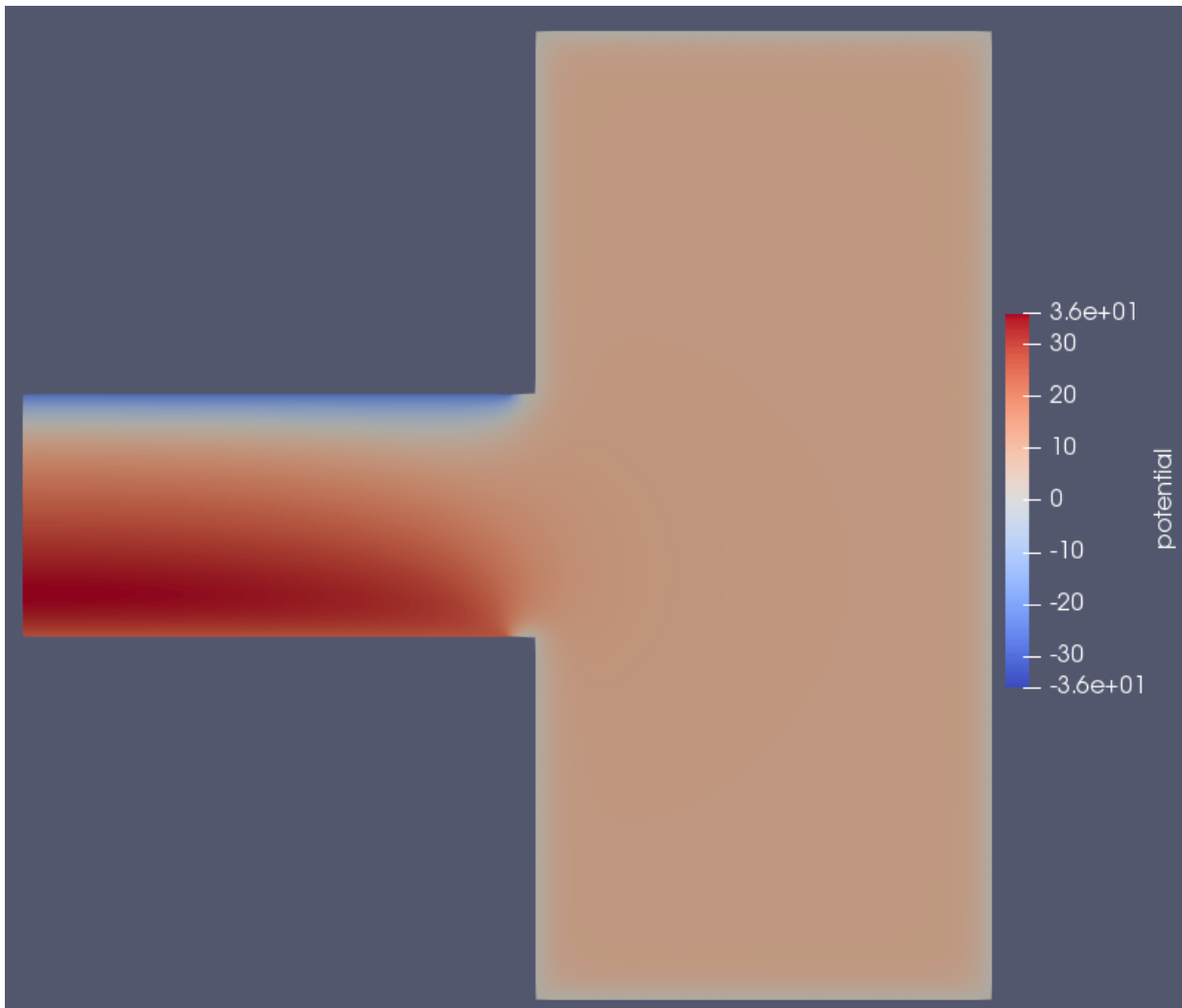
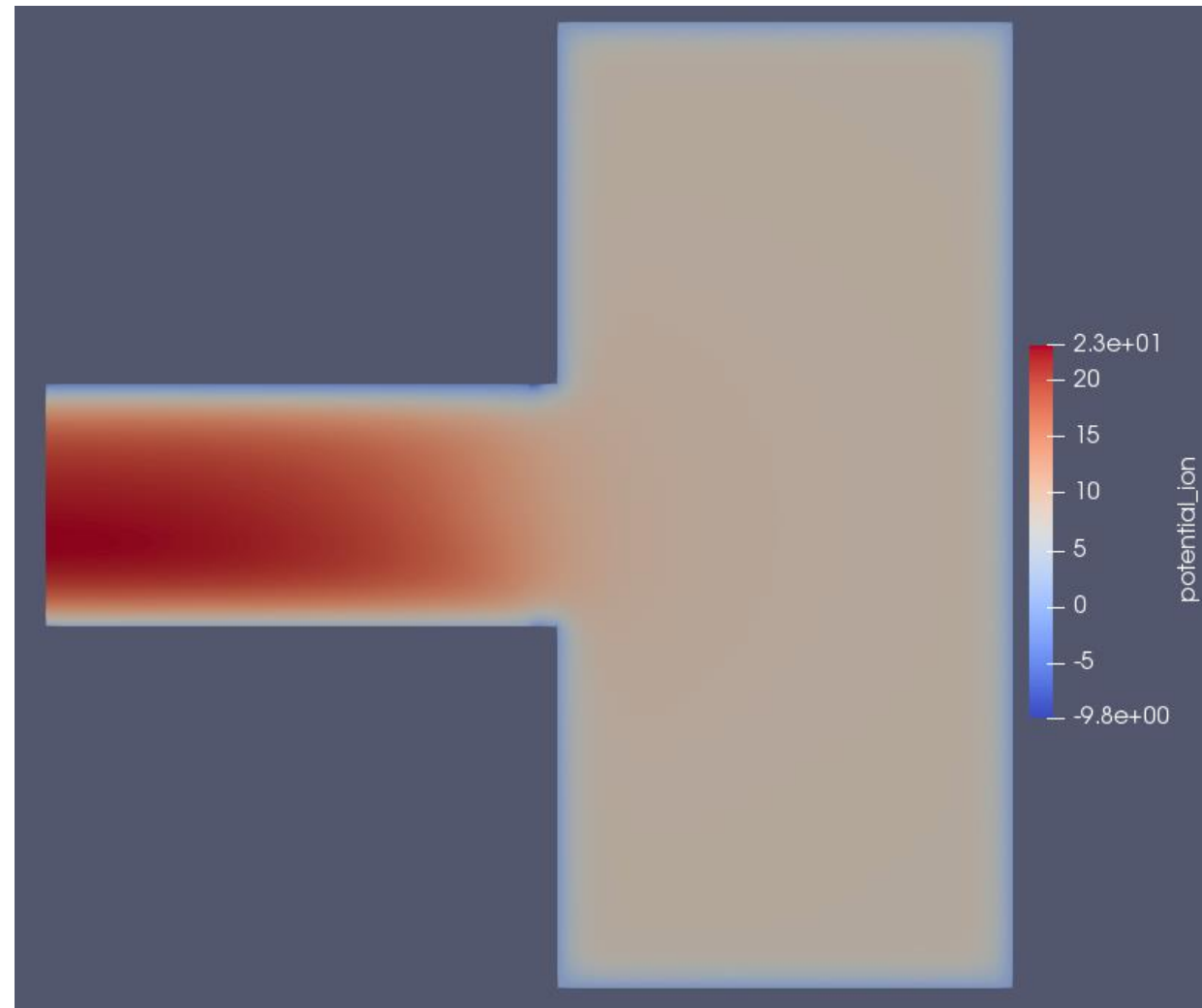
## Bottom Boundary

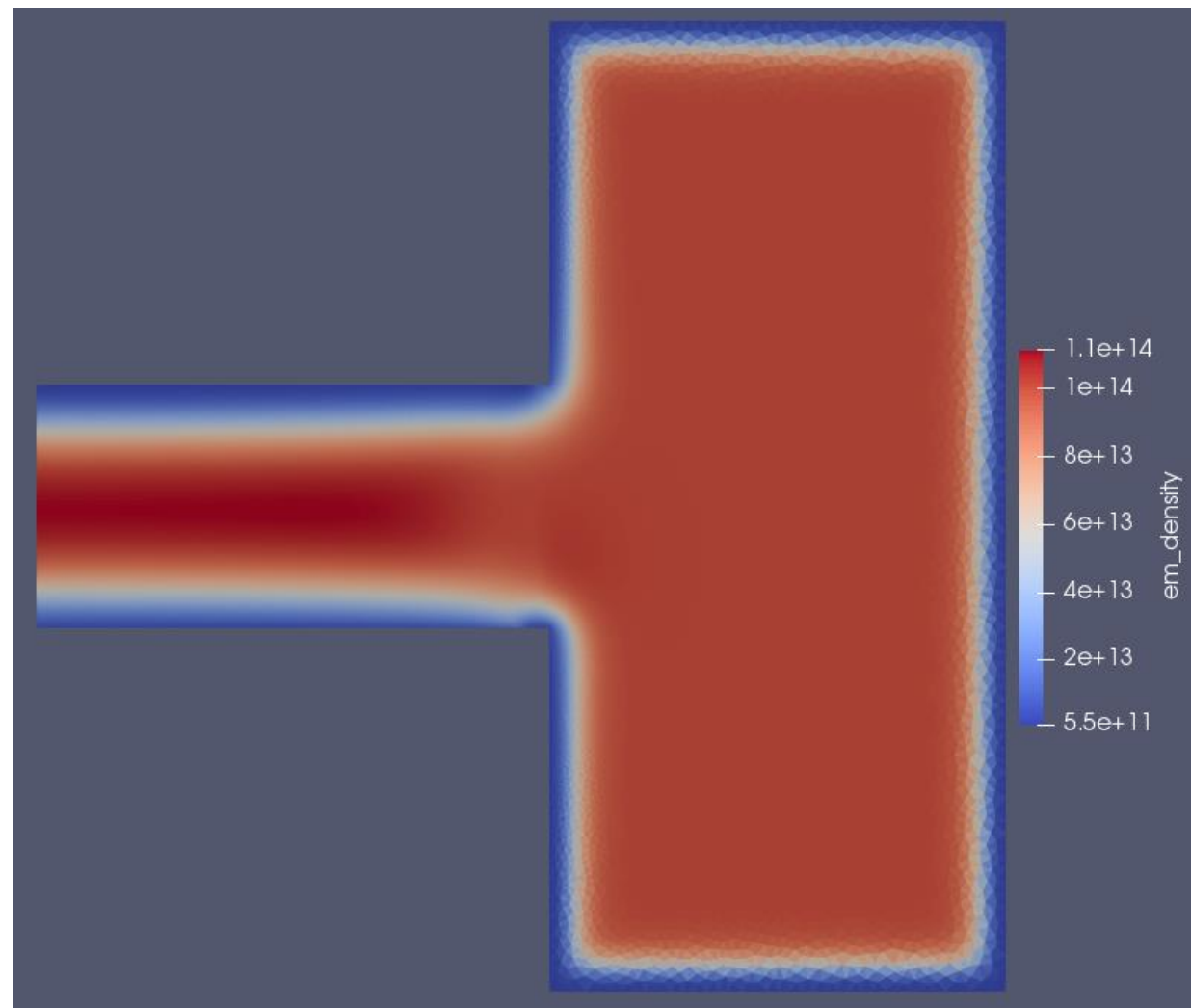


## Top Boundary

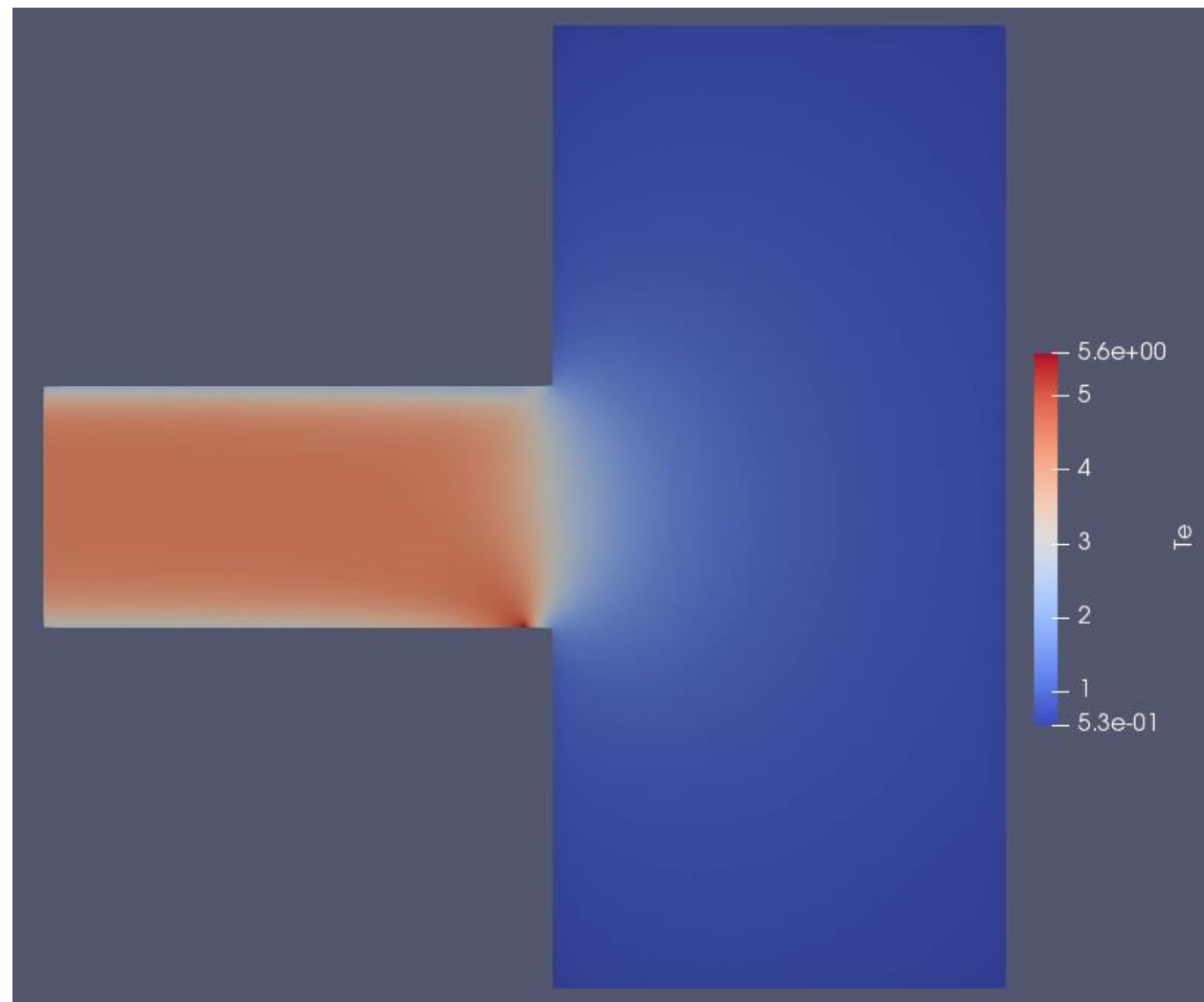


# Results for Rearranged BC / Actions / Standard Mesh

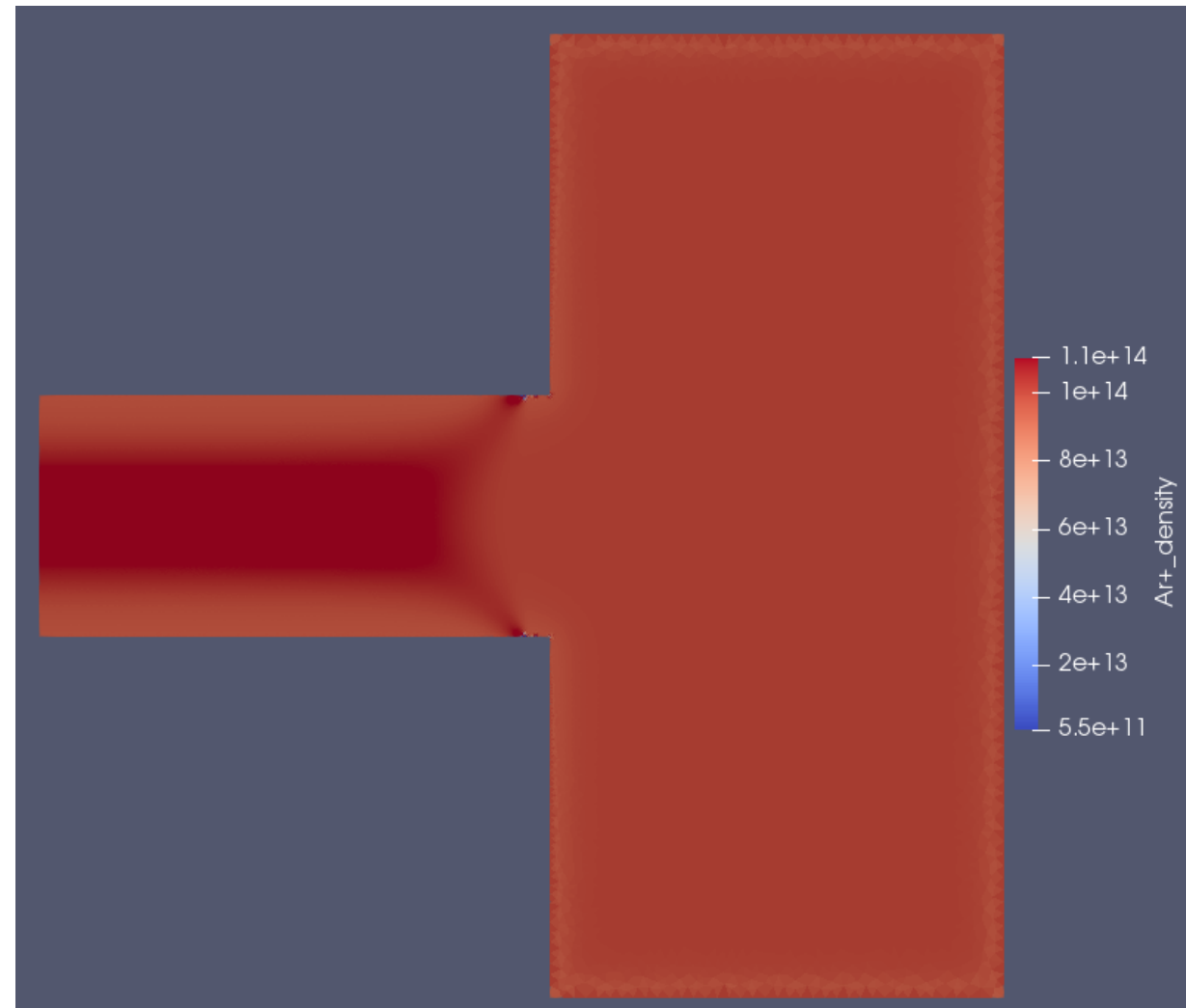
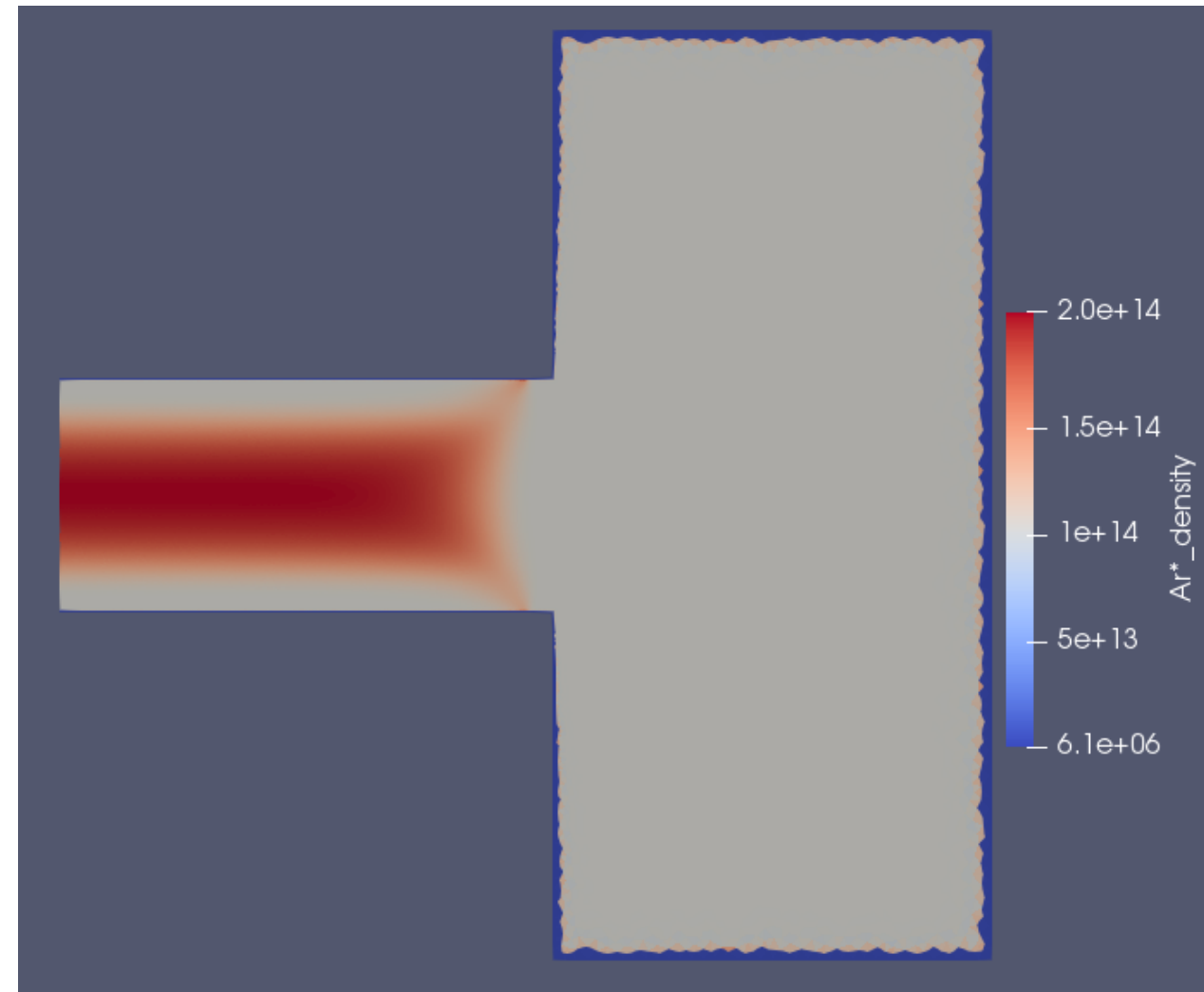
**Potential [V]****Ion Potential [V]**

Electron Density [ $\text{m}^3$ ]

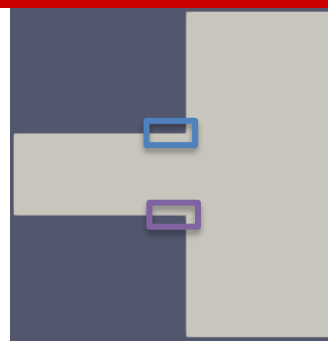
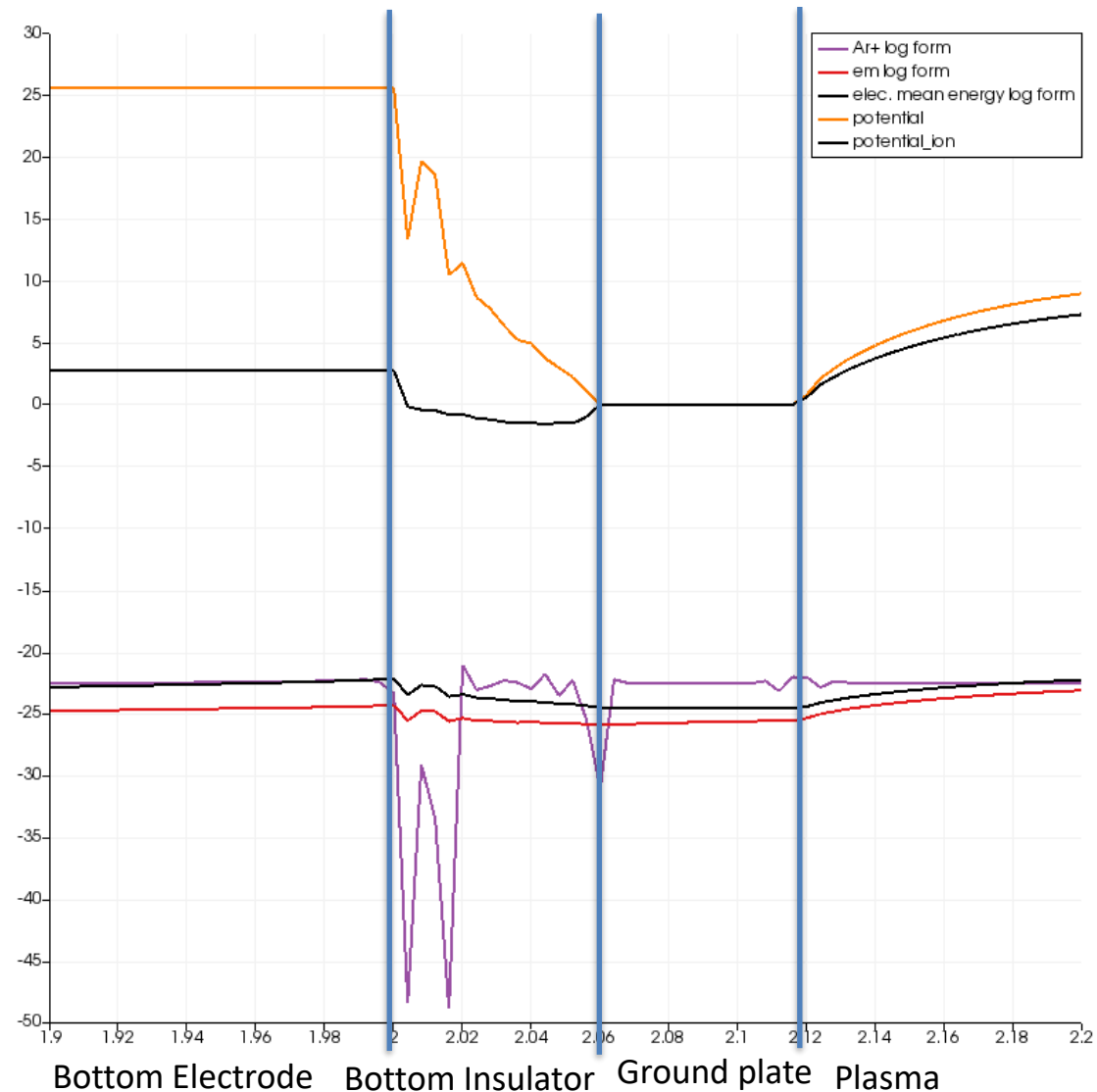
Electron Temperature [V]



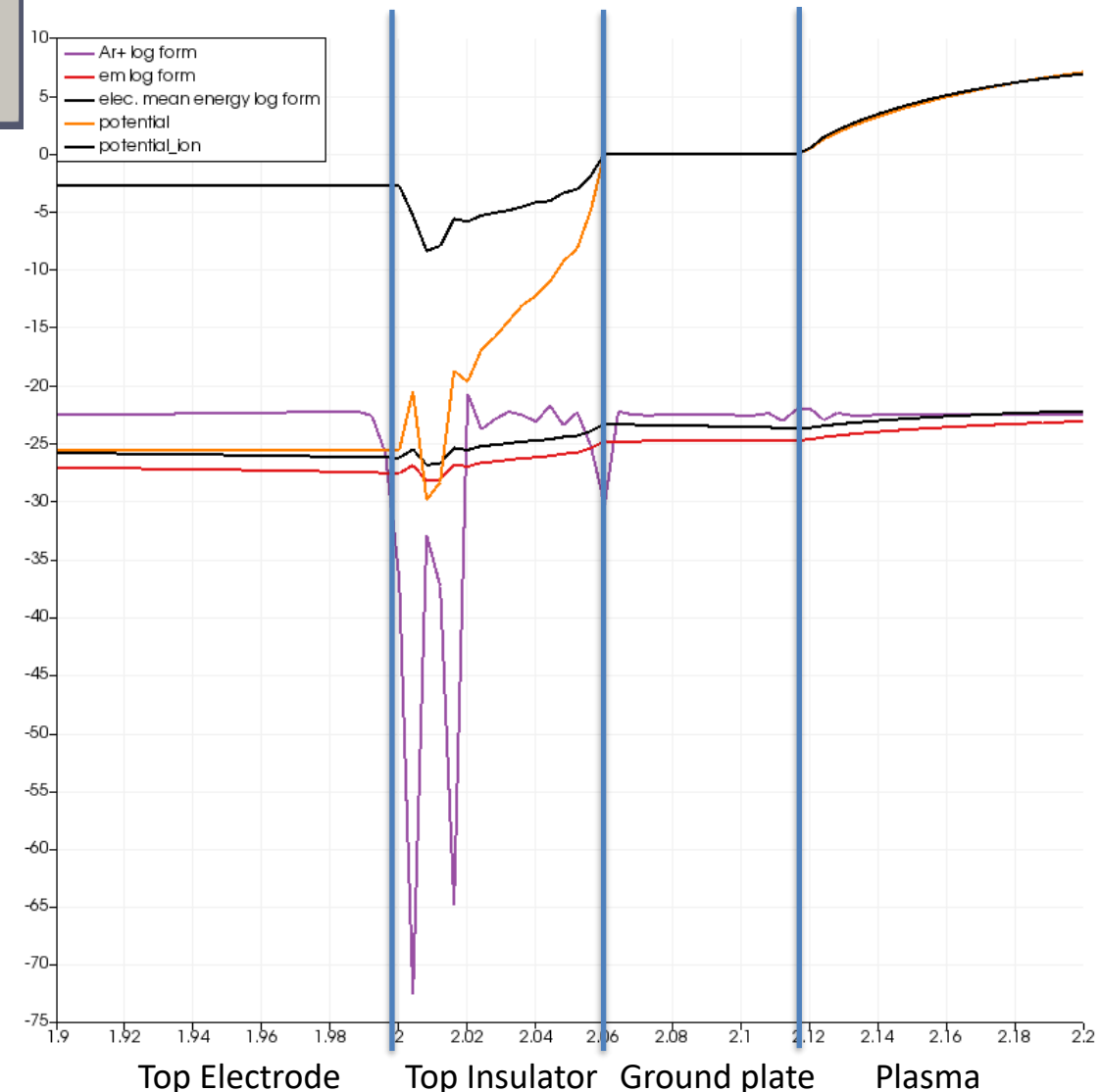


Ion Density [ $\text{m}^3$ ]Metastable Density [ $\text{m}^3$ ]

## Bottom Boundary

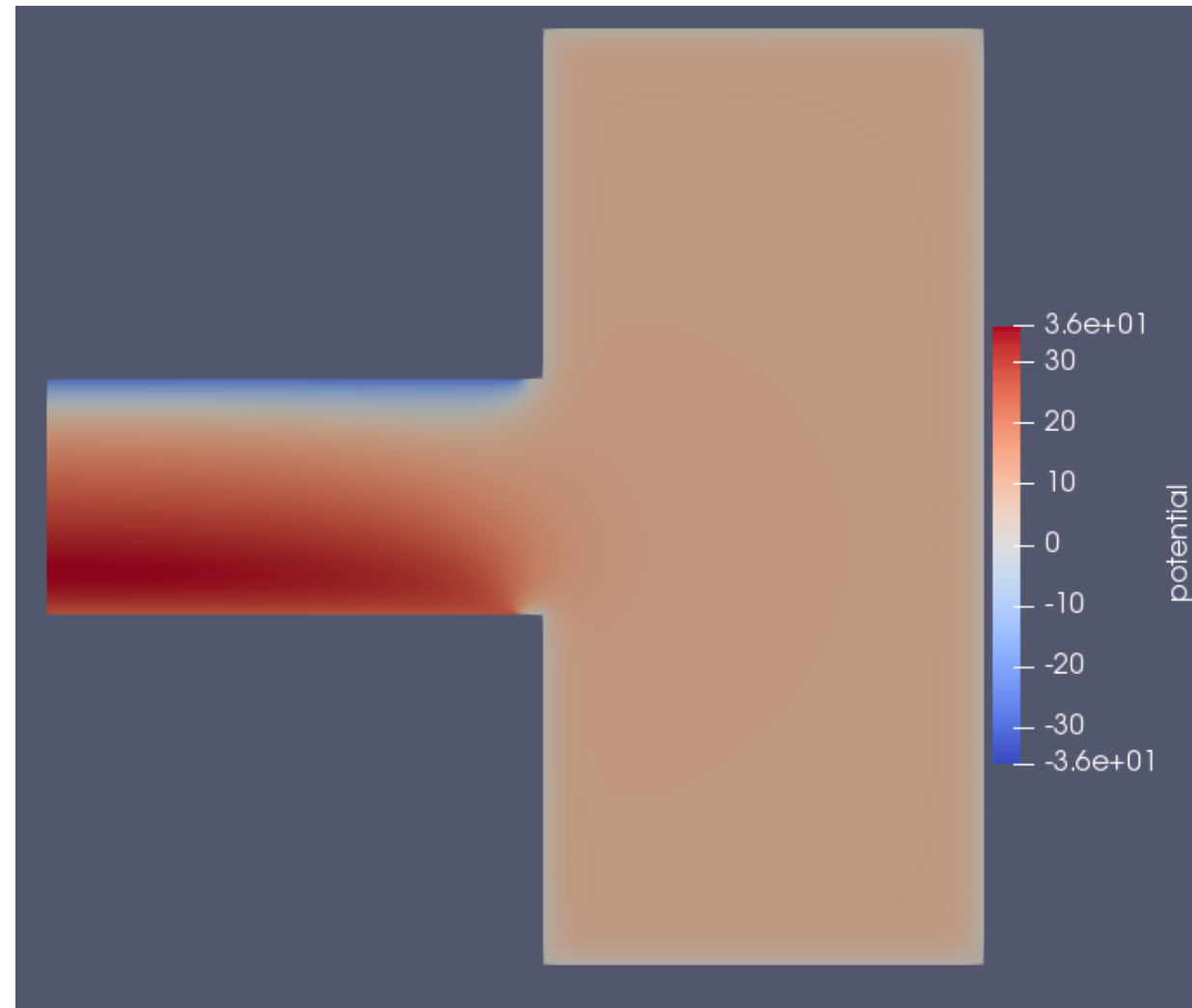


## Top Boundary

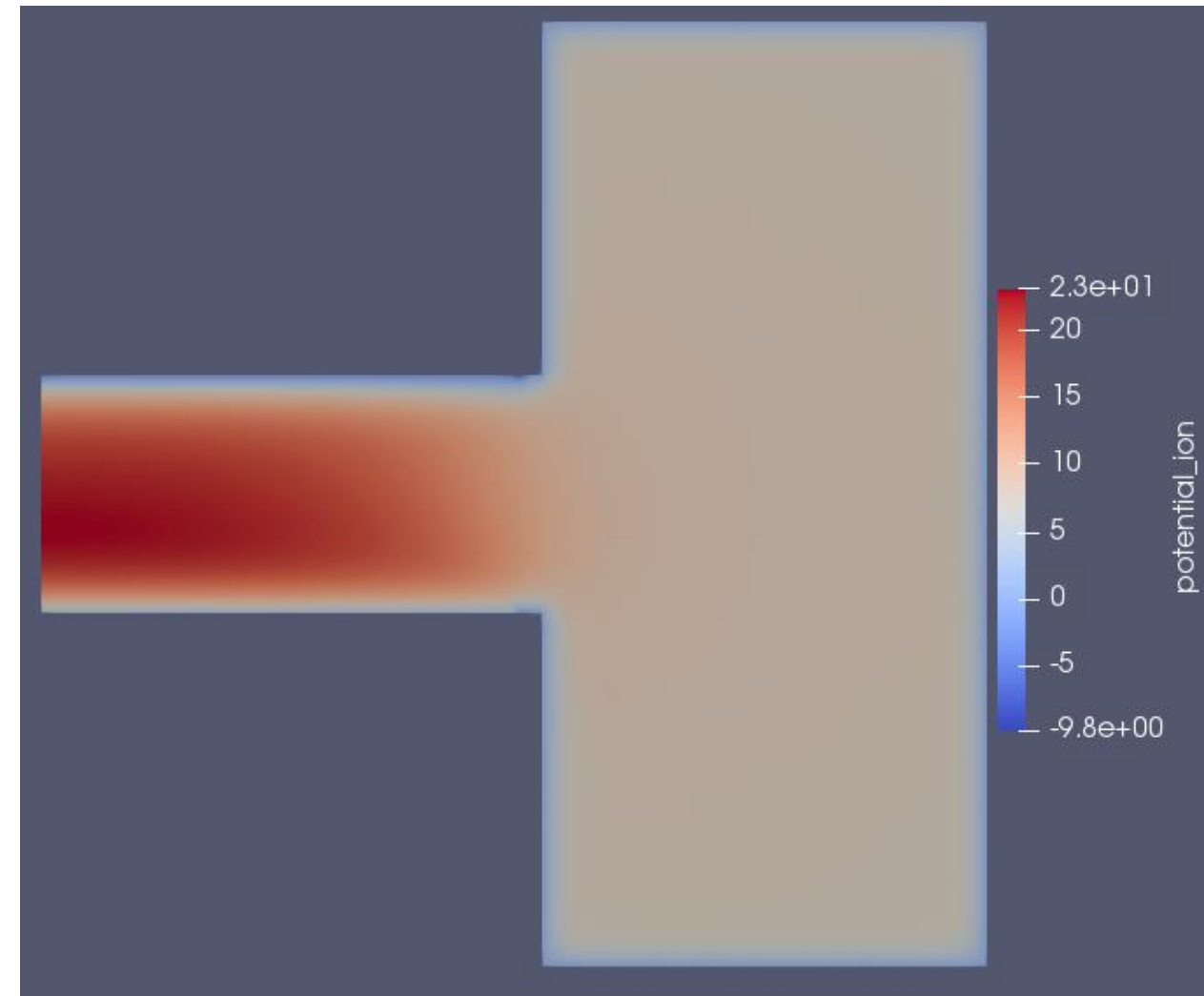


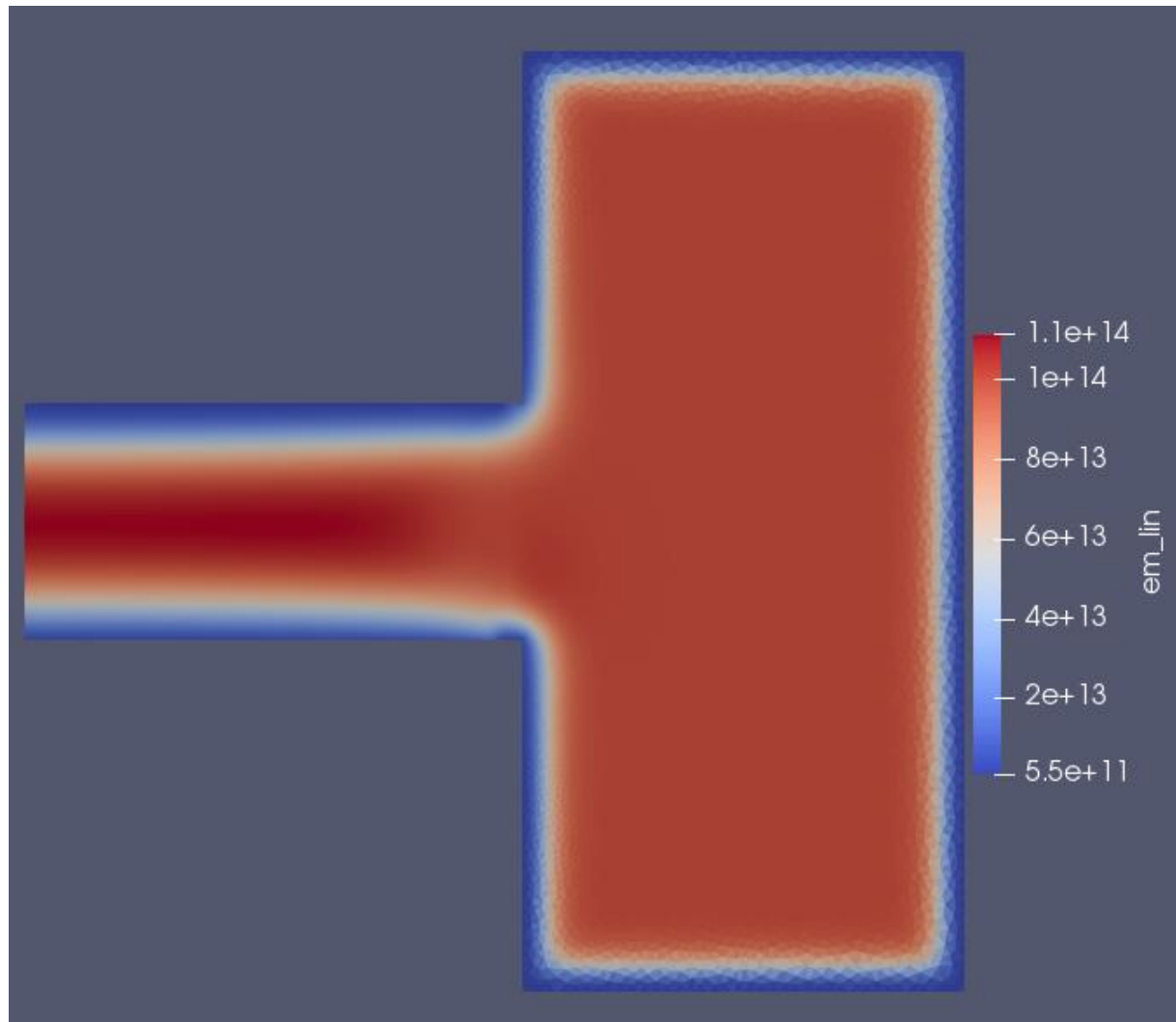
# Results for Rearranged BC / No Actions / Standard Mesh

Potential [V]

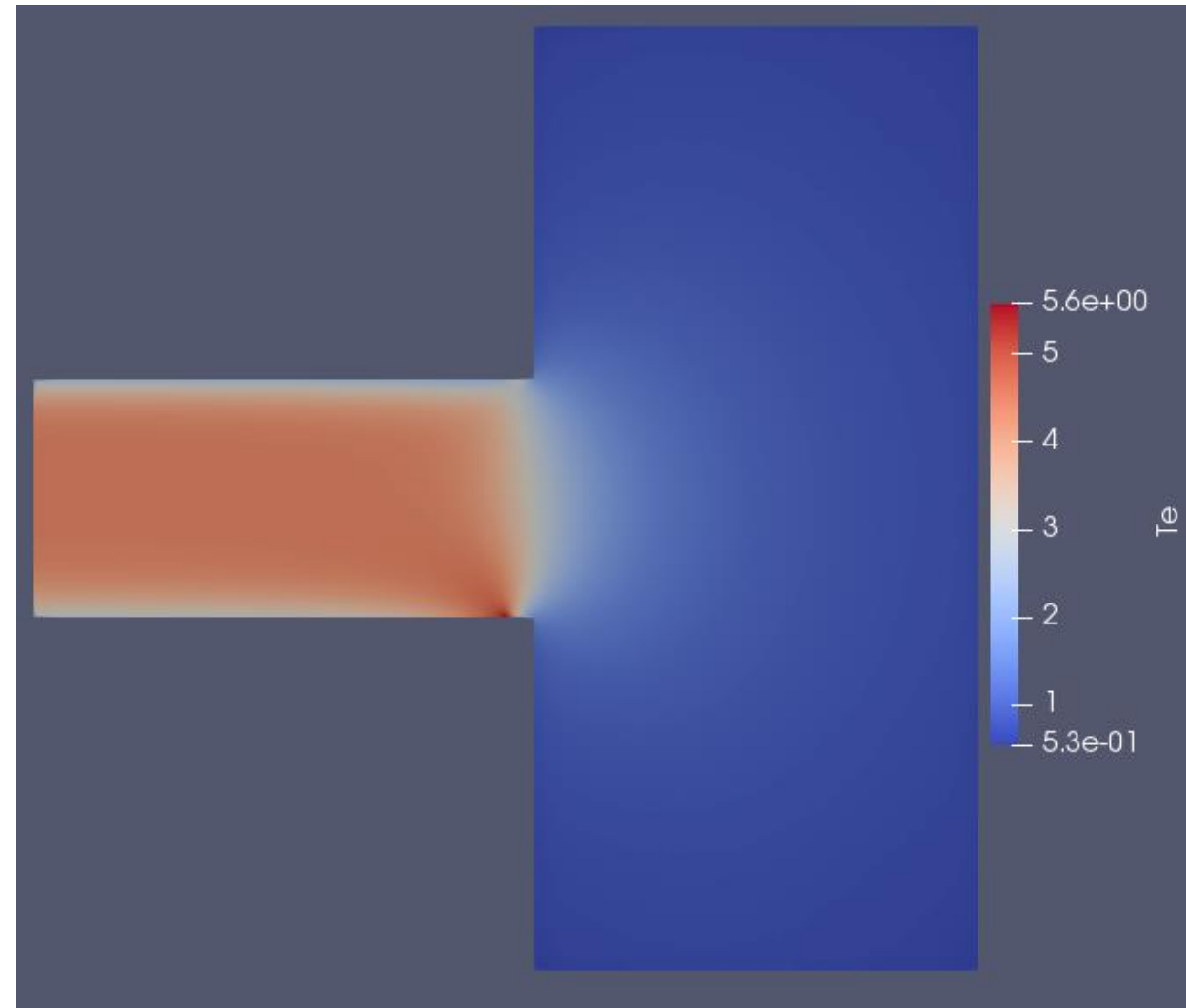


Ion Potential [V]

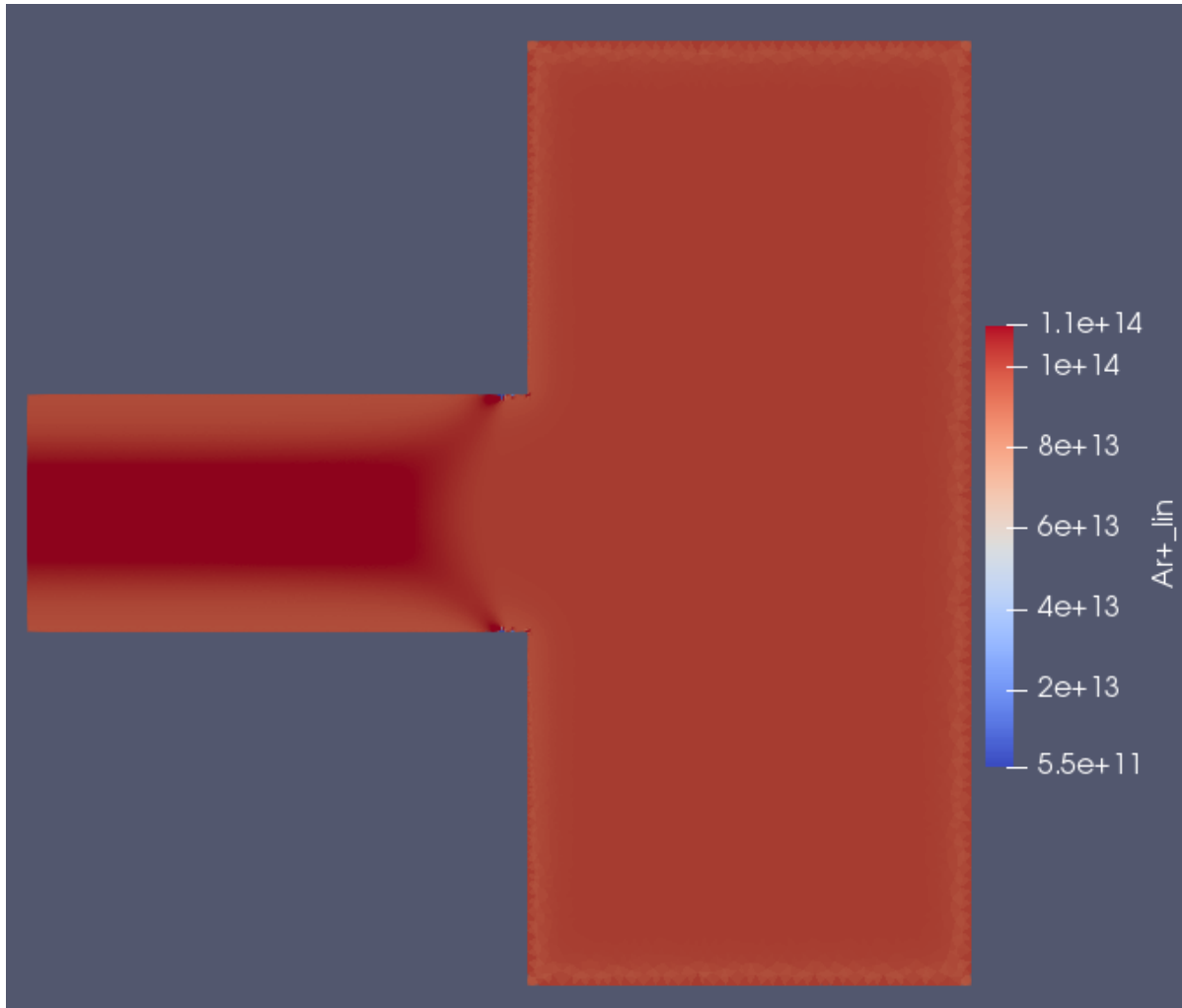


Electron Density [ $\text{m}^3$ ]

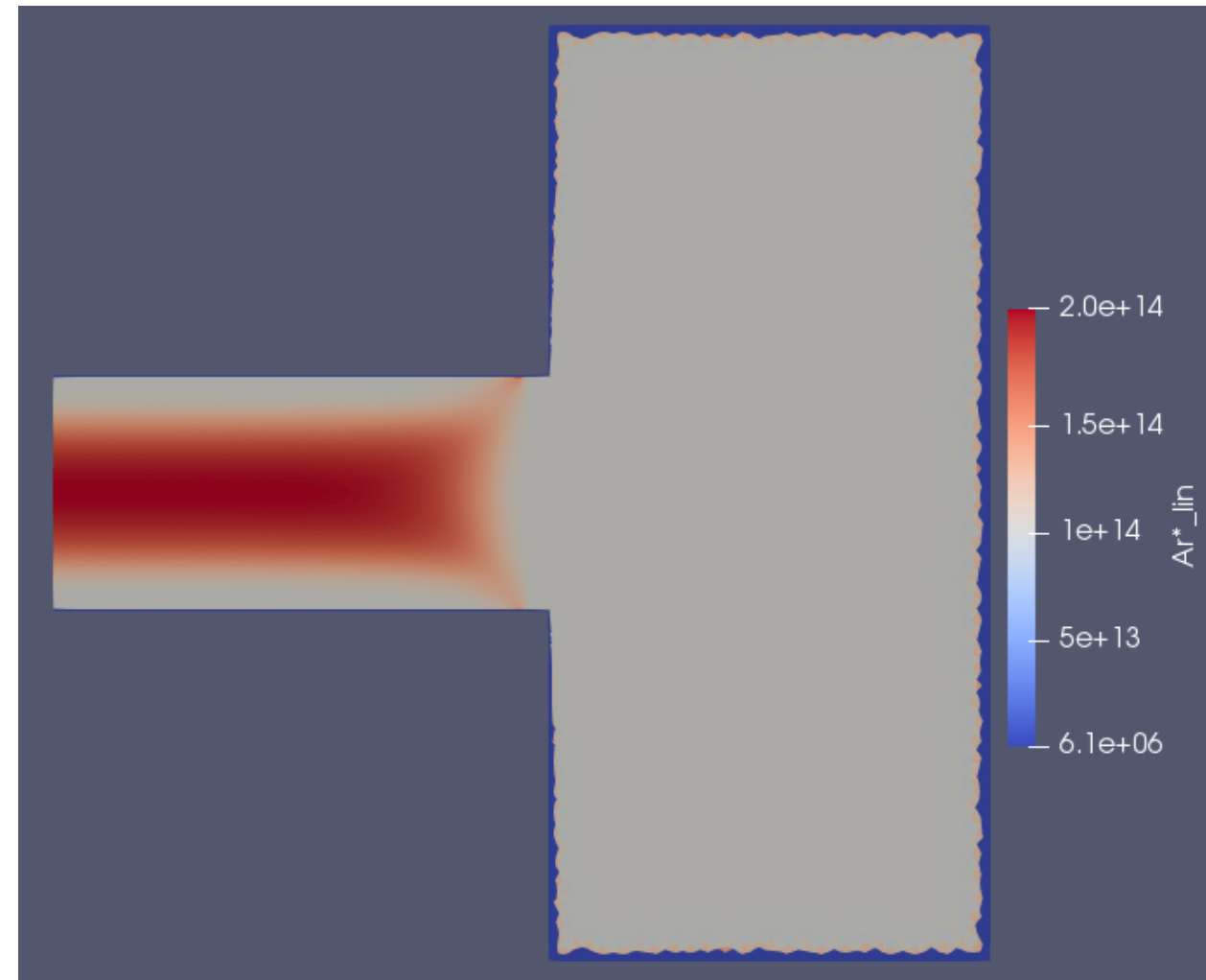
Electron Temperature [V]



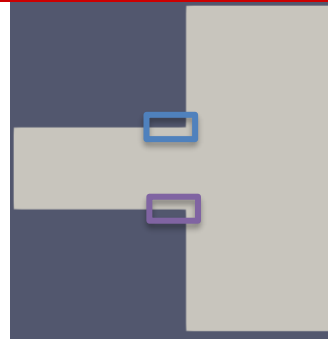
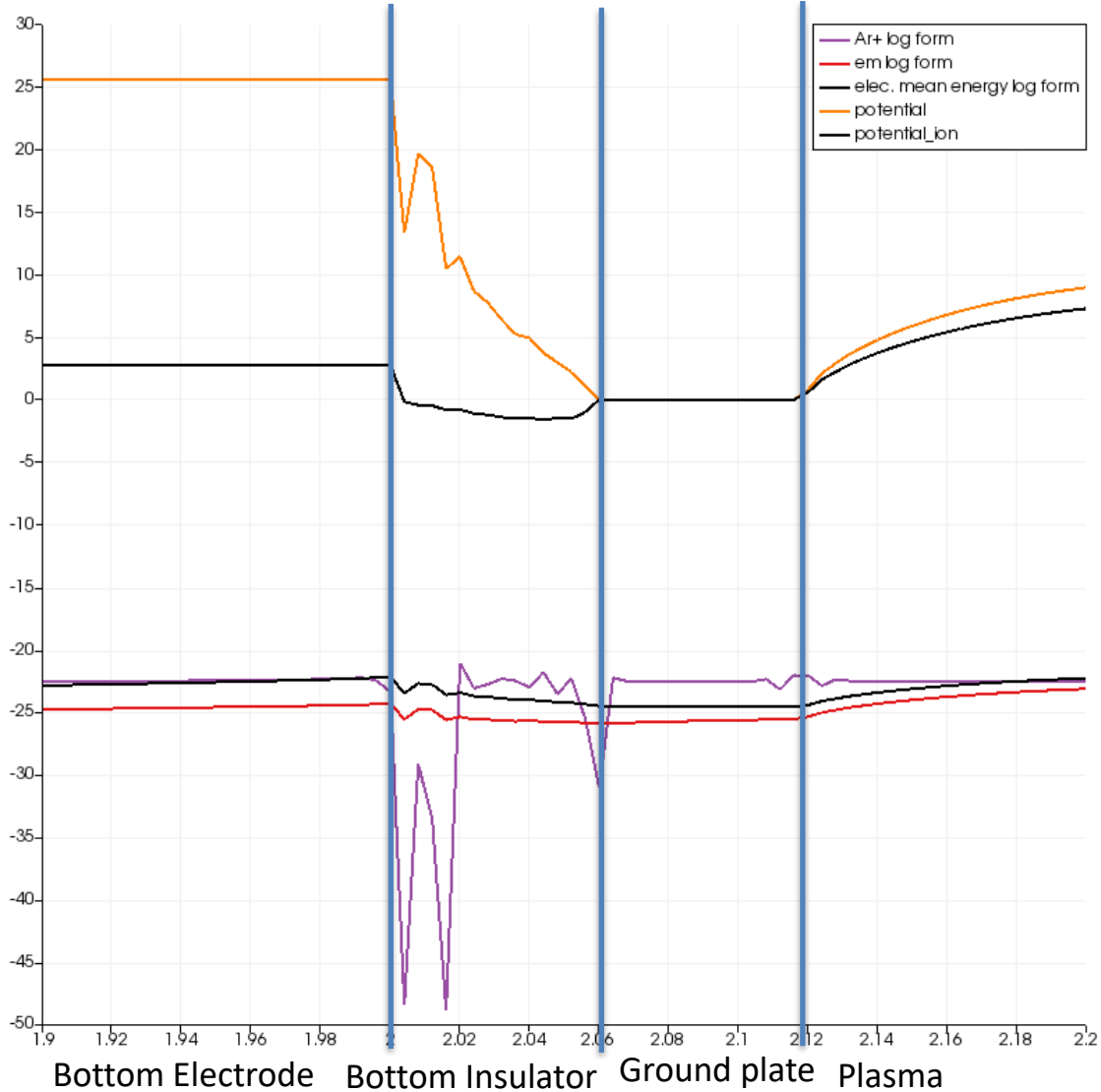
Ion Density [ $m^3$ ]



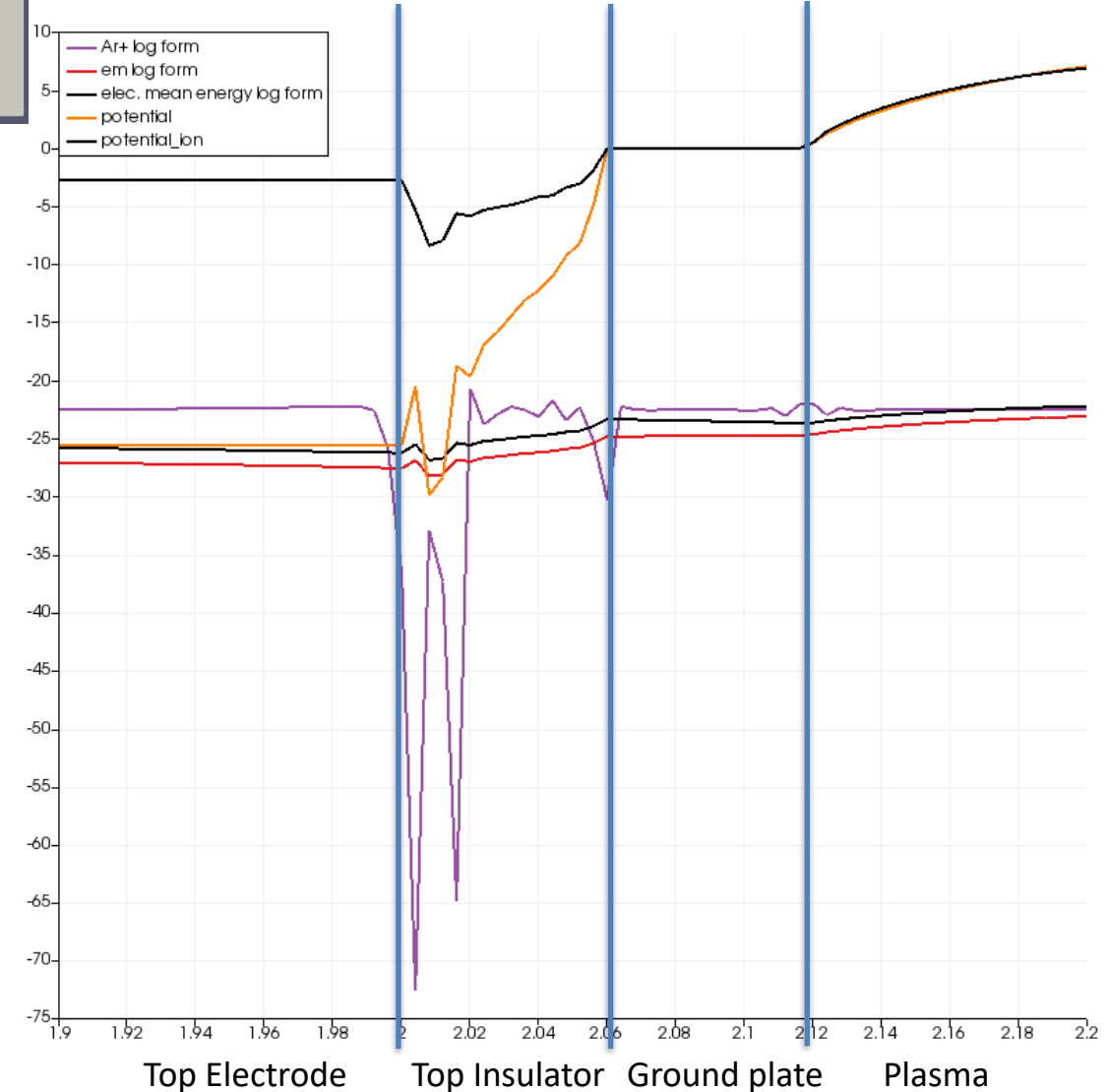
Metastable Density [ $m^3$ ]



## Bottom Boundary



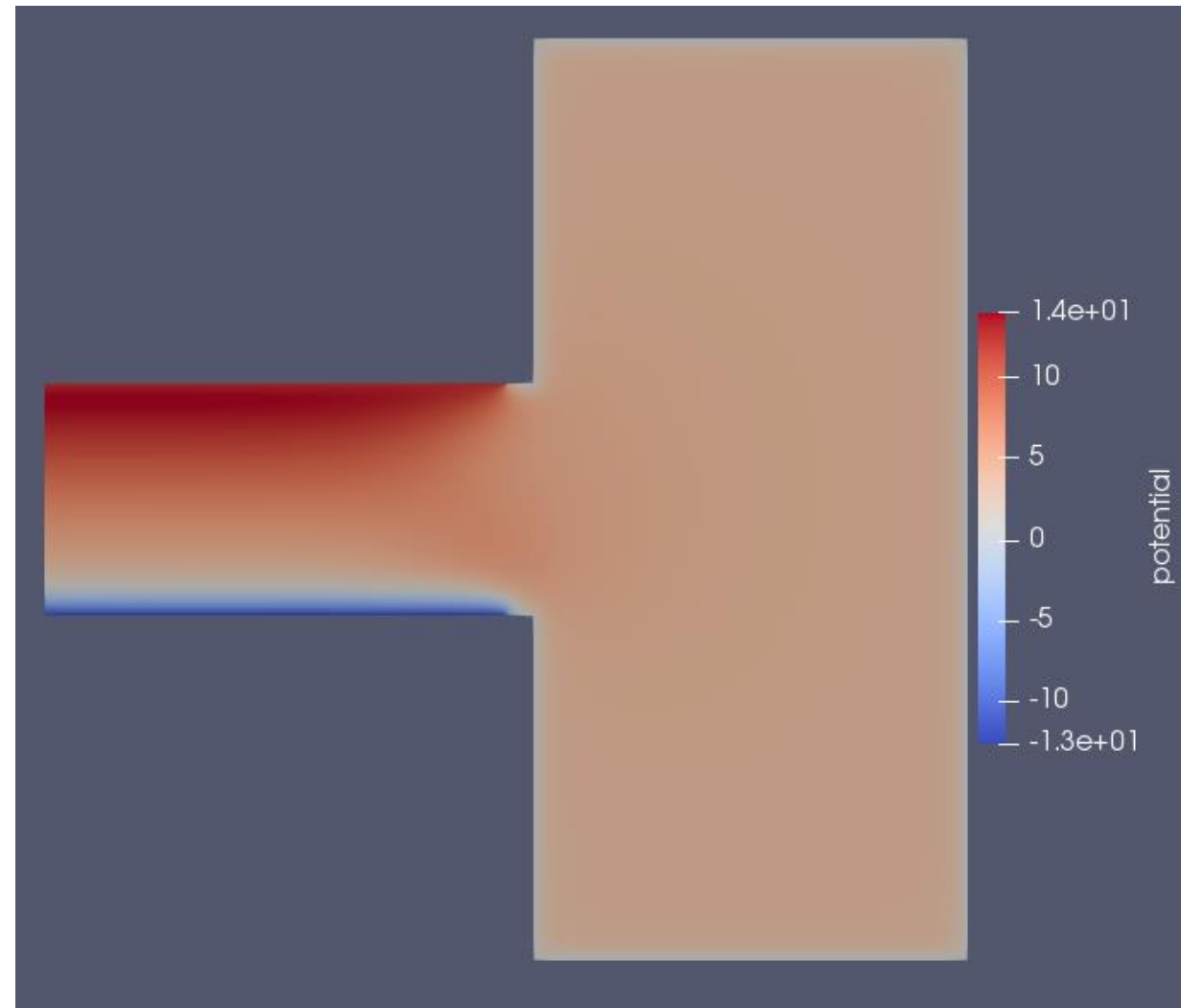
## Top Boundary



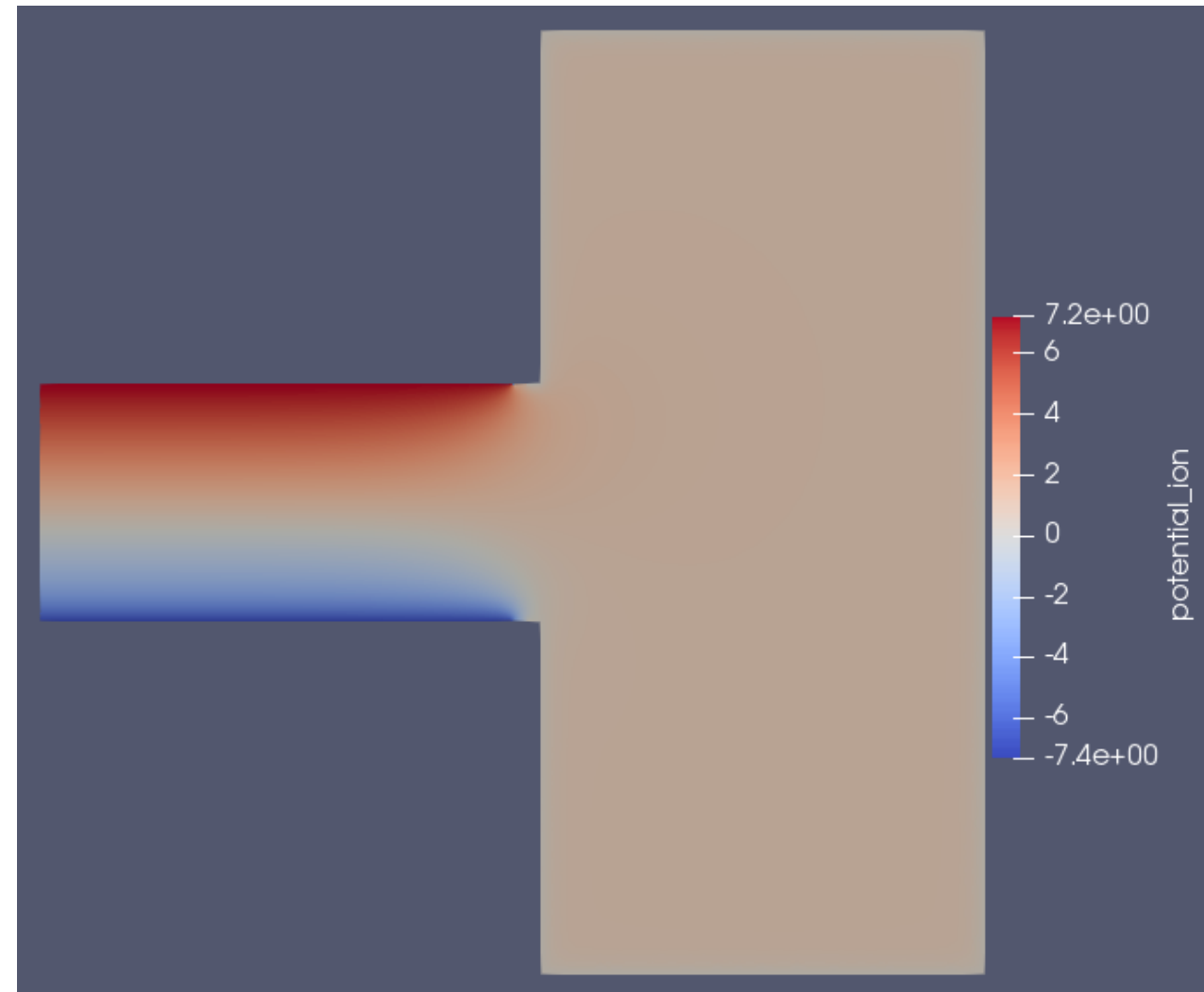
# **Results for Default BC / Actions / No Dimensional Scaling Mesh**



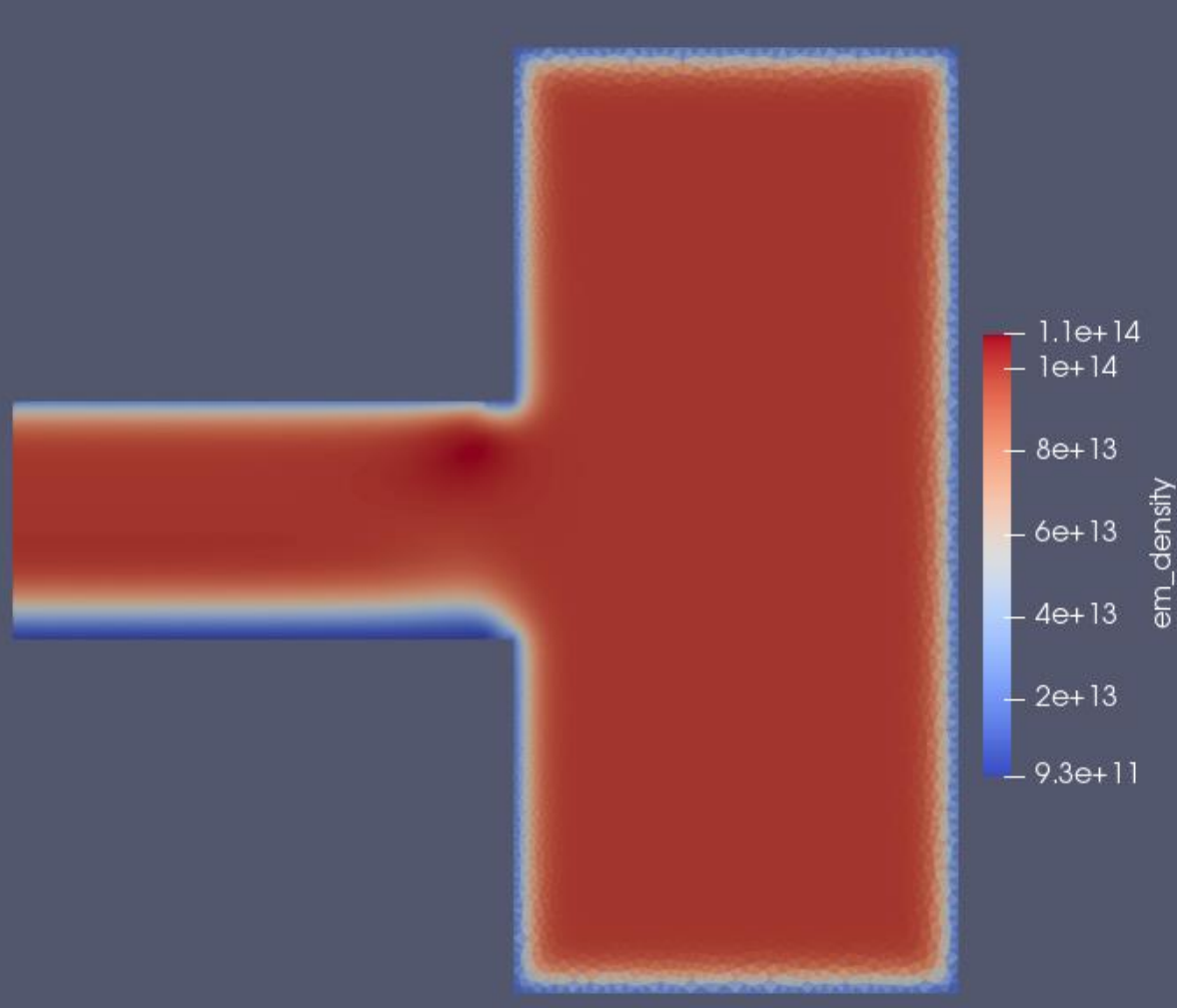
Potential [V]



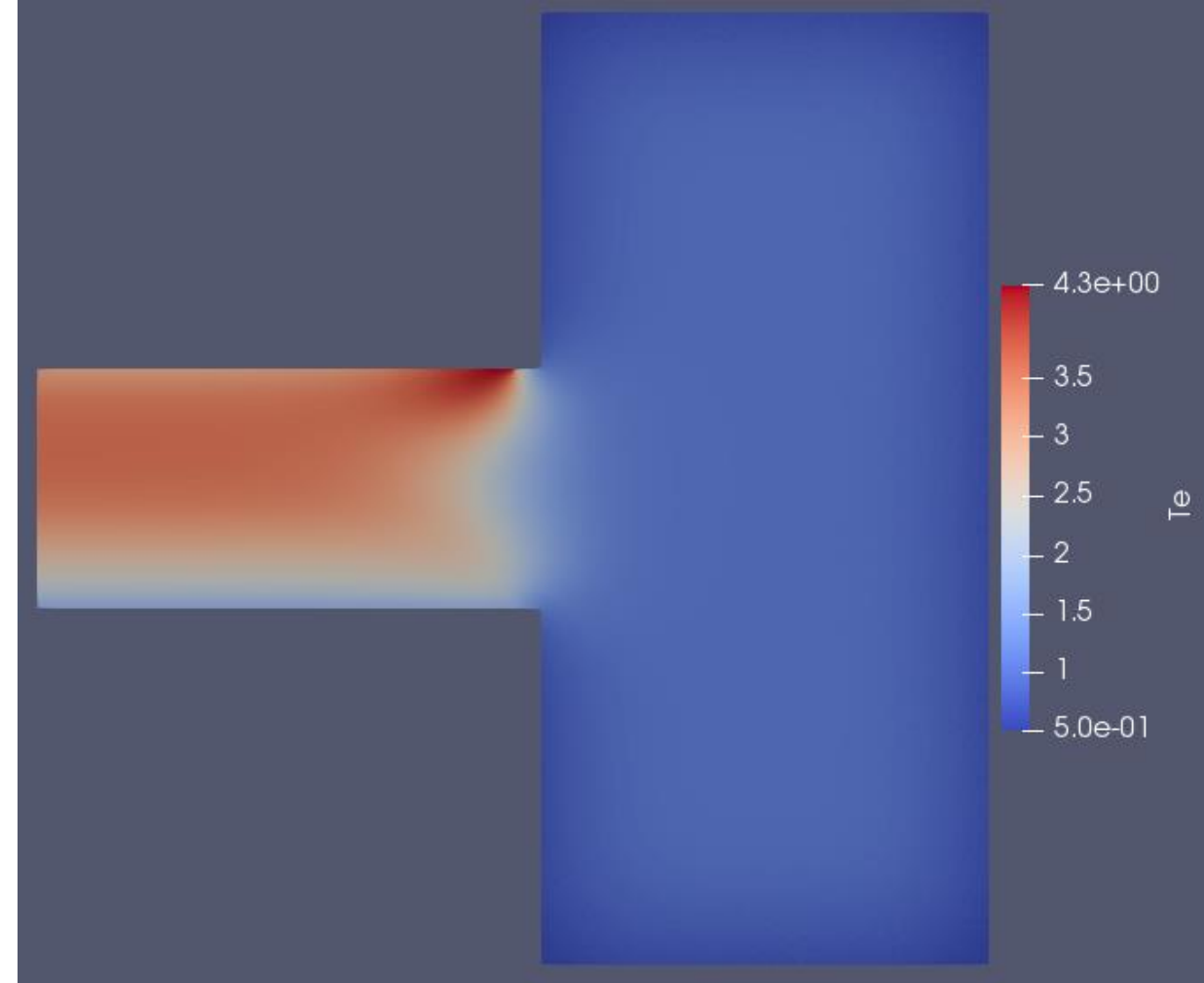
Ion Potential [V]



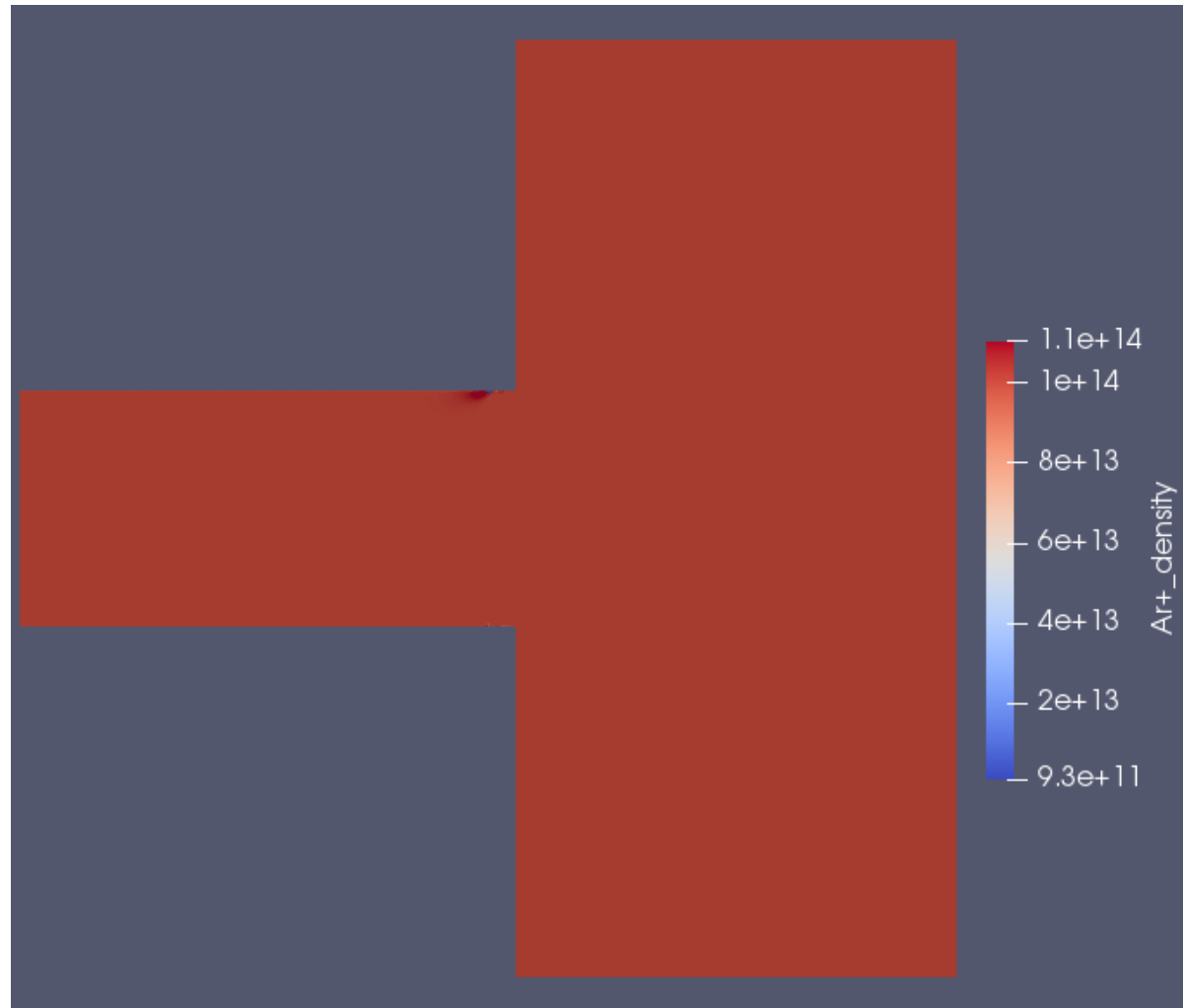
Electron Density [ $\text{m}^3$ ]



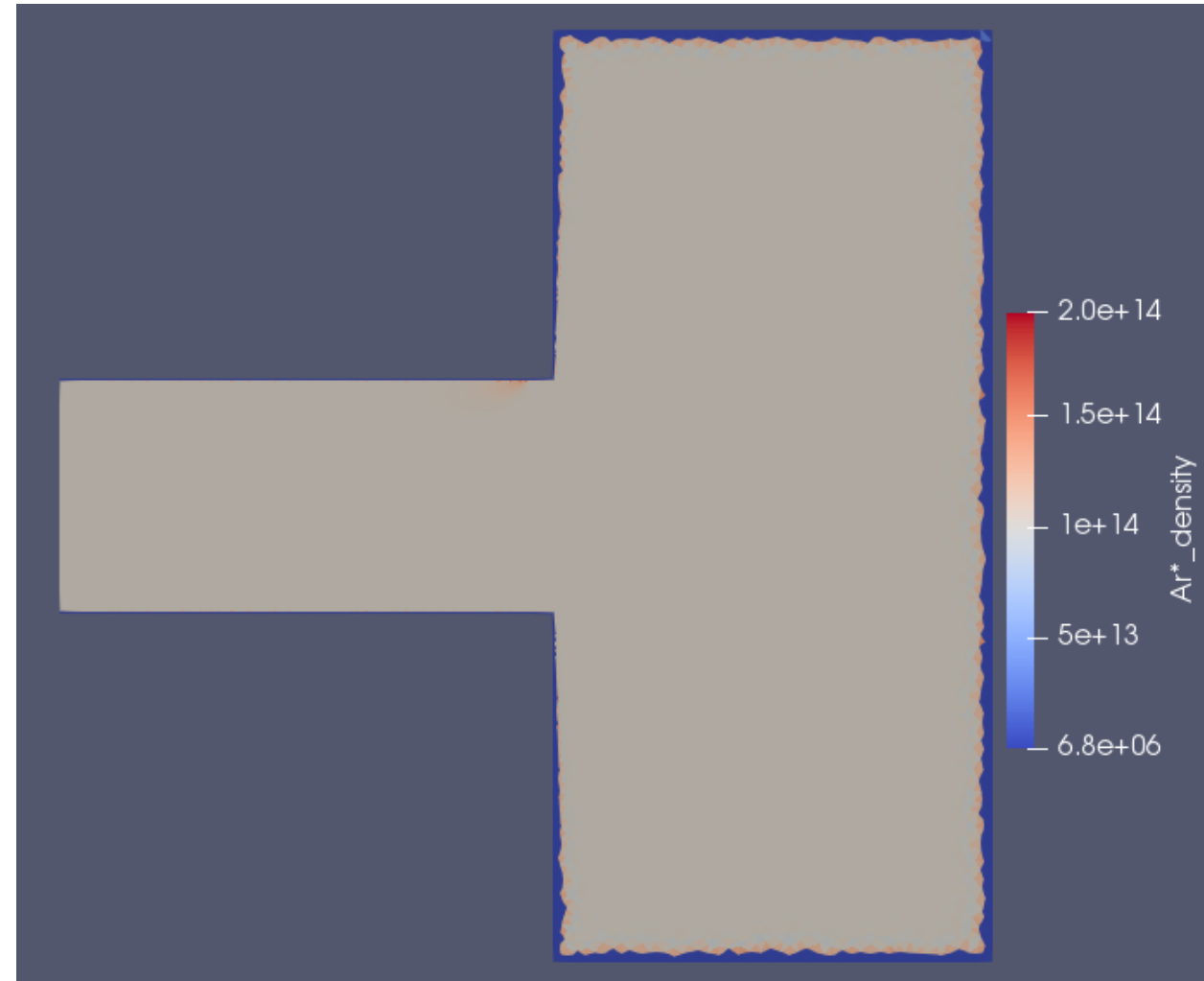
Electron Temperature [V]



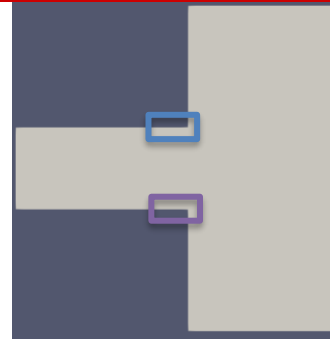
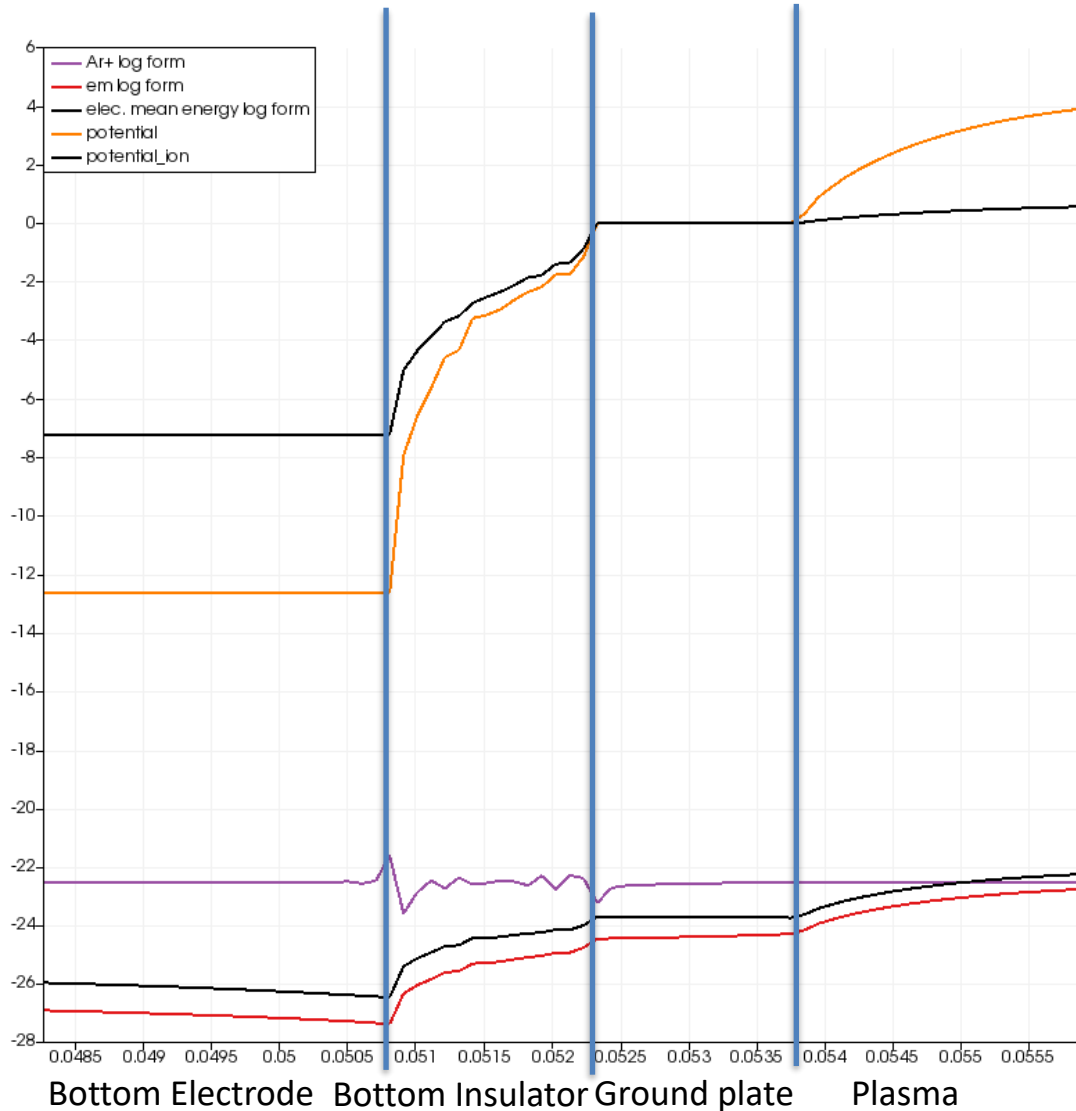
**Ion Density [m<sup>3</sup>]**



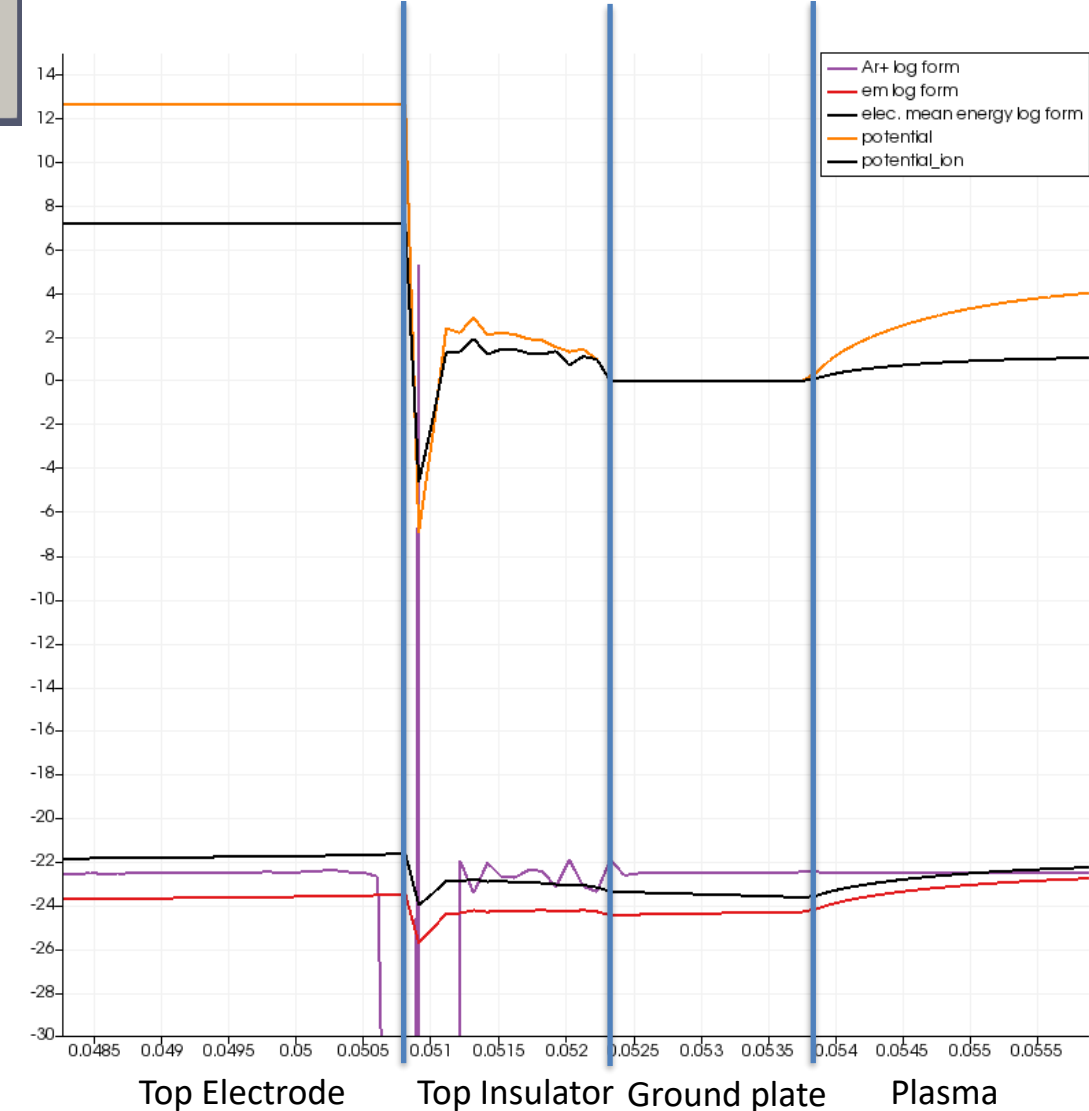
**Metastable Density [m<sup>3</sup>]**



## Bottom Boundary



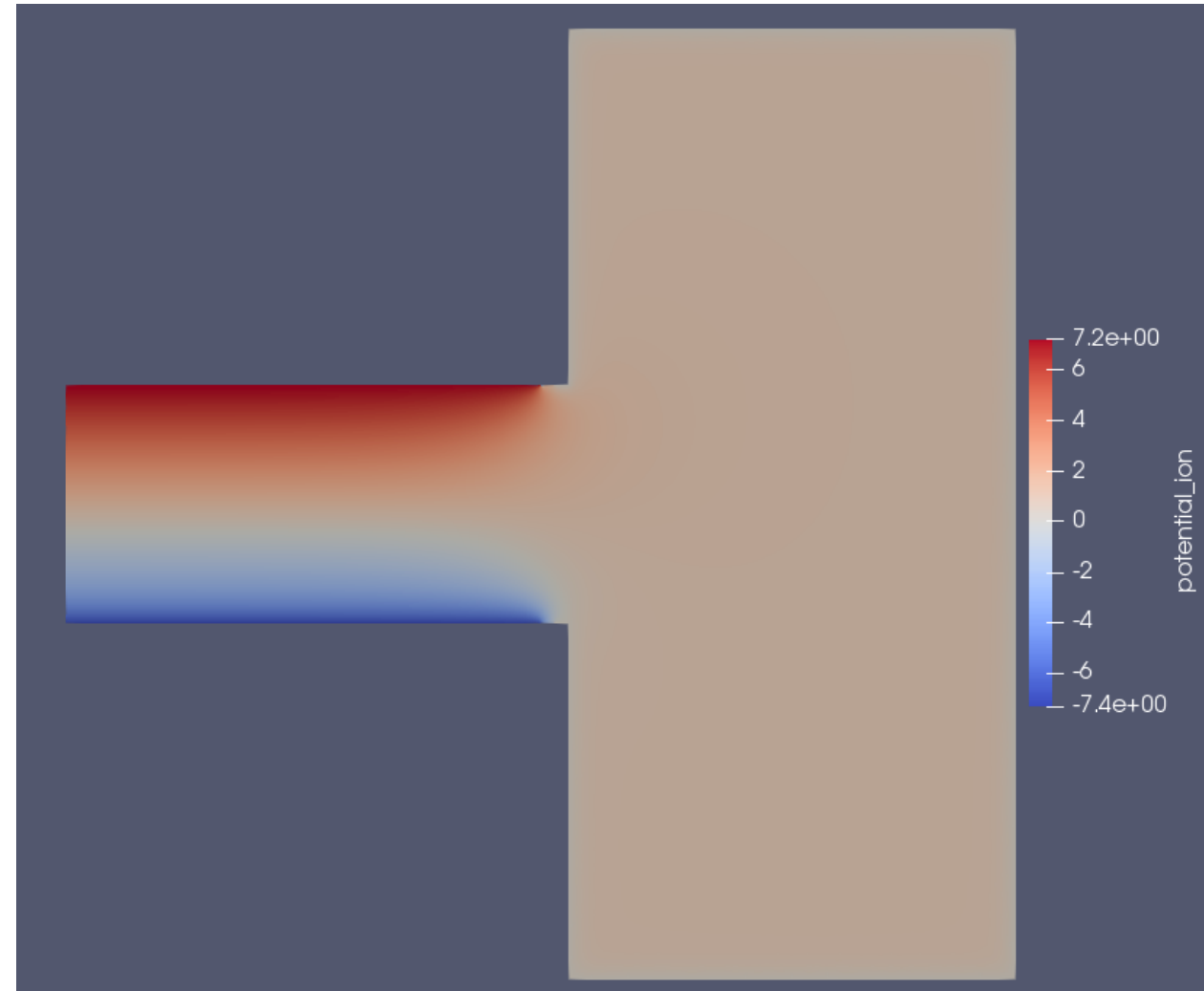
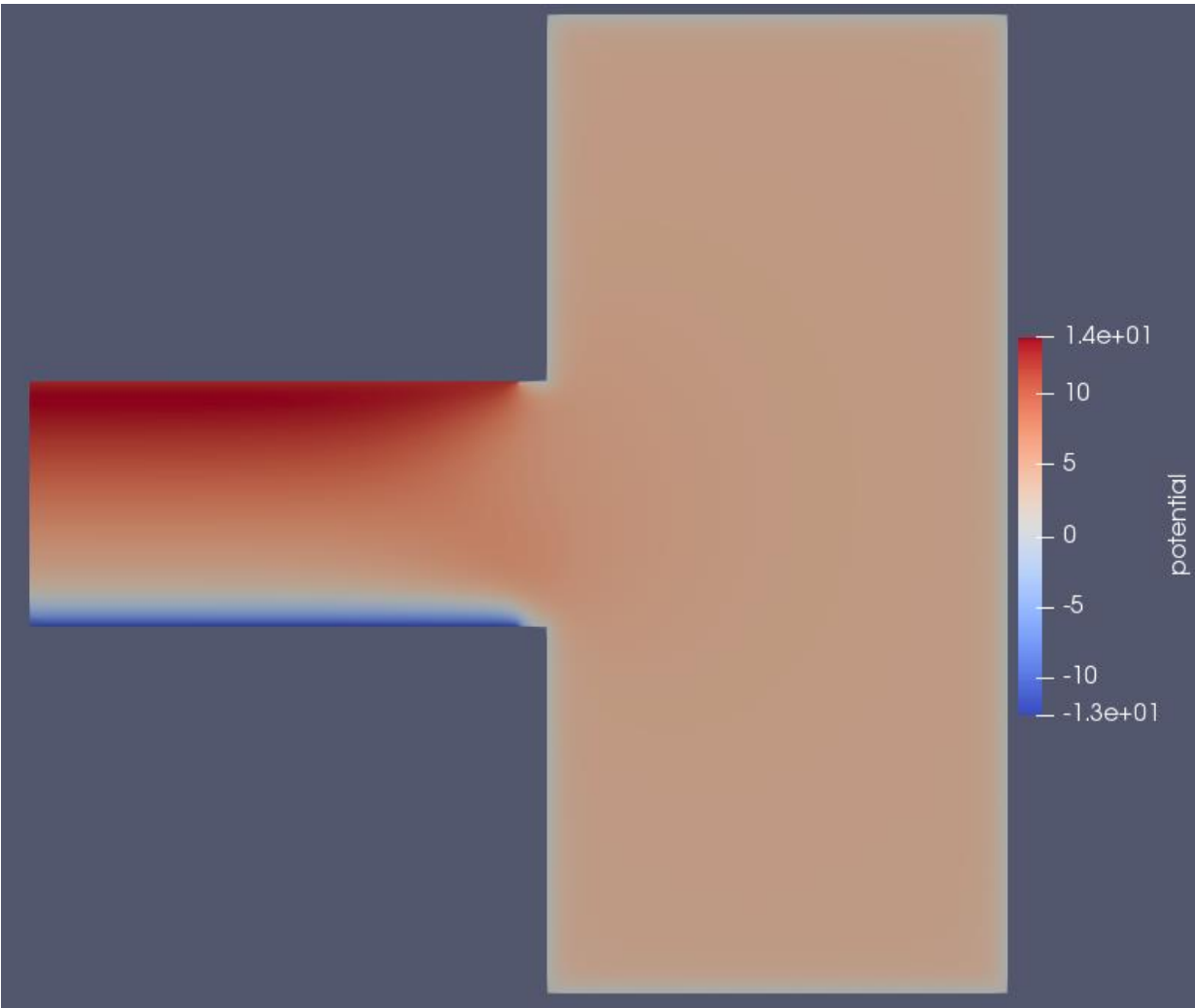
## Top Boundary



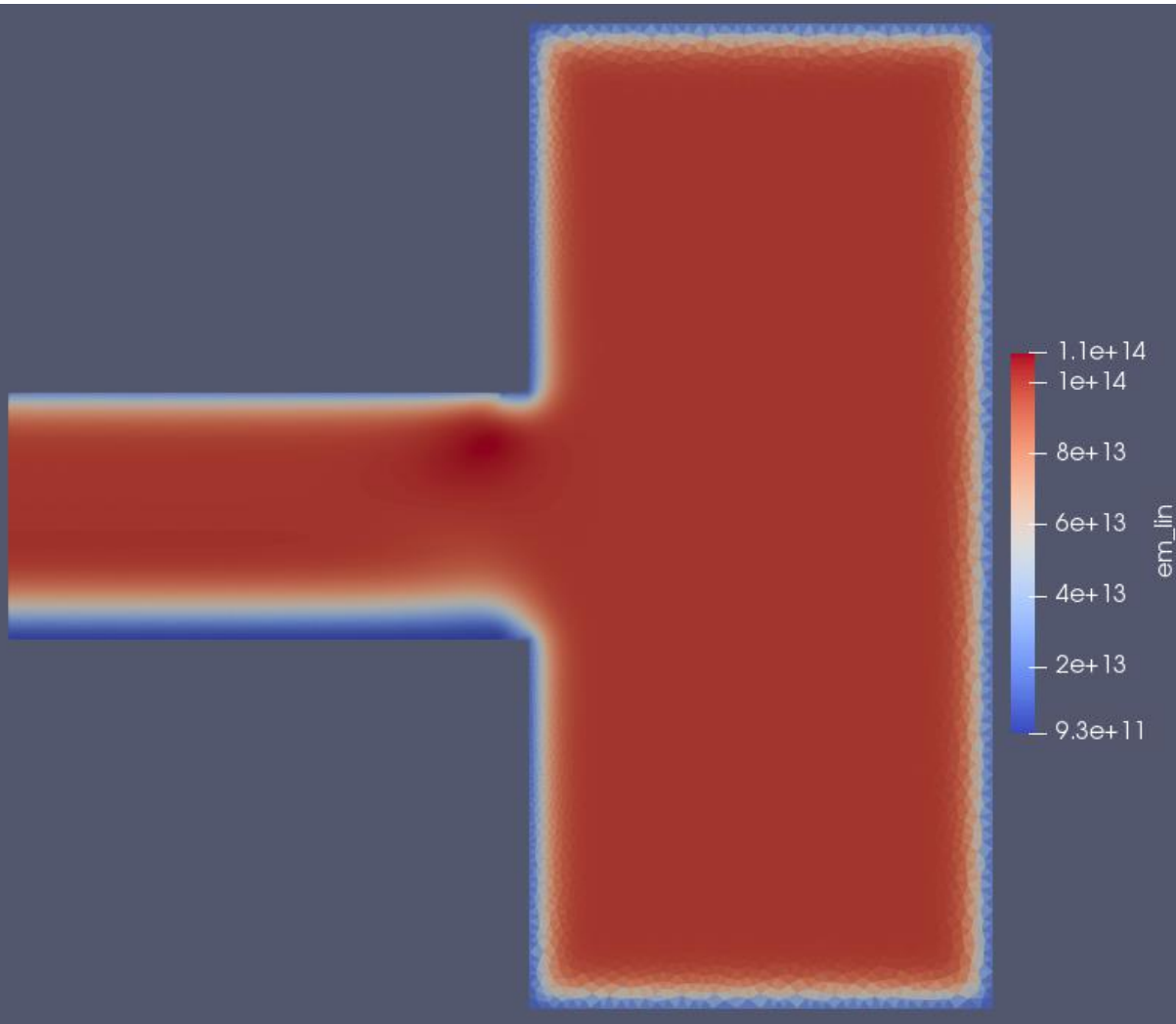
# **Results for Default BC / No Actions / No Dimensional Scaling Mesh**

Potential [V]

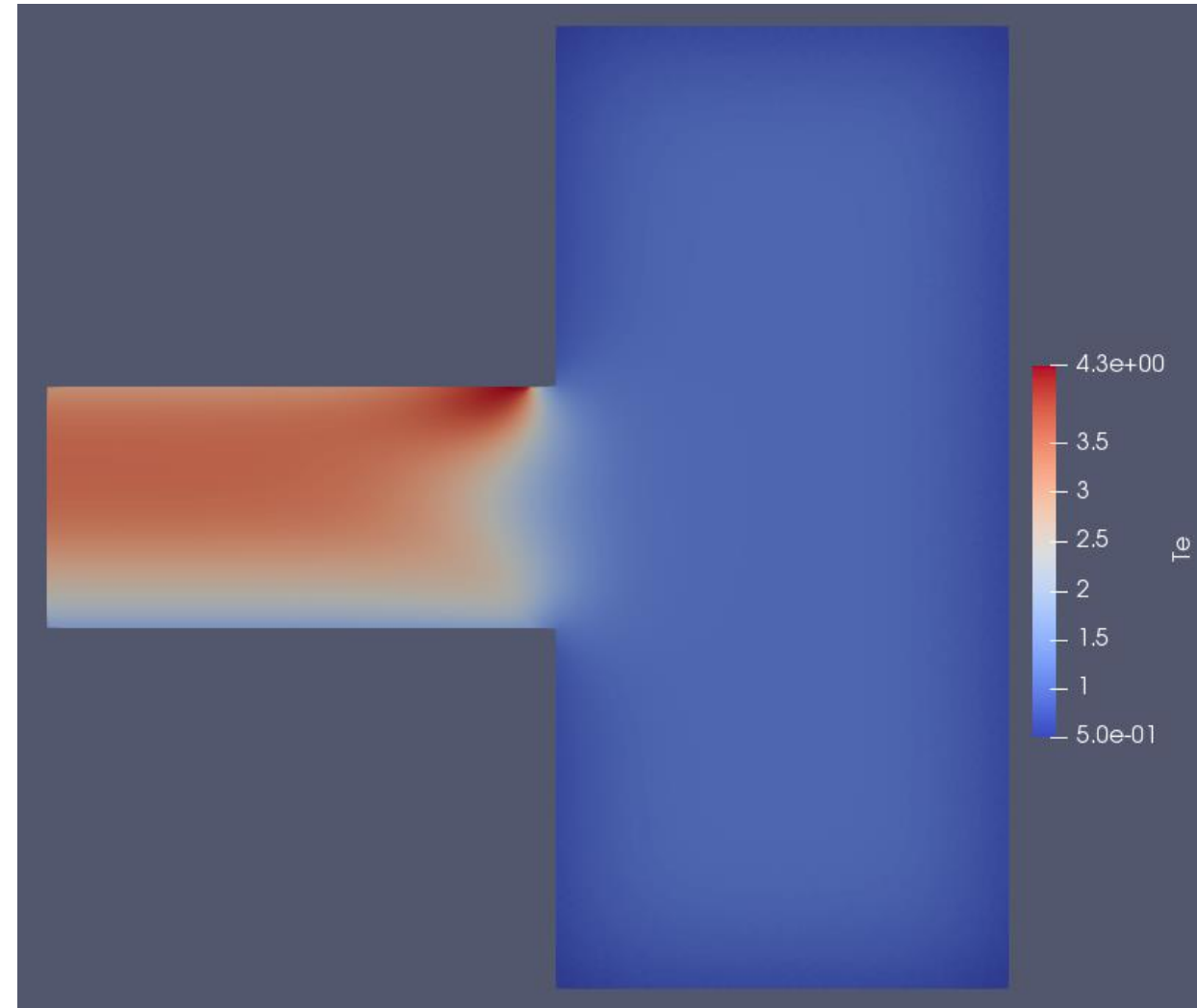
Ion Potential [V]



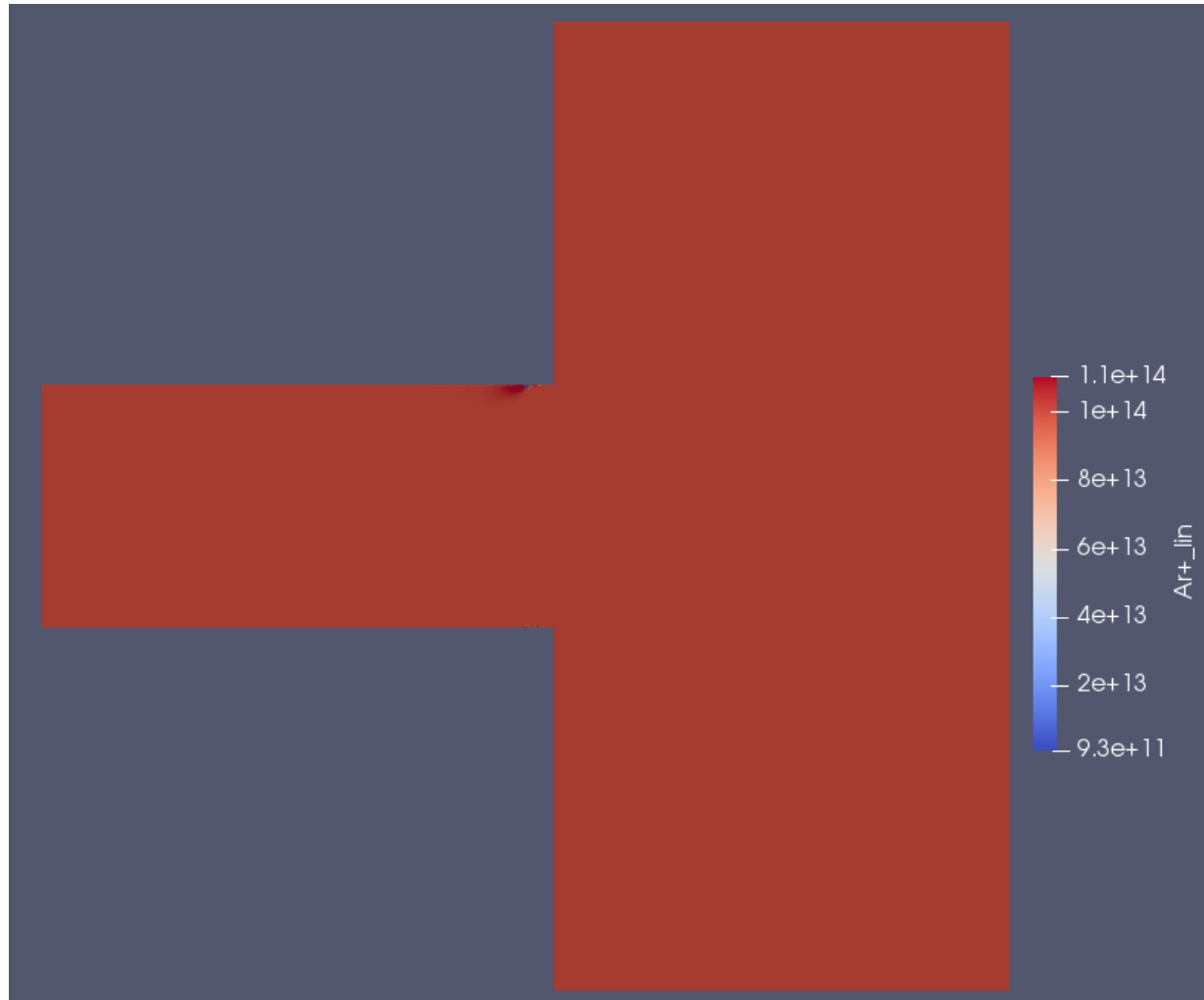
Electron Density [ $\text{m}^3$ ]



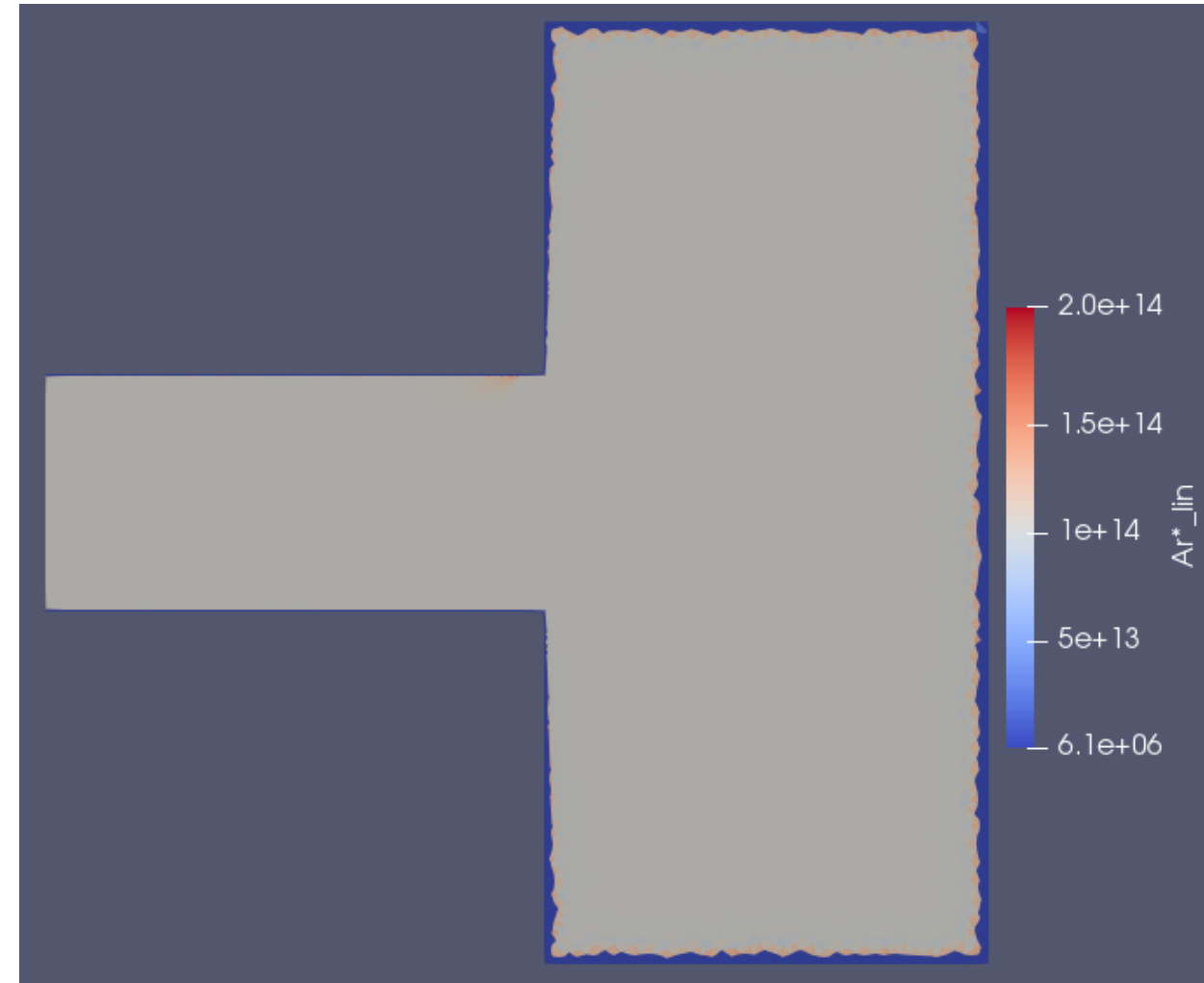
Electron Temperature [V]



Ion Density [m<sup>3</sup>]

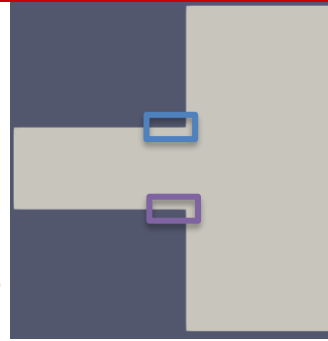
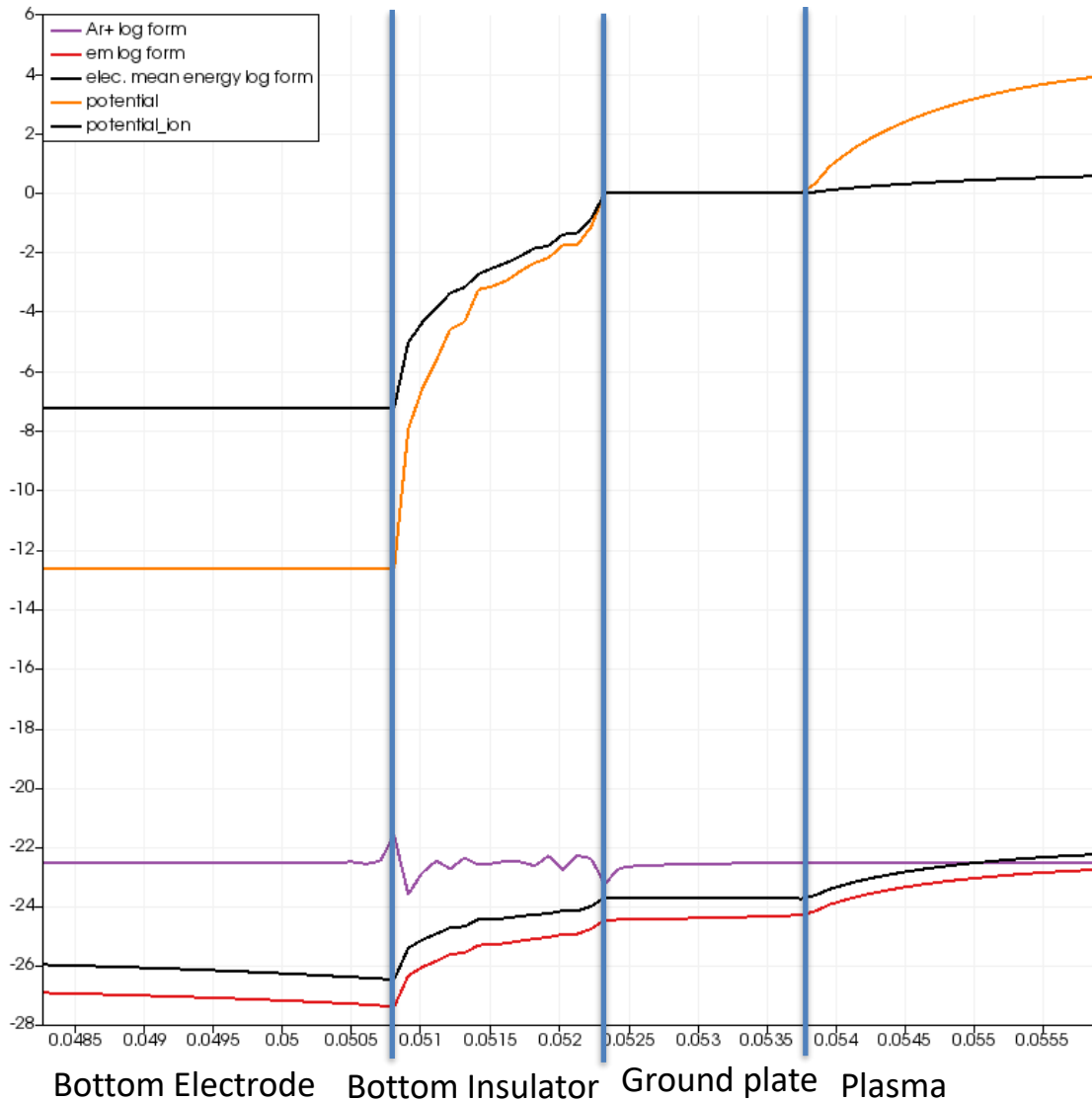


Metastable Density [m<sup>3</sup>]

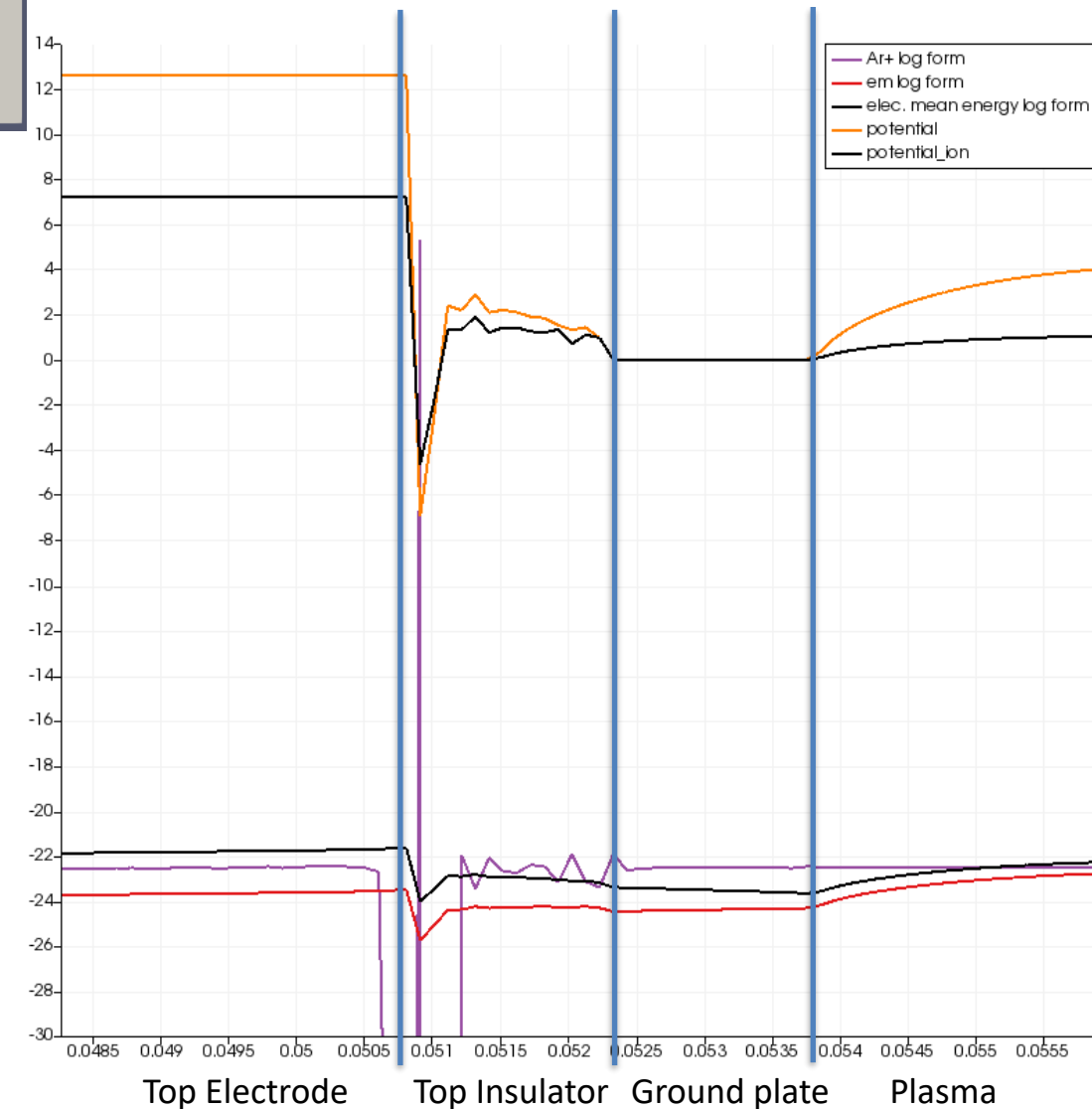




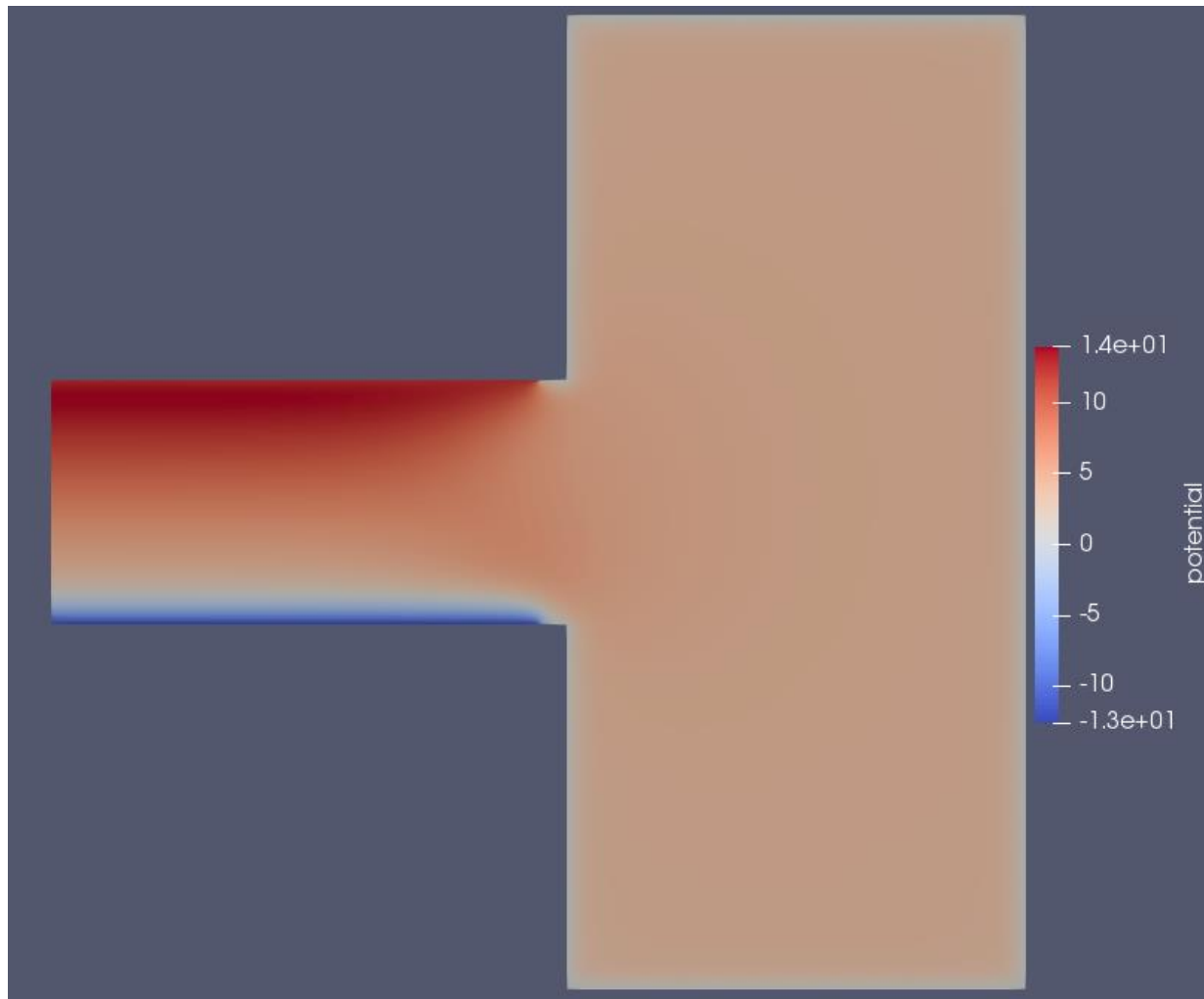
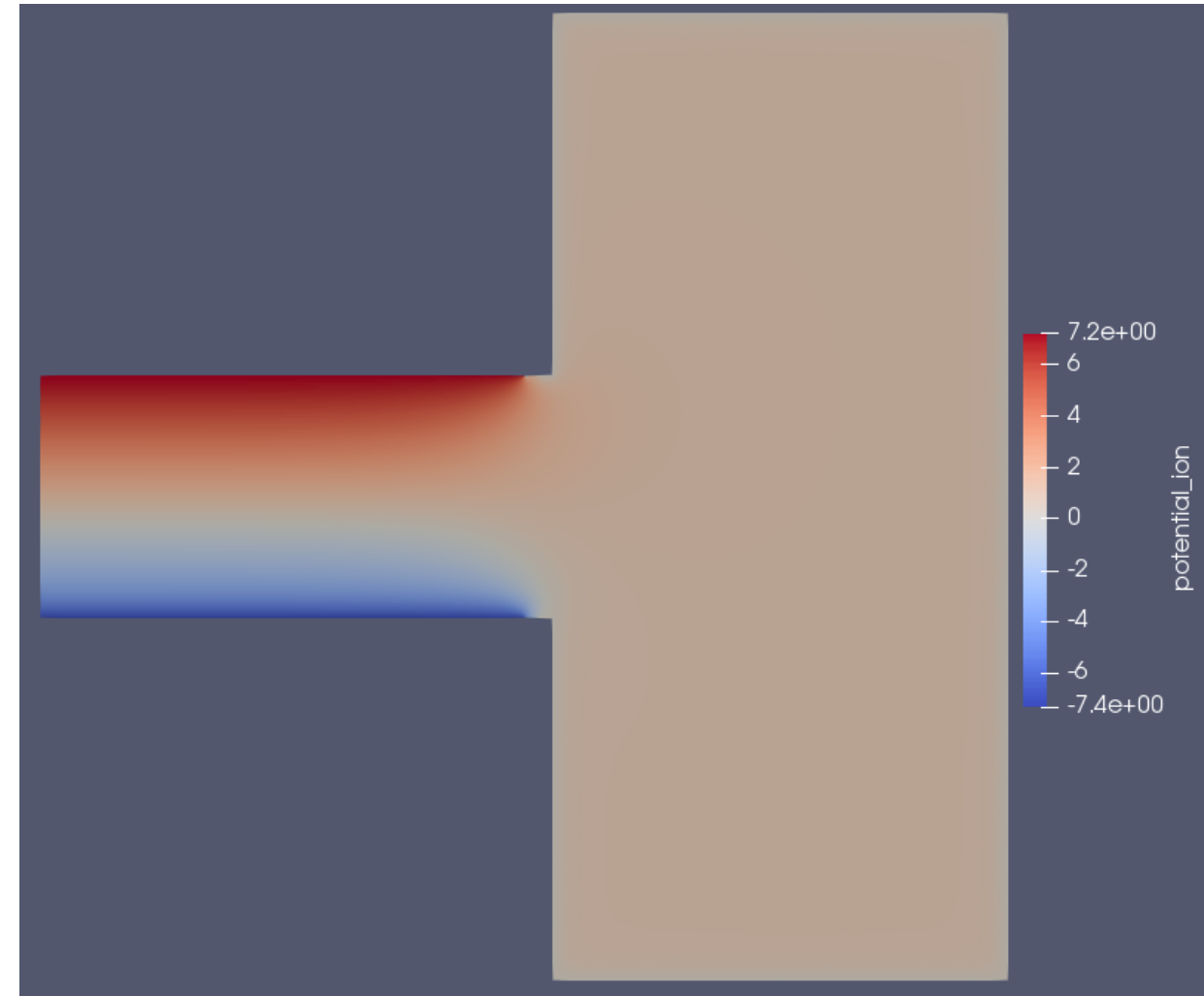
## Bottom Boundary

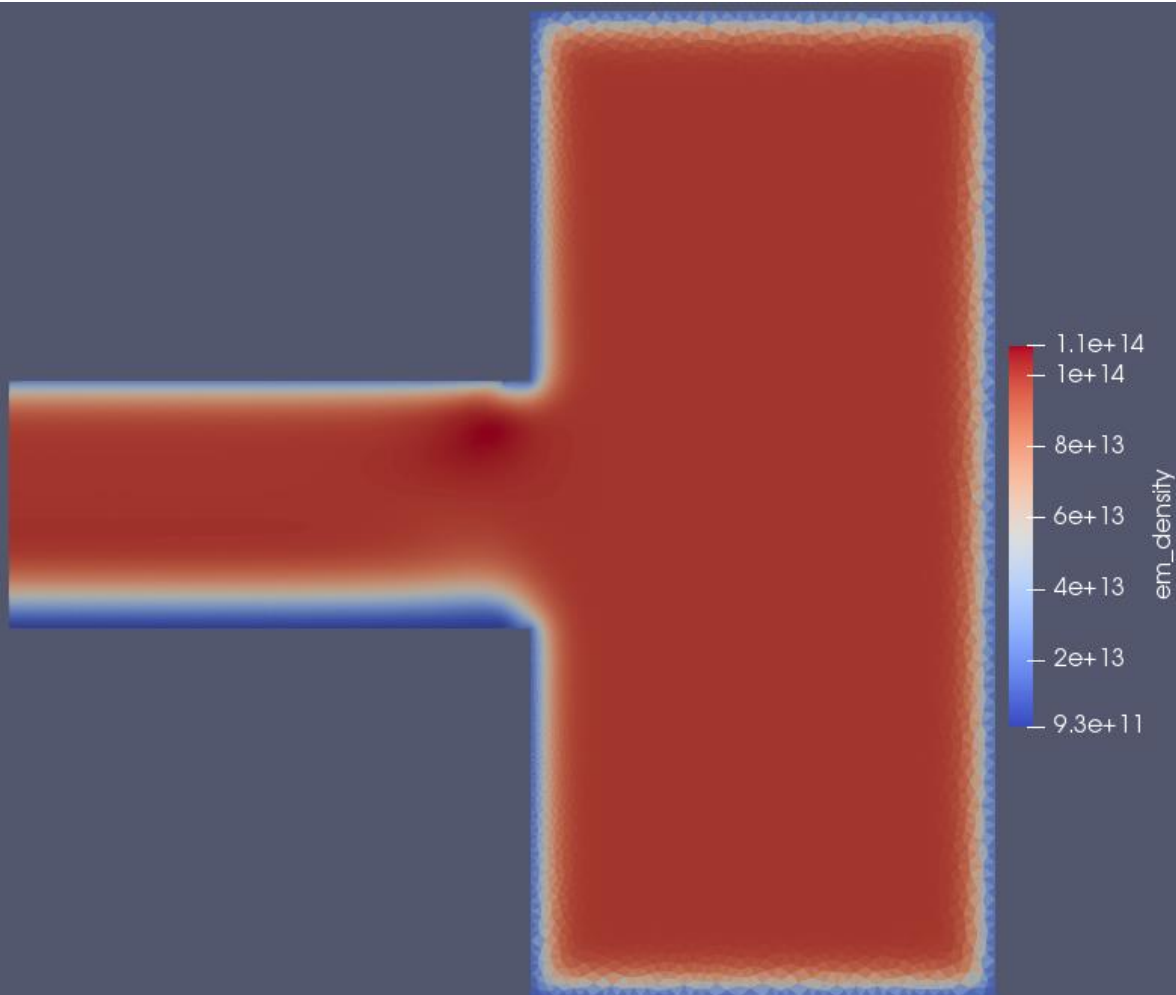


## Top Boundary

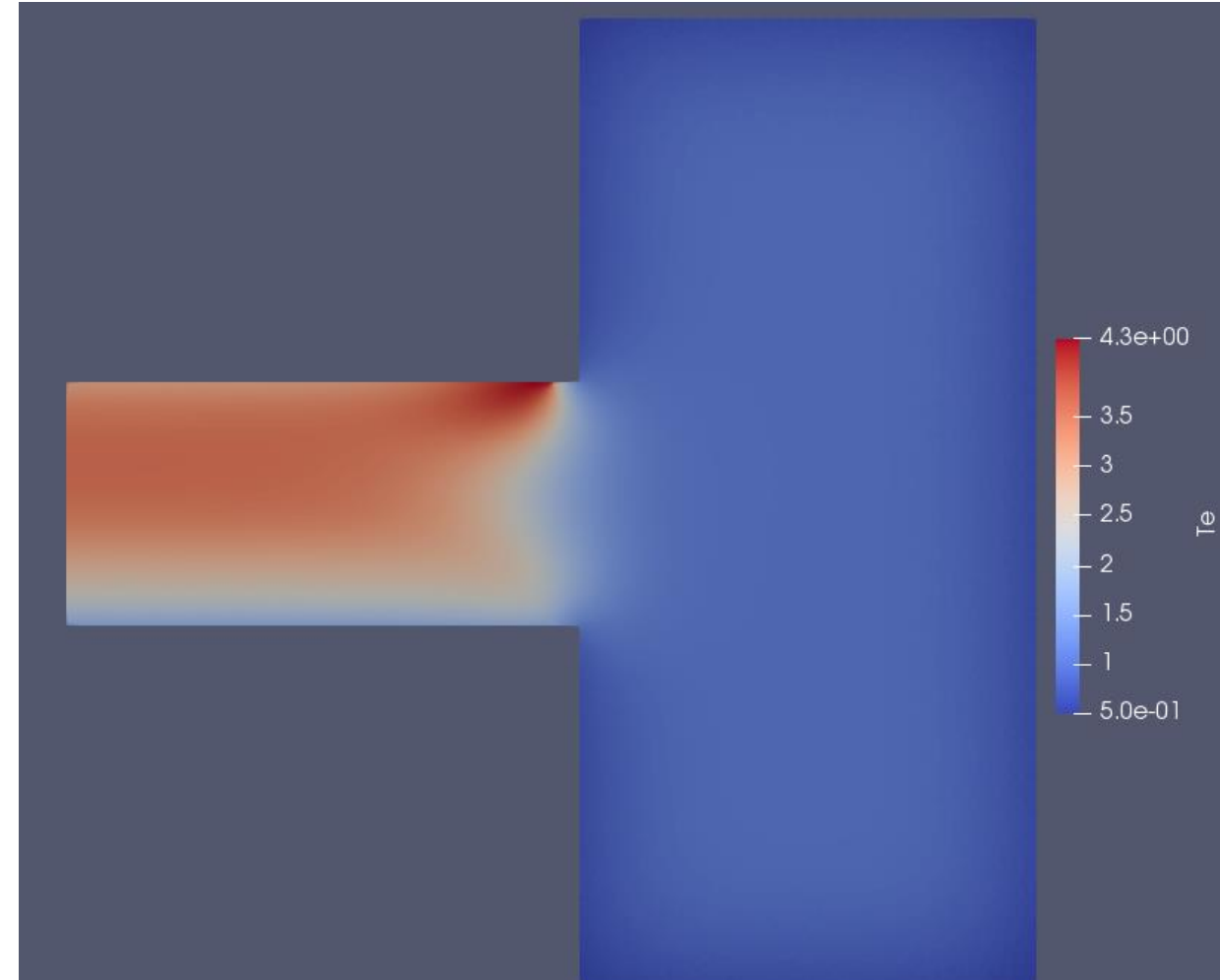


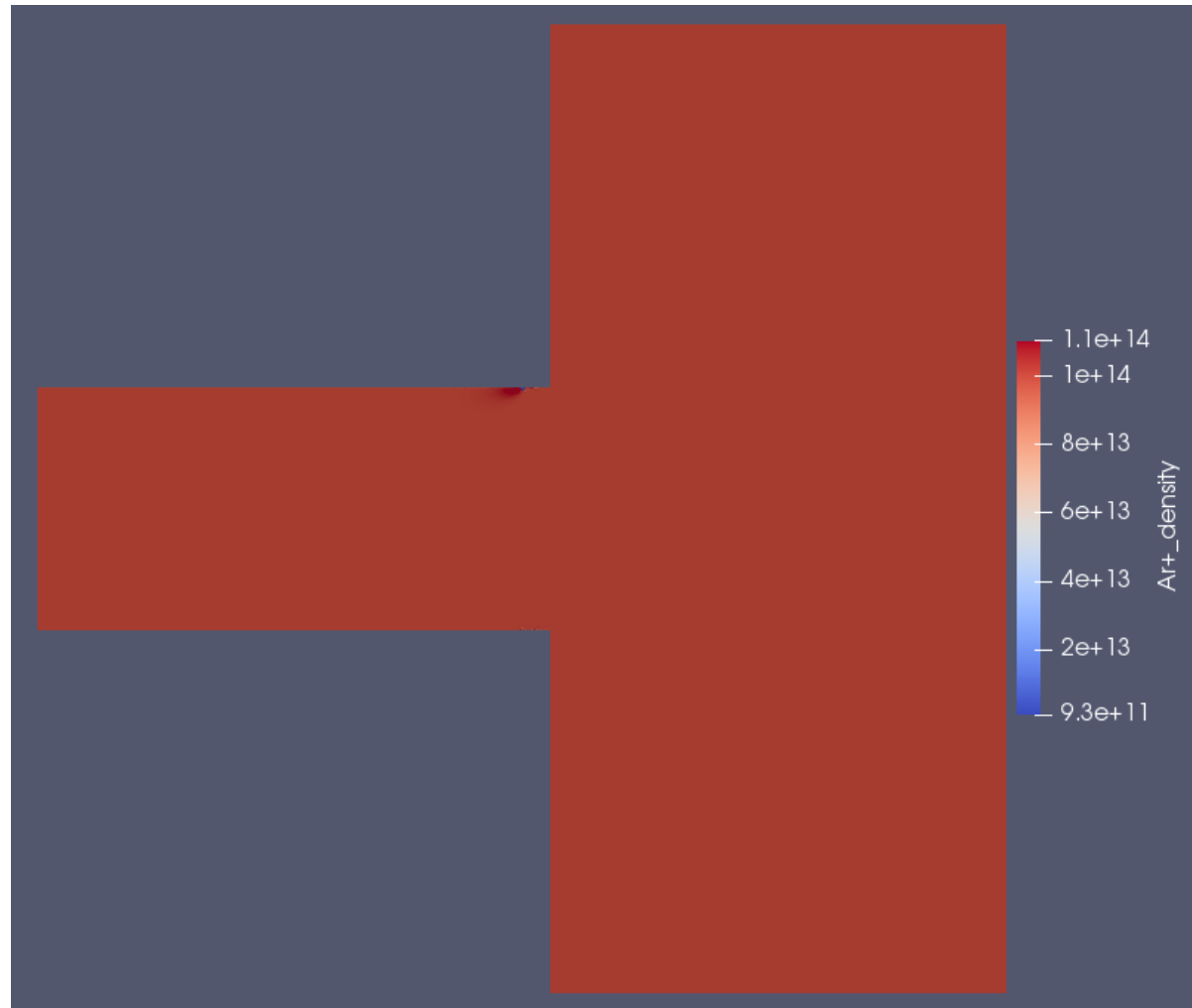
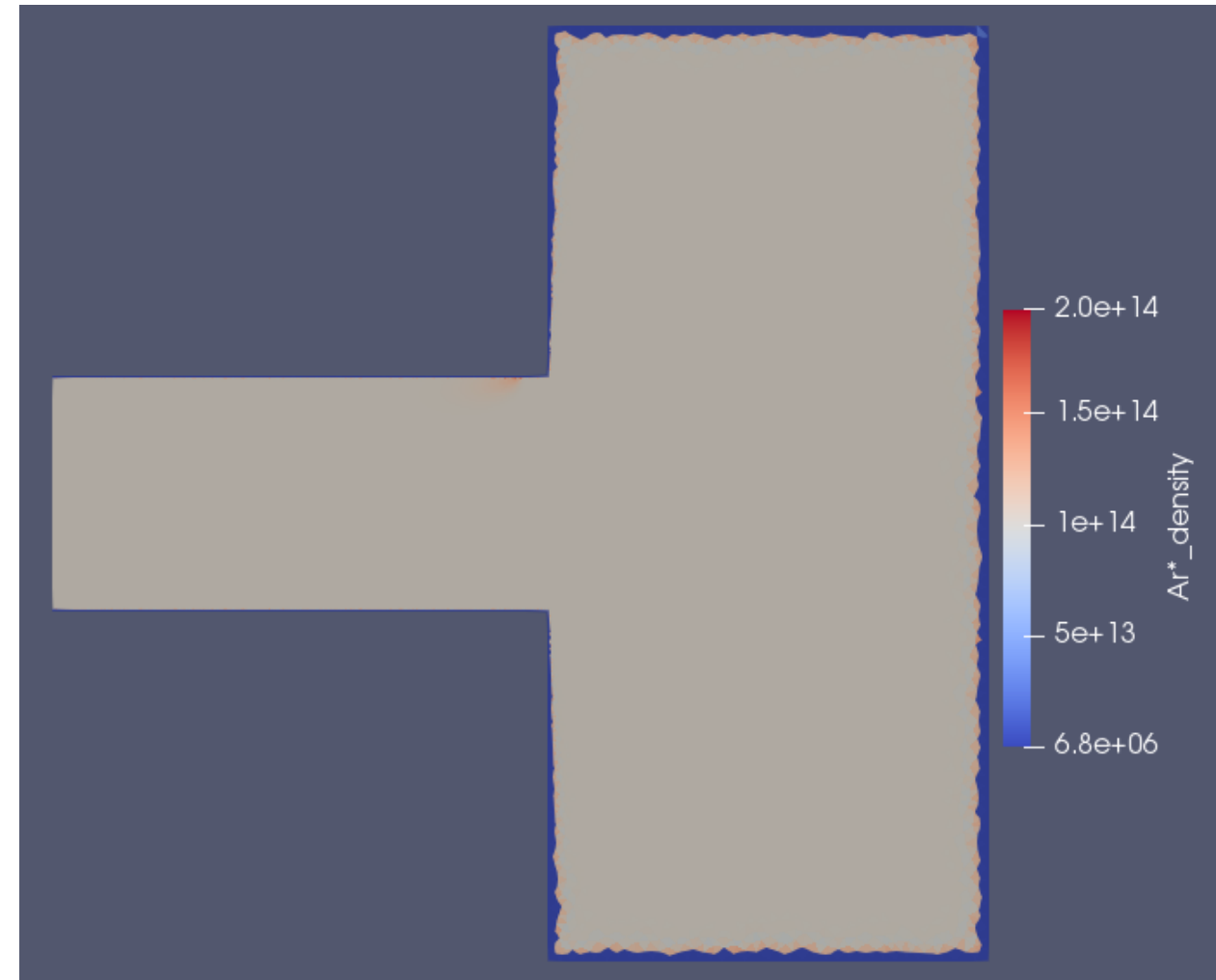
# **Results for Rearranged BC / Actions / No Dimensional Scaling Mesh**

**Potential [V]****Ion Potential [V]**

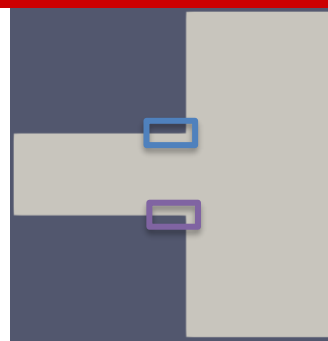
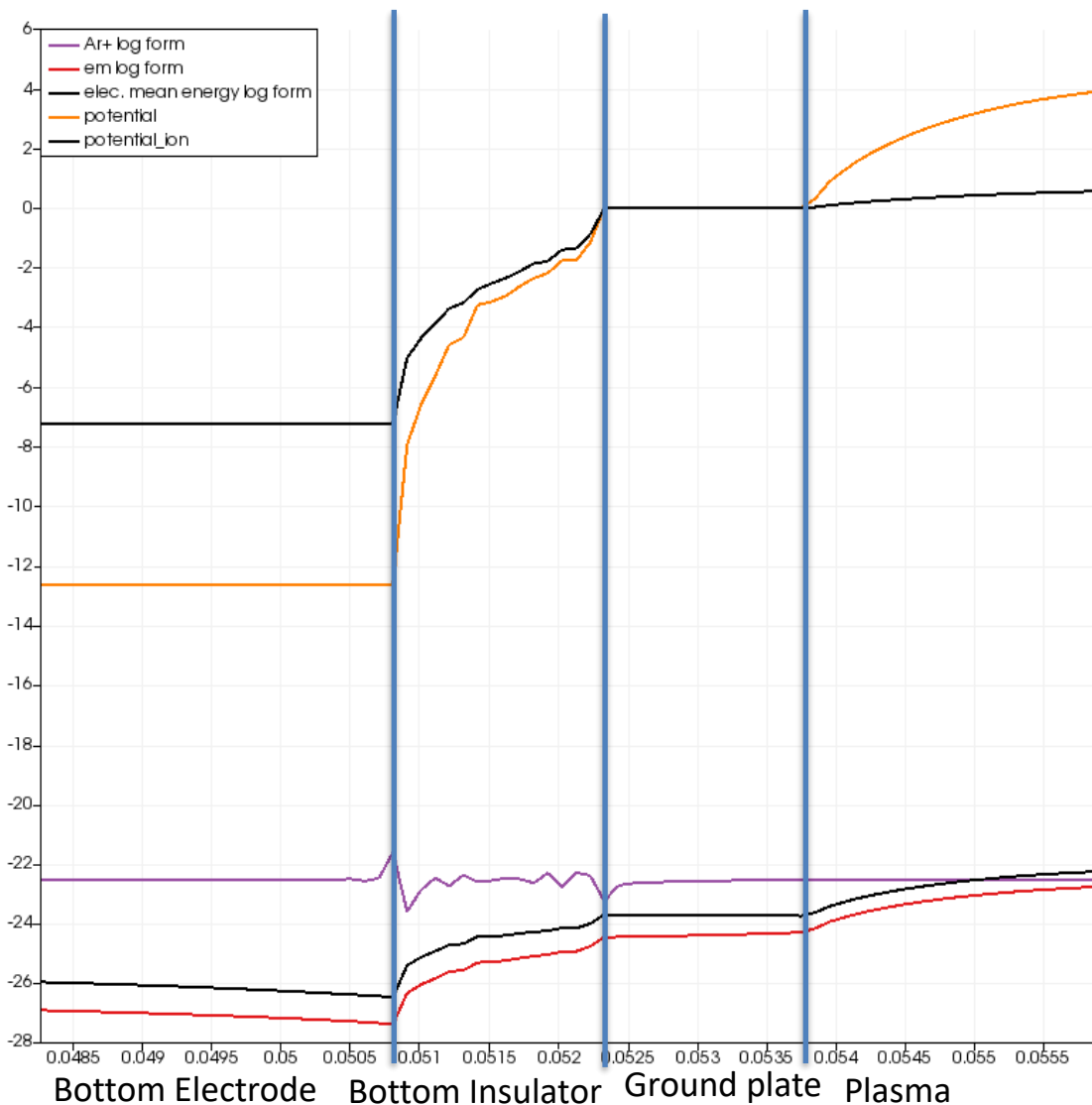
Electron Density [ $\text{m}^3$ ]

Electron Temperature [V]

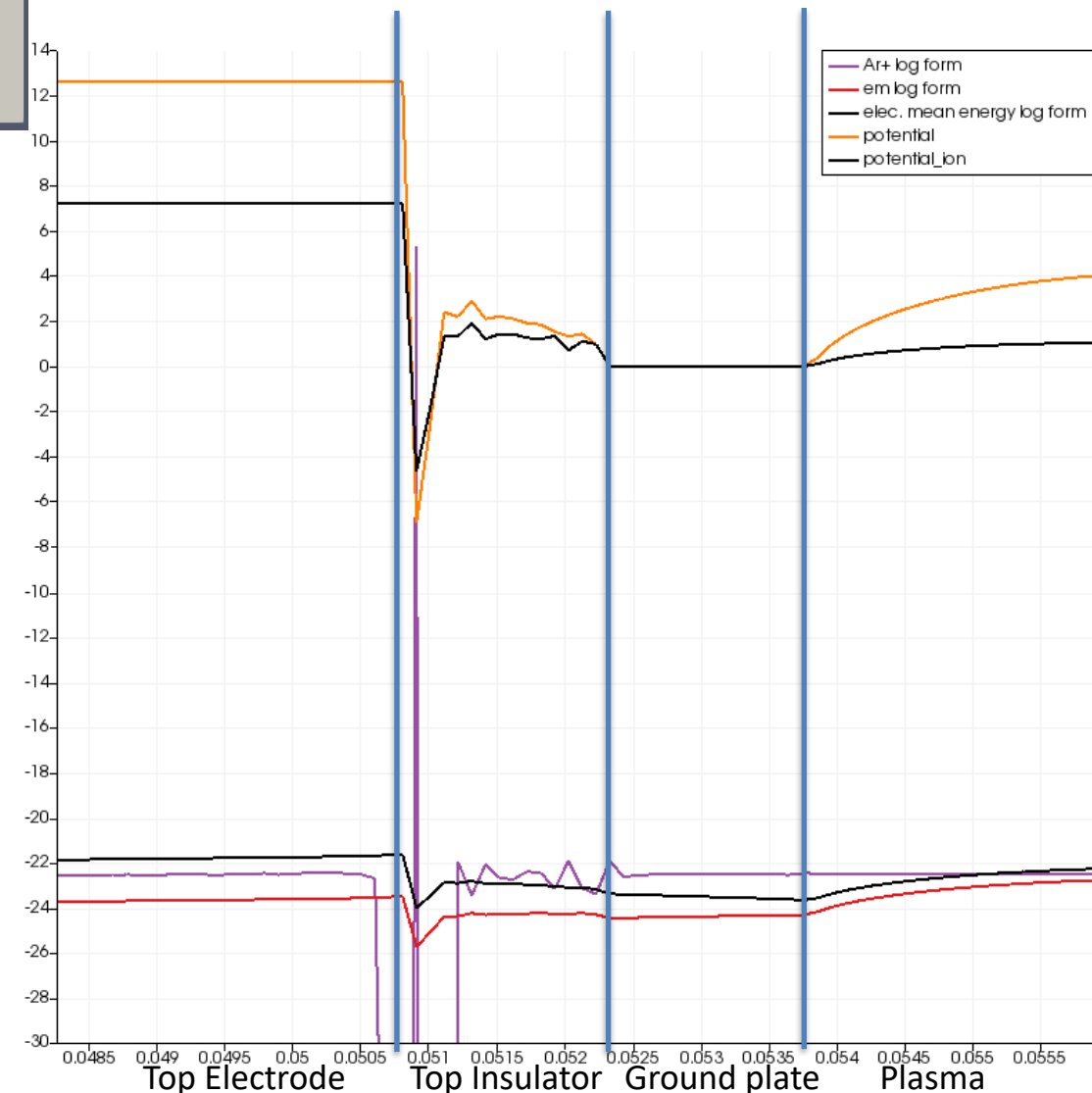


**Ion Density [ $\text{m}^3$ ]****Metastable Density [ $\text{m}^3$ ]**

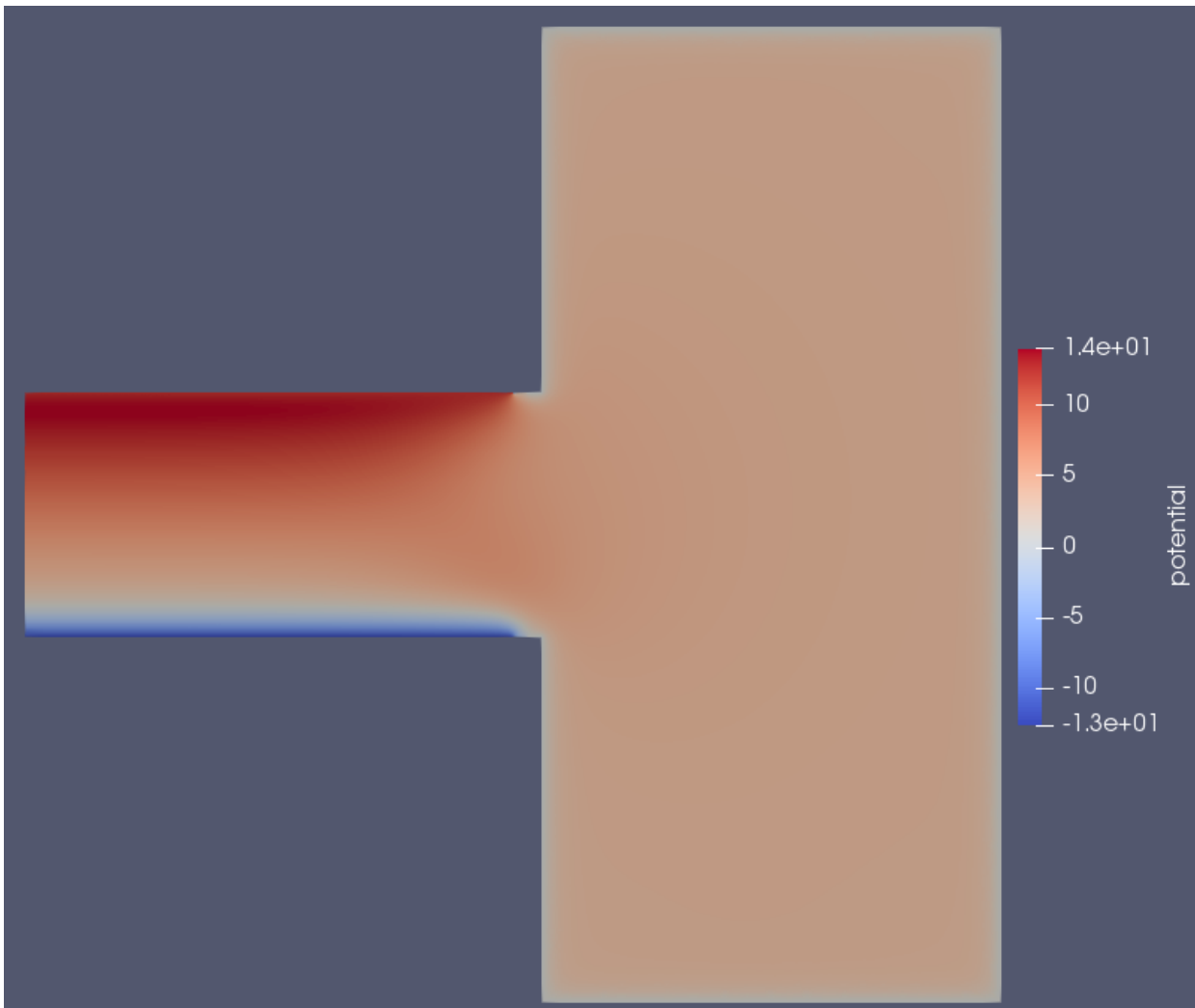
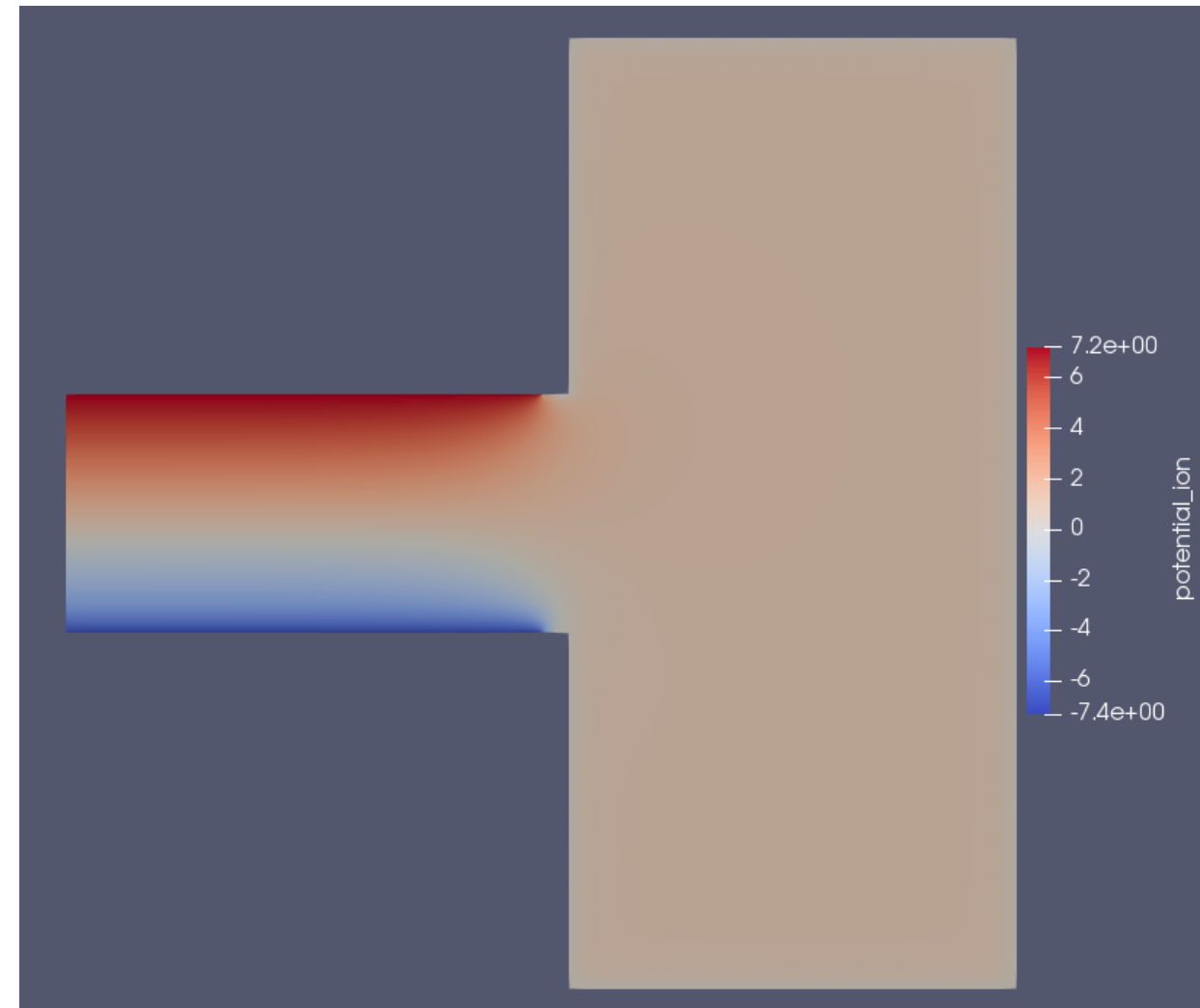
## Bottom Boundary



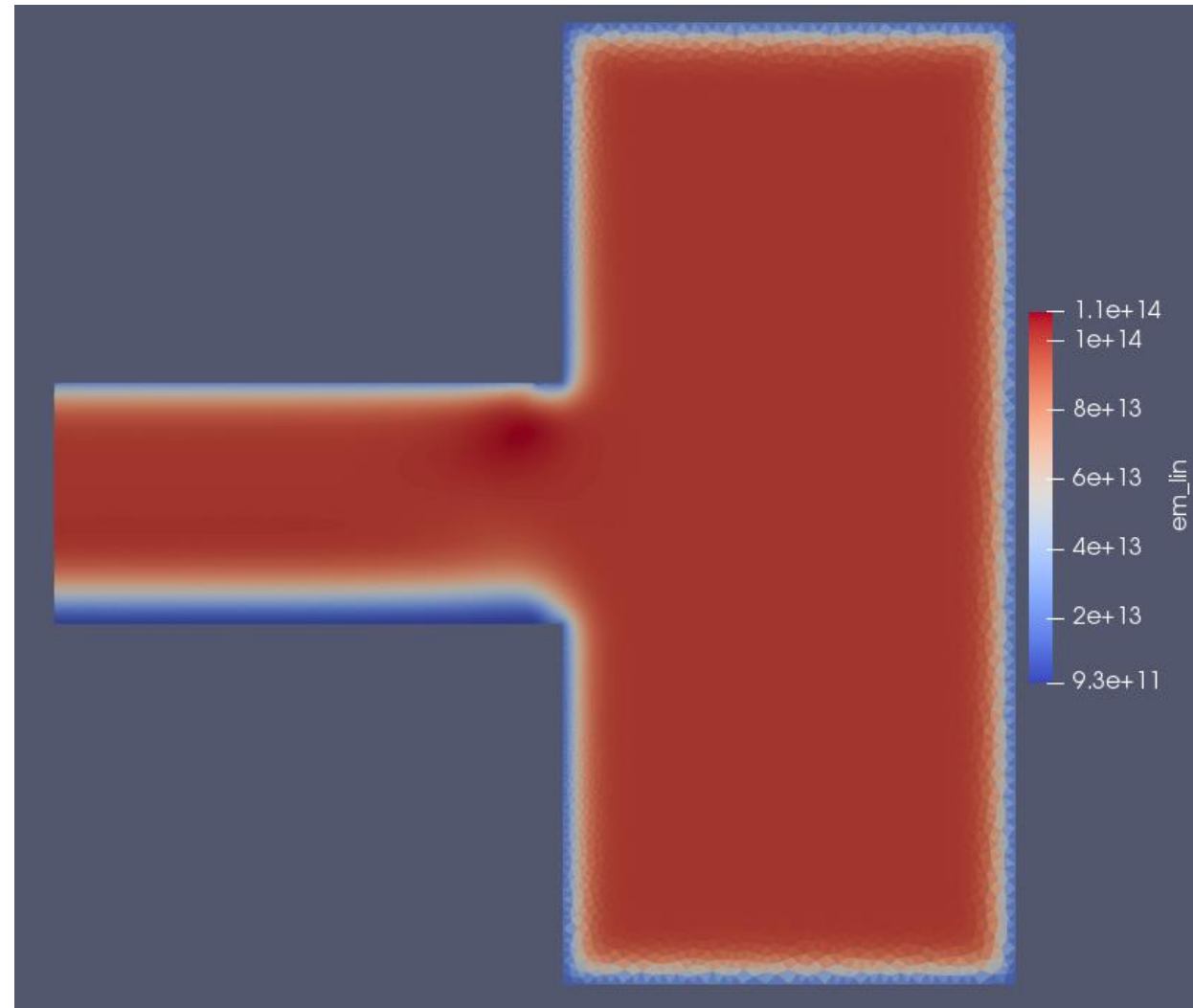
## Top Boundary



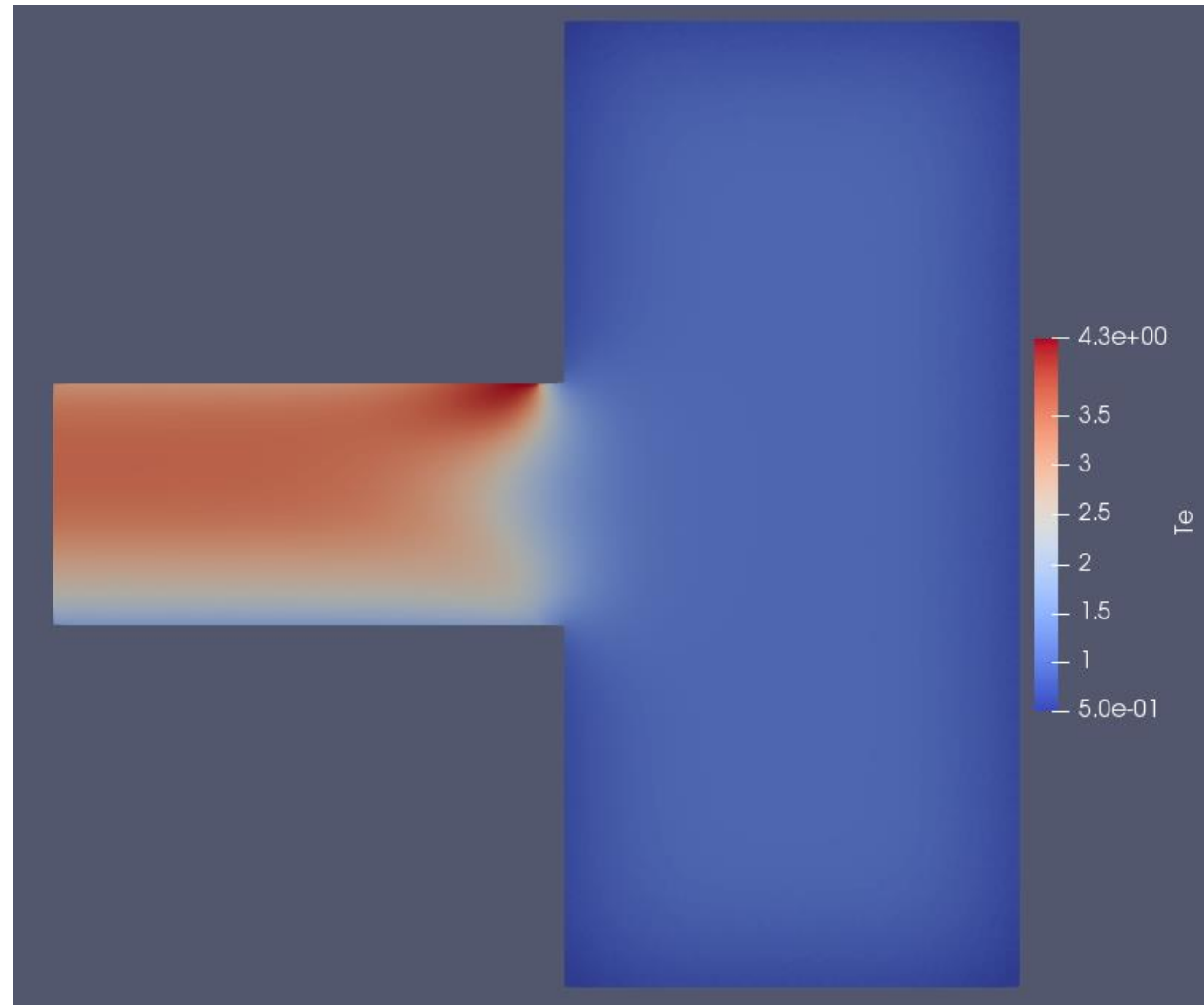
# **Results for Rearranged BC / No Actions / No Dimensional Scaling Mesh**

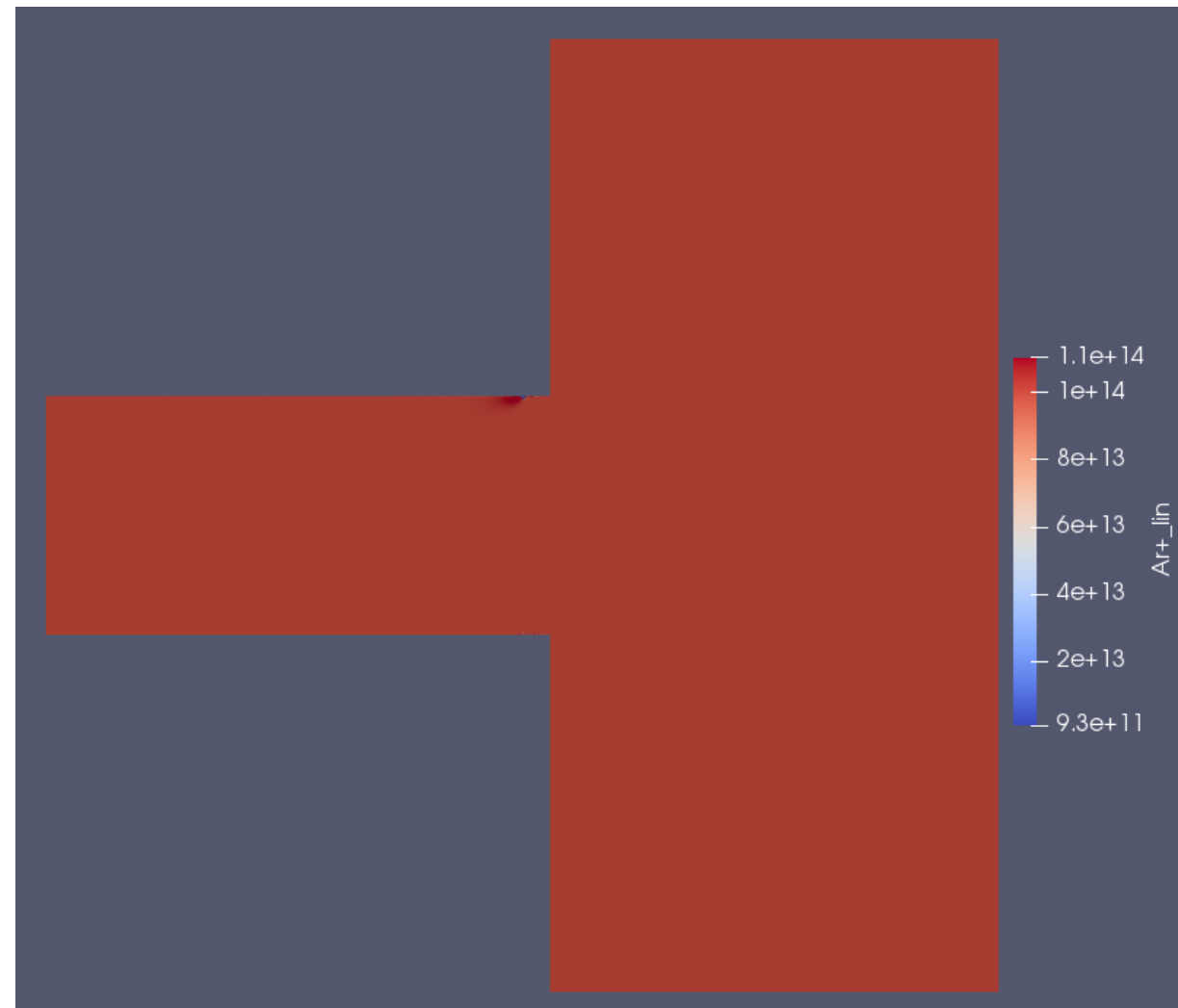
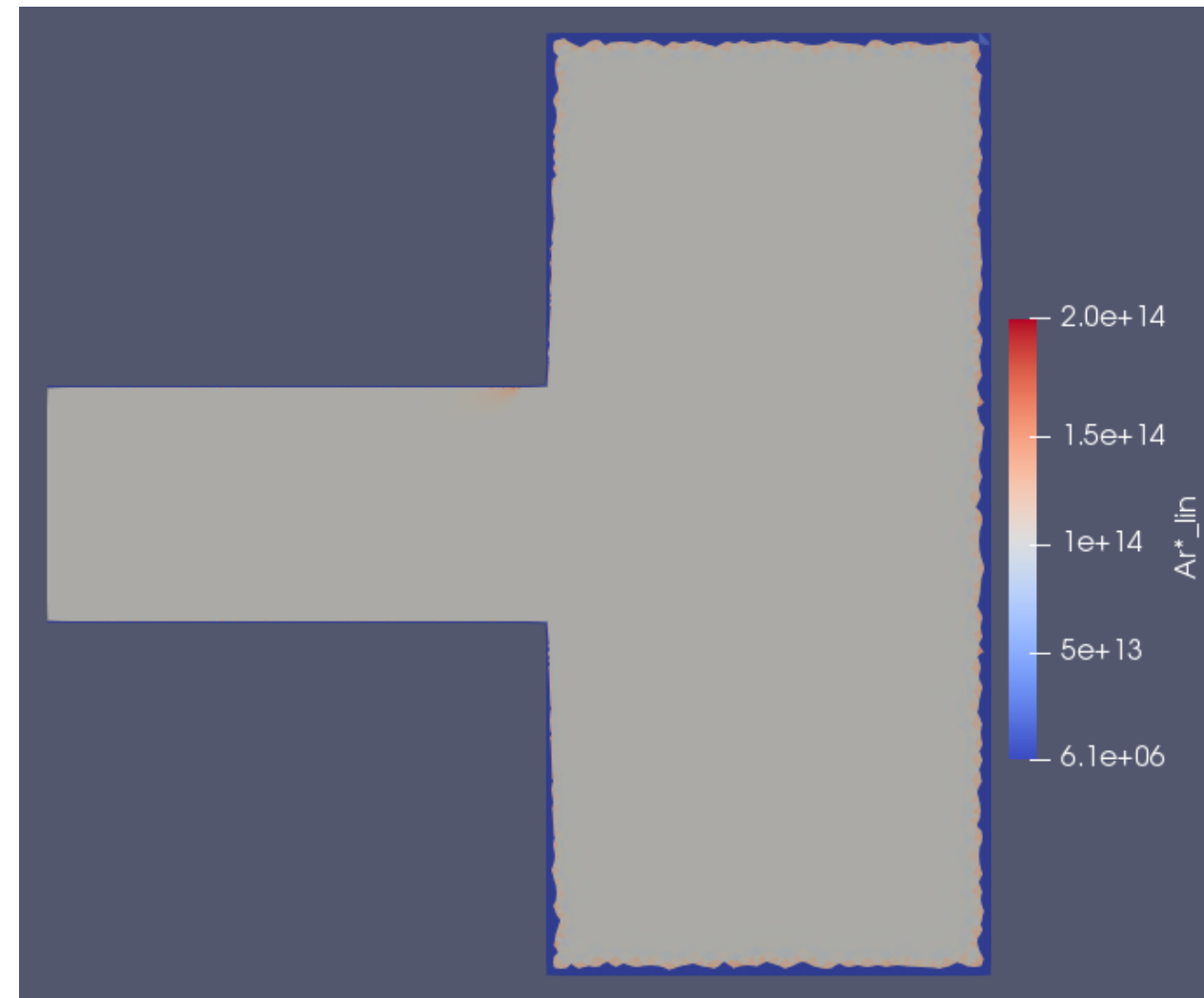
**Potential [V]****Ion Potential [V]**



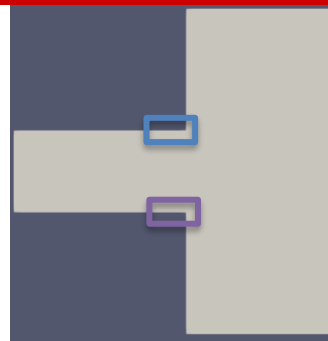
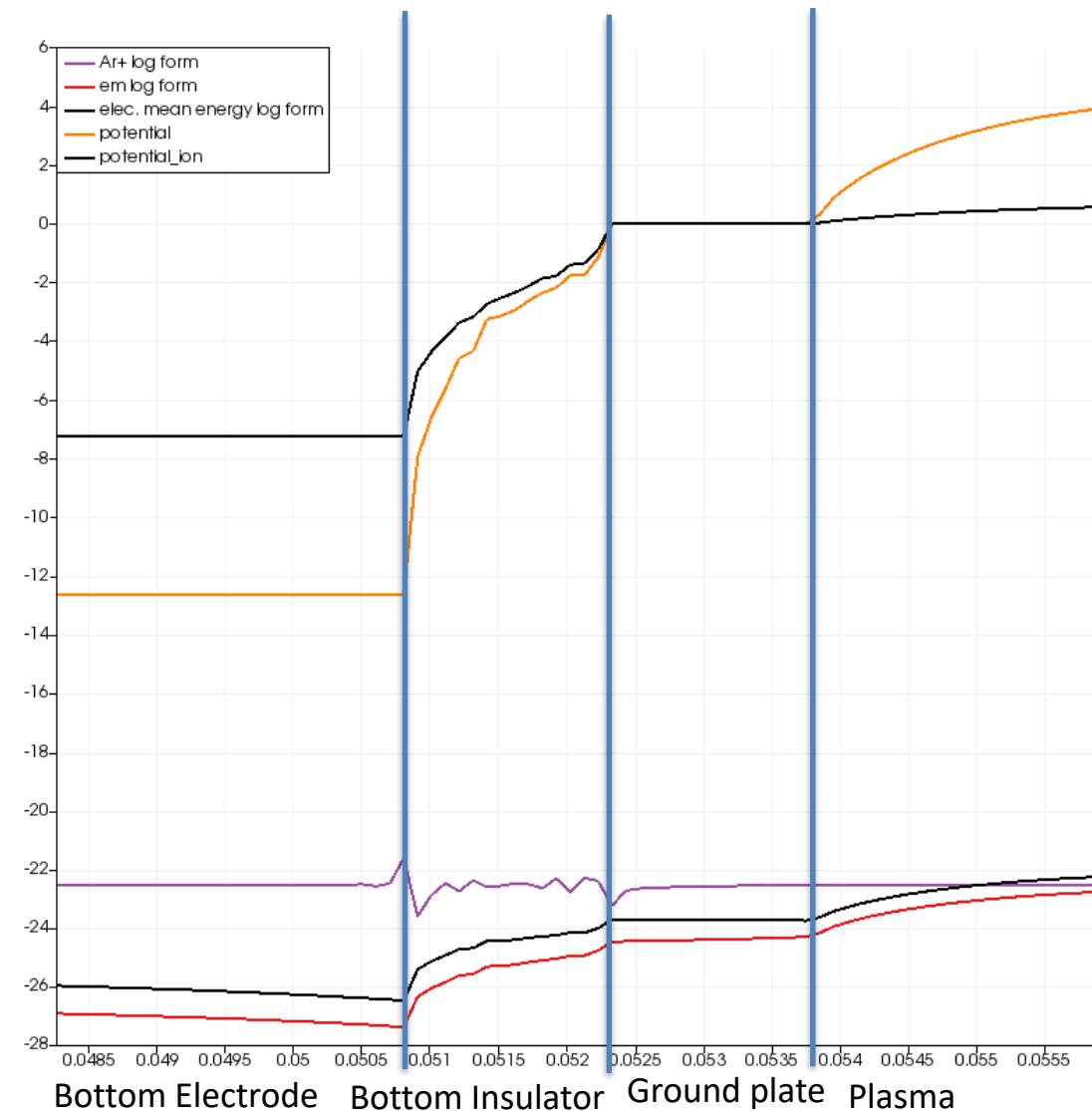
Electron Density [ $\text{m}^3$ ]

Electron Temperature [V]

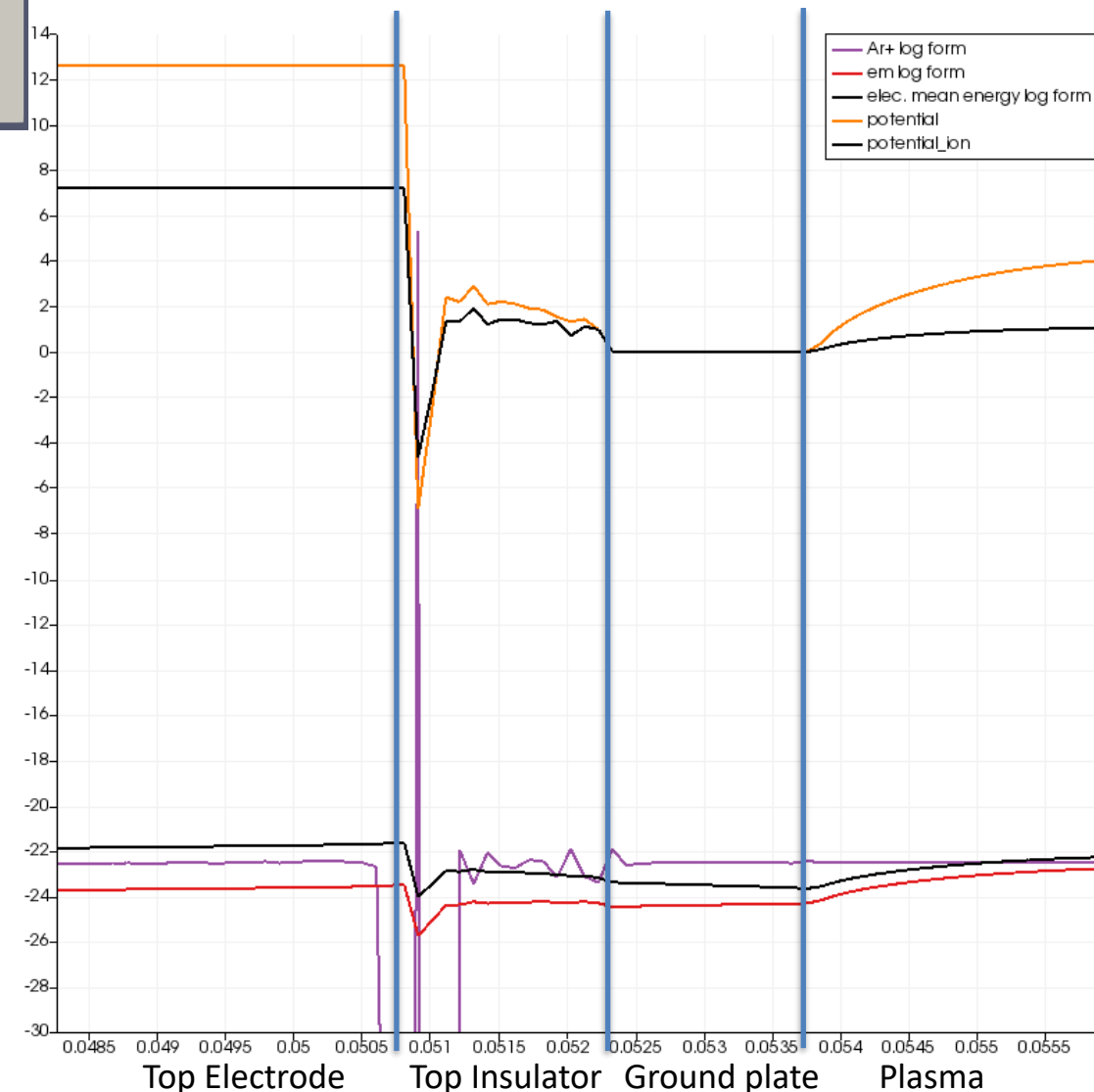


Ion Density [ $\text{m}^3$ ]Metastable Density [ $\text{m}^3$ ]

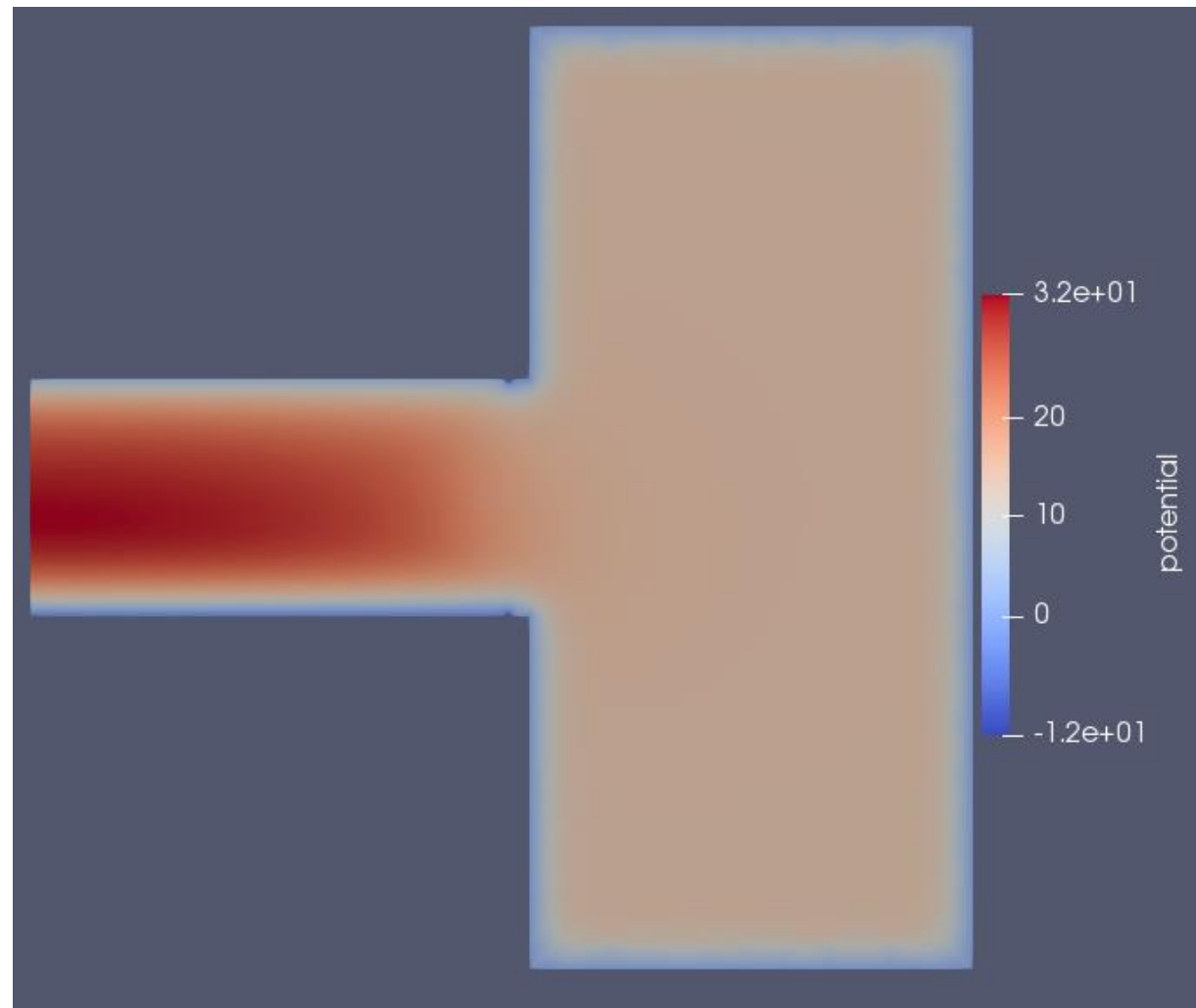
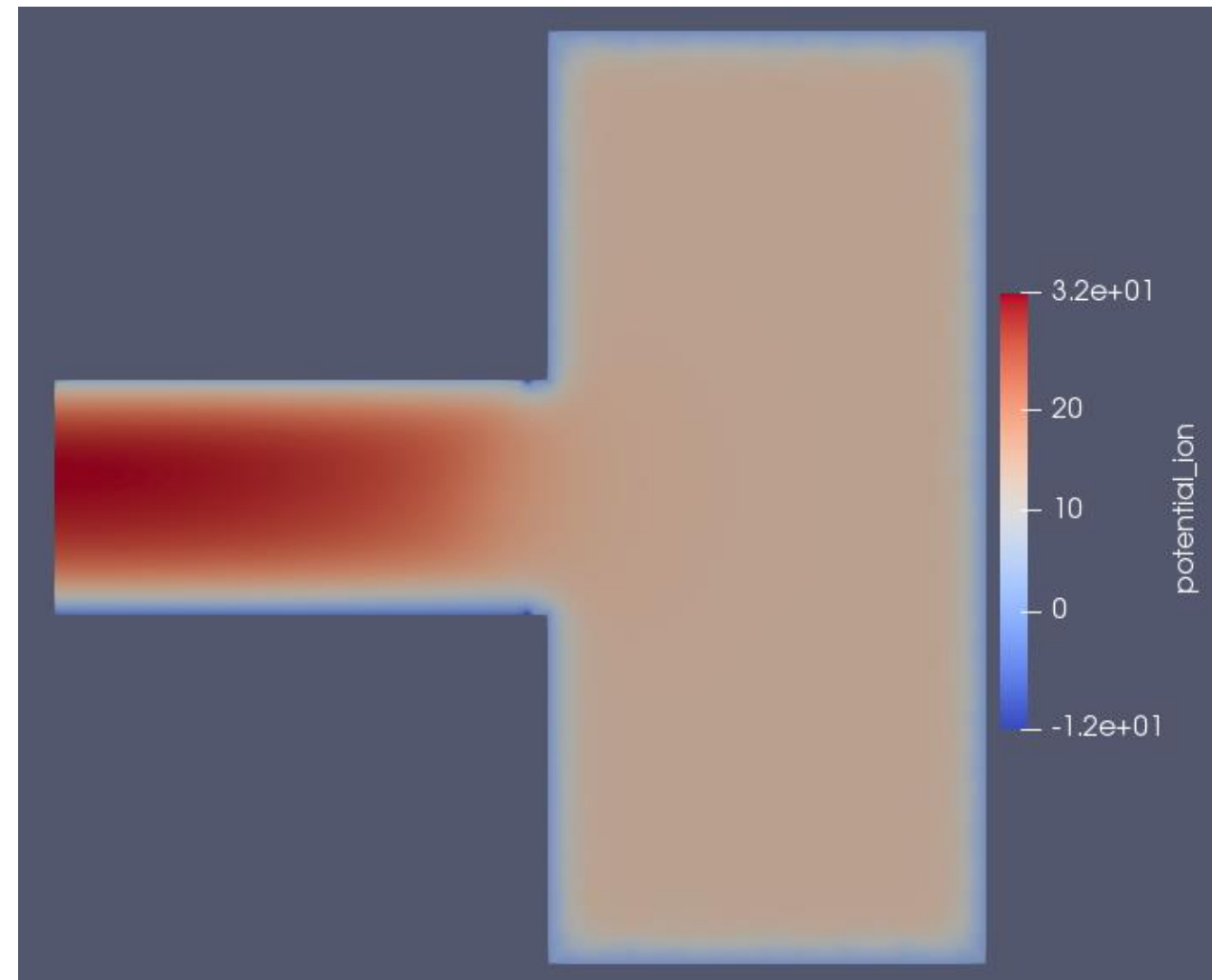
## Bottom Boundary

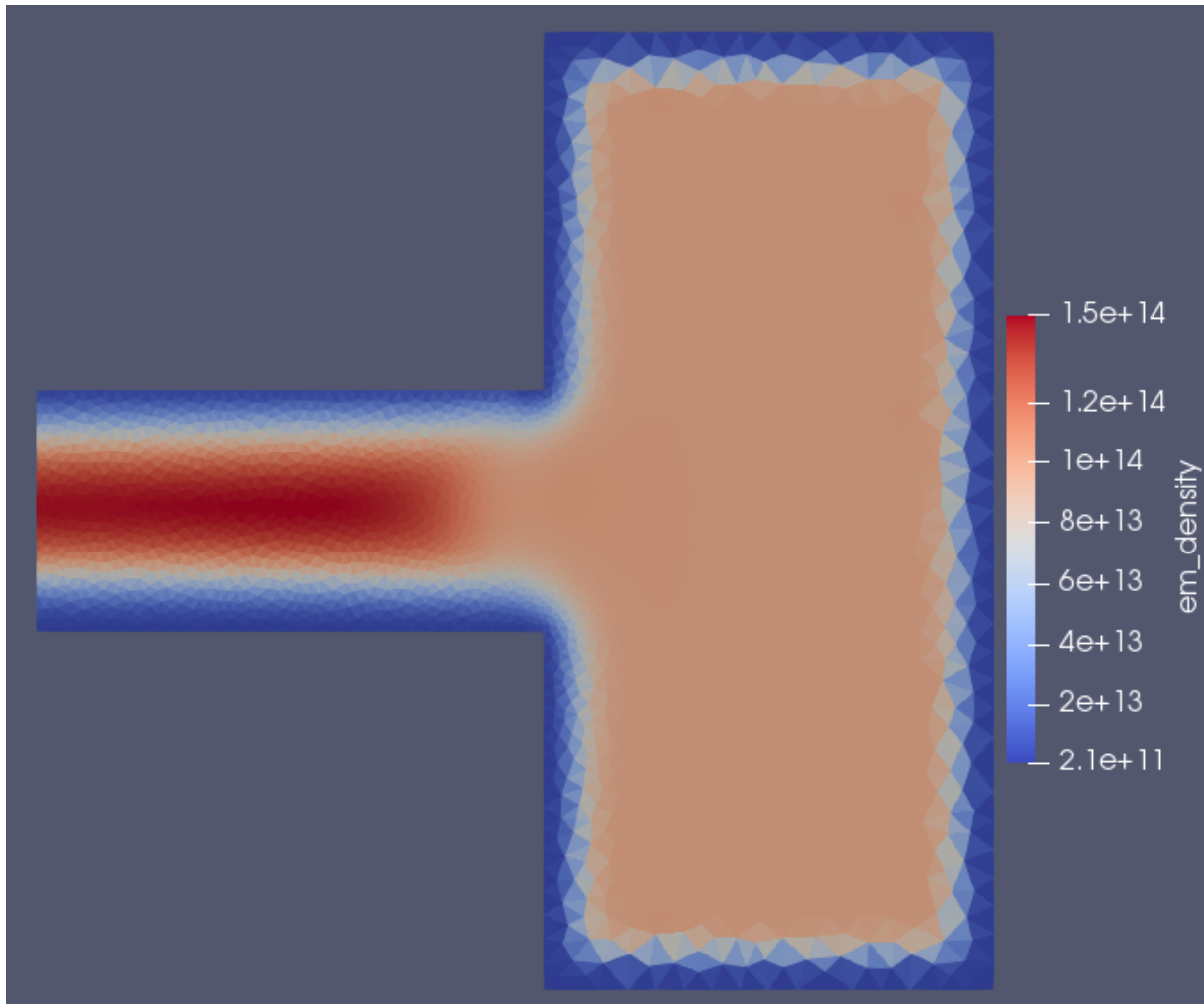


## Top Boundary

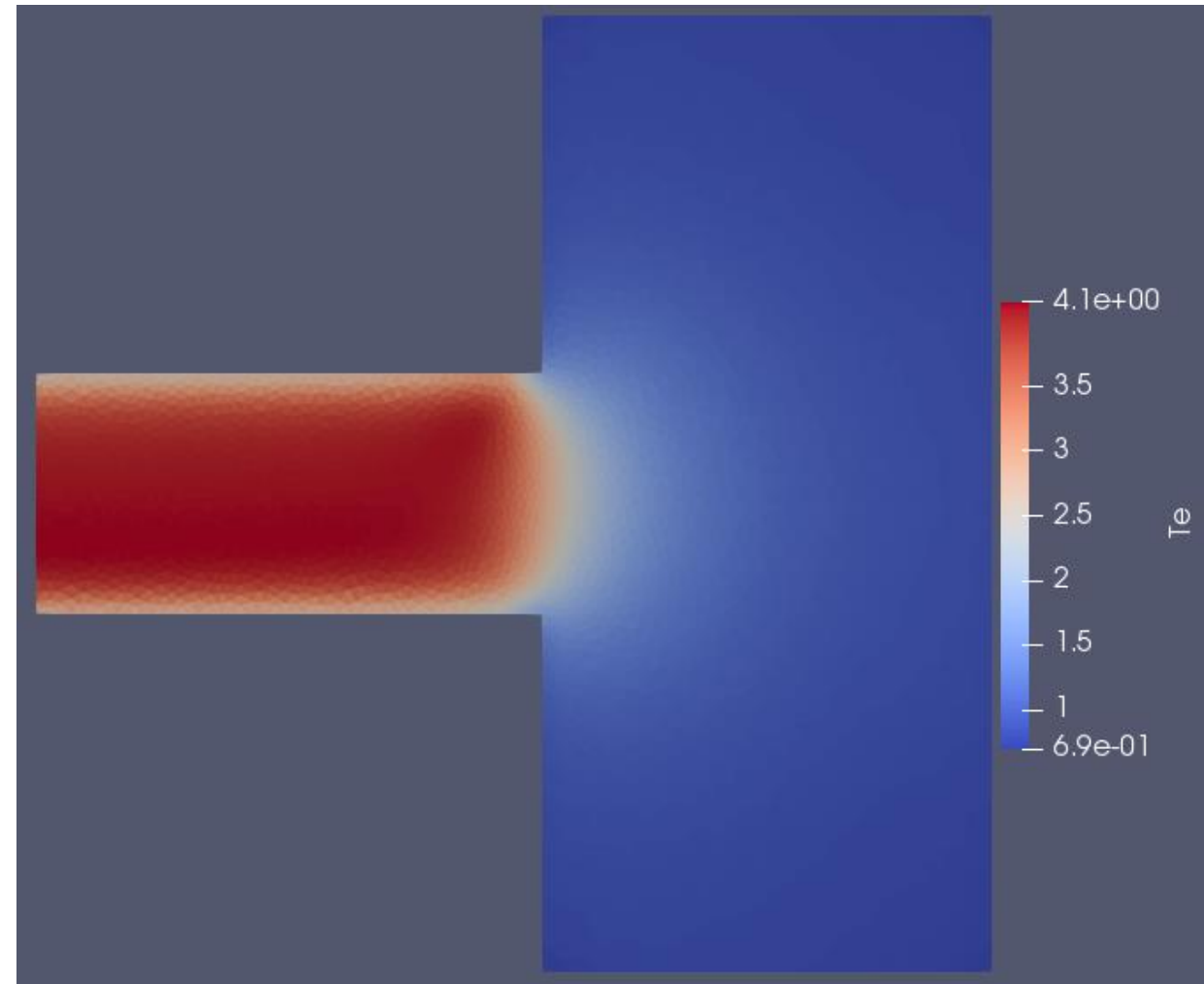


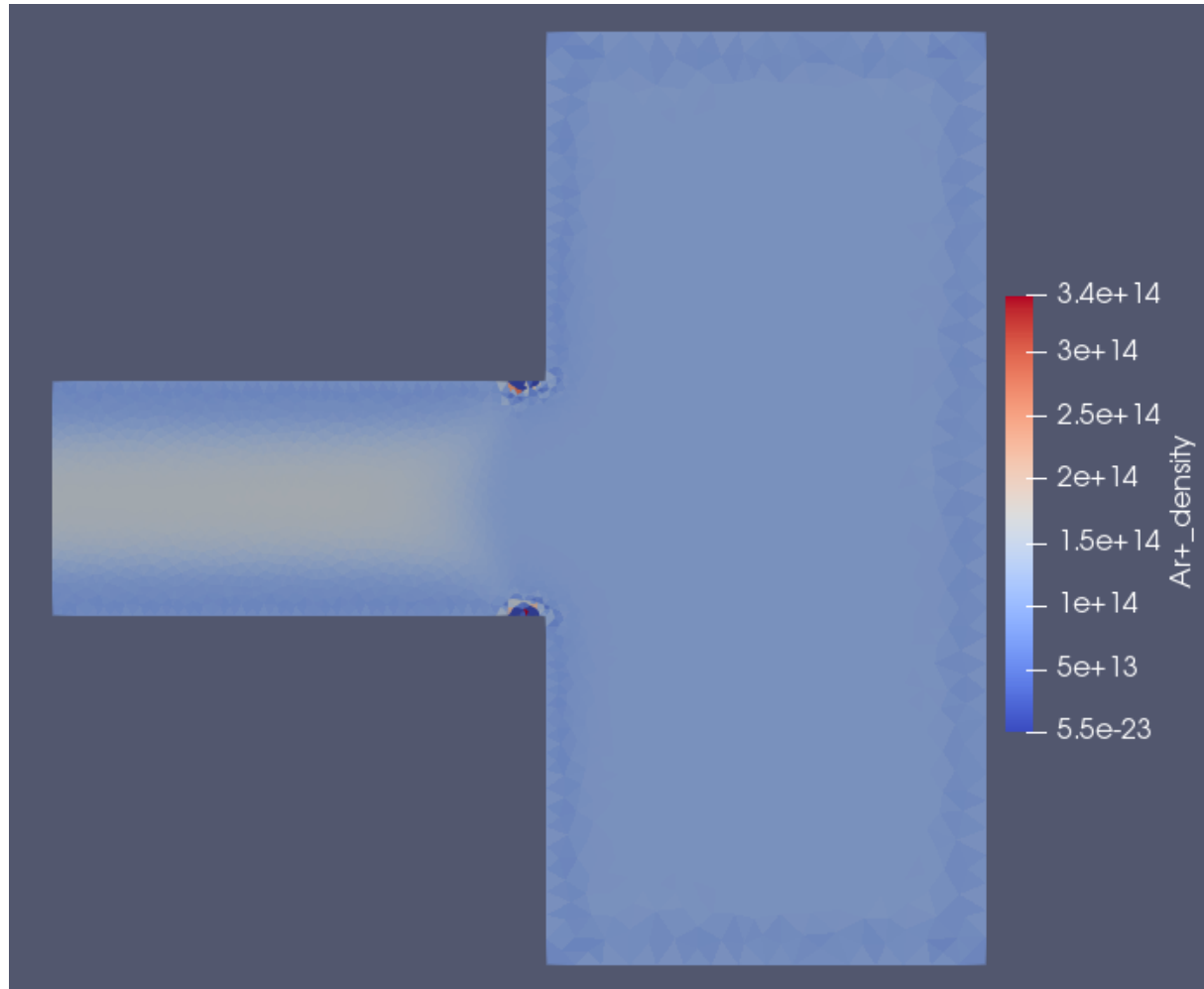
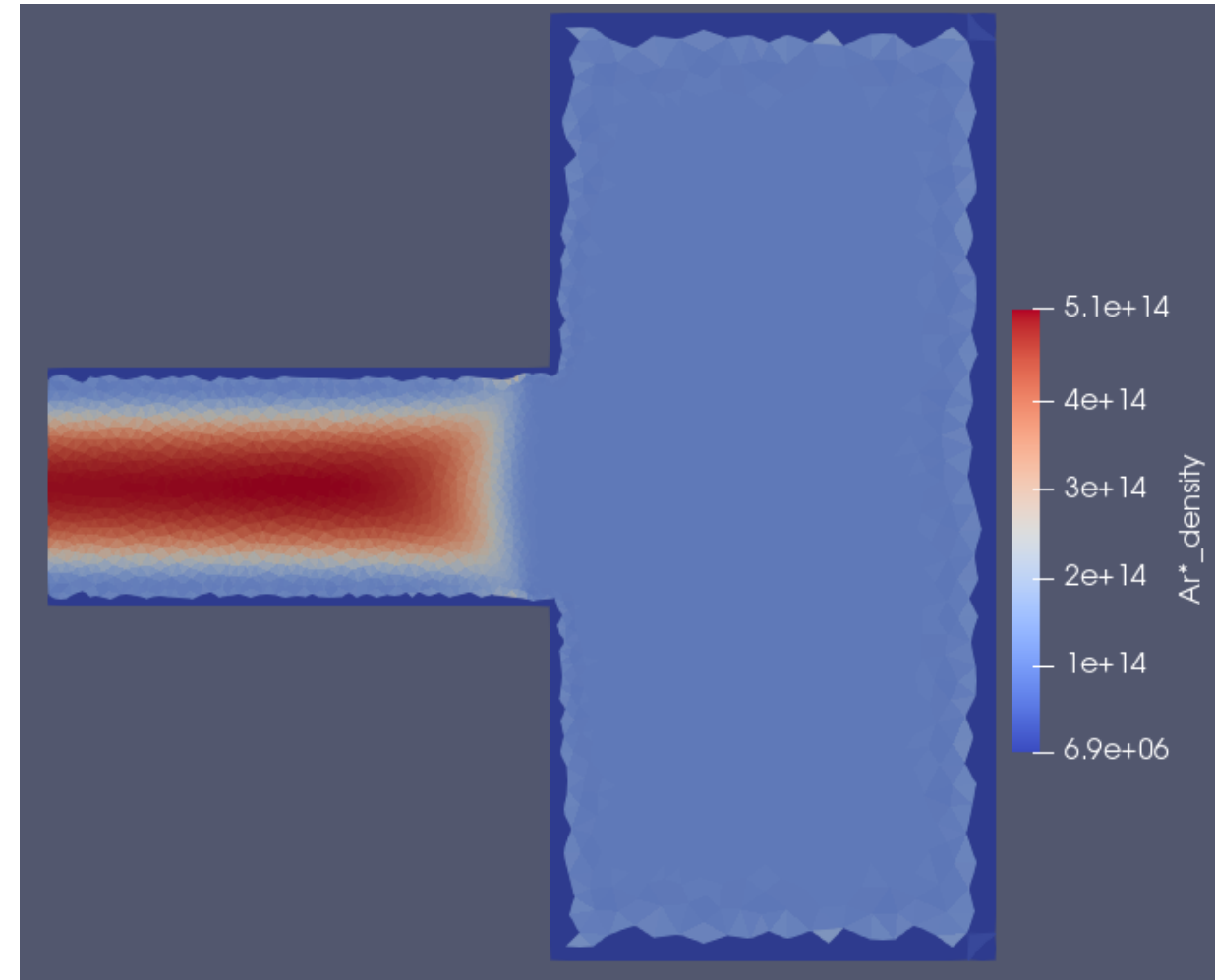
# Results for Rearranged BC / Actions / Coarse Mesh

**Potential [V]****Ion Potential [V]**

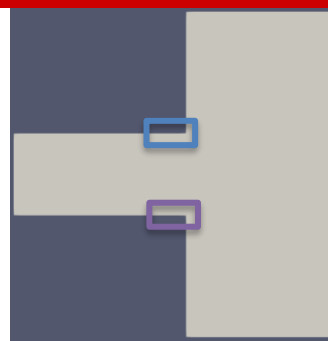
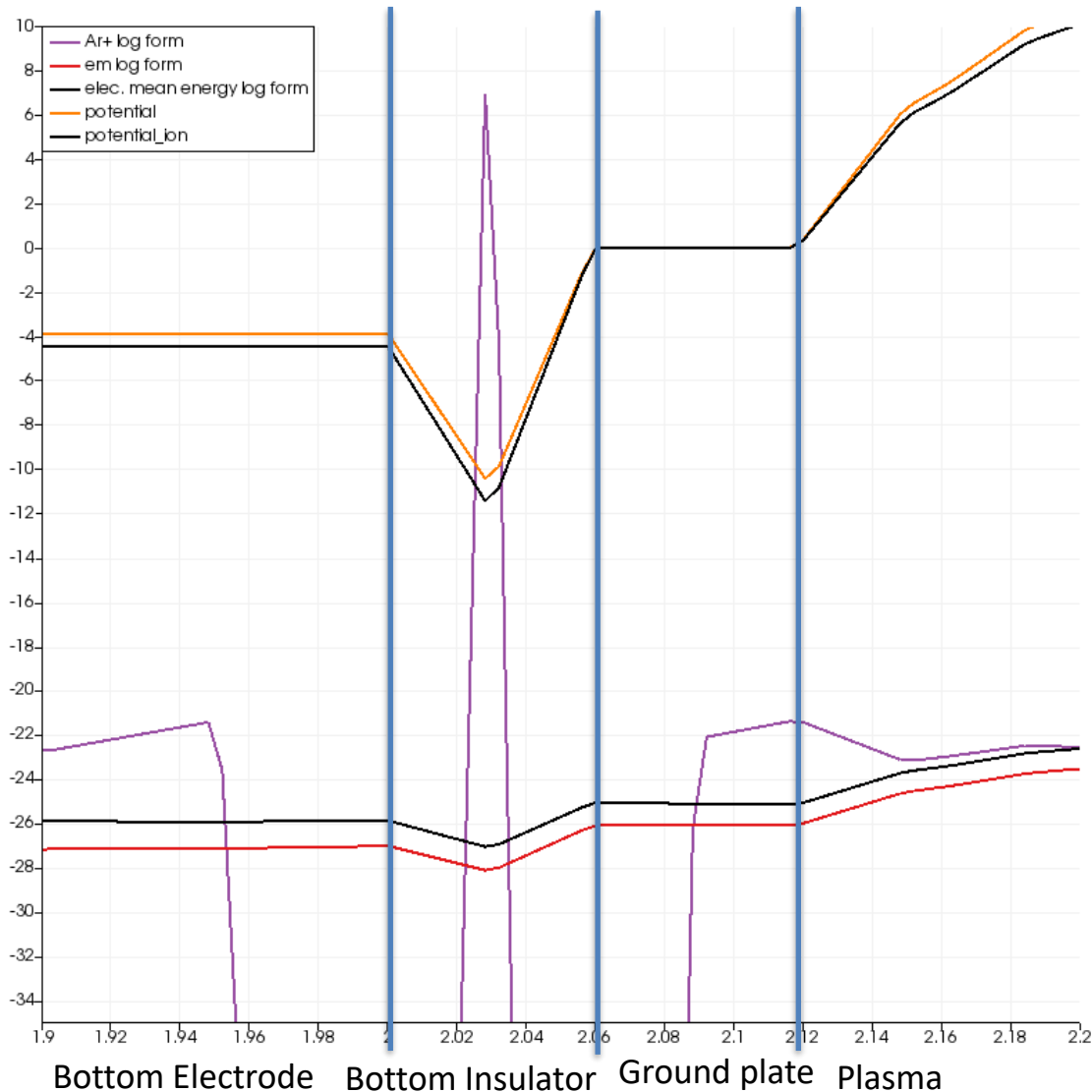
Electron Density [ $\text{m}^3$ ]

Electron Temperature [V]

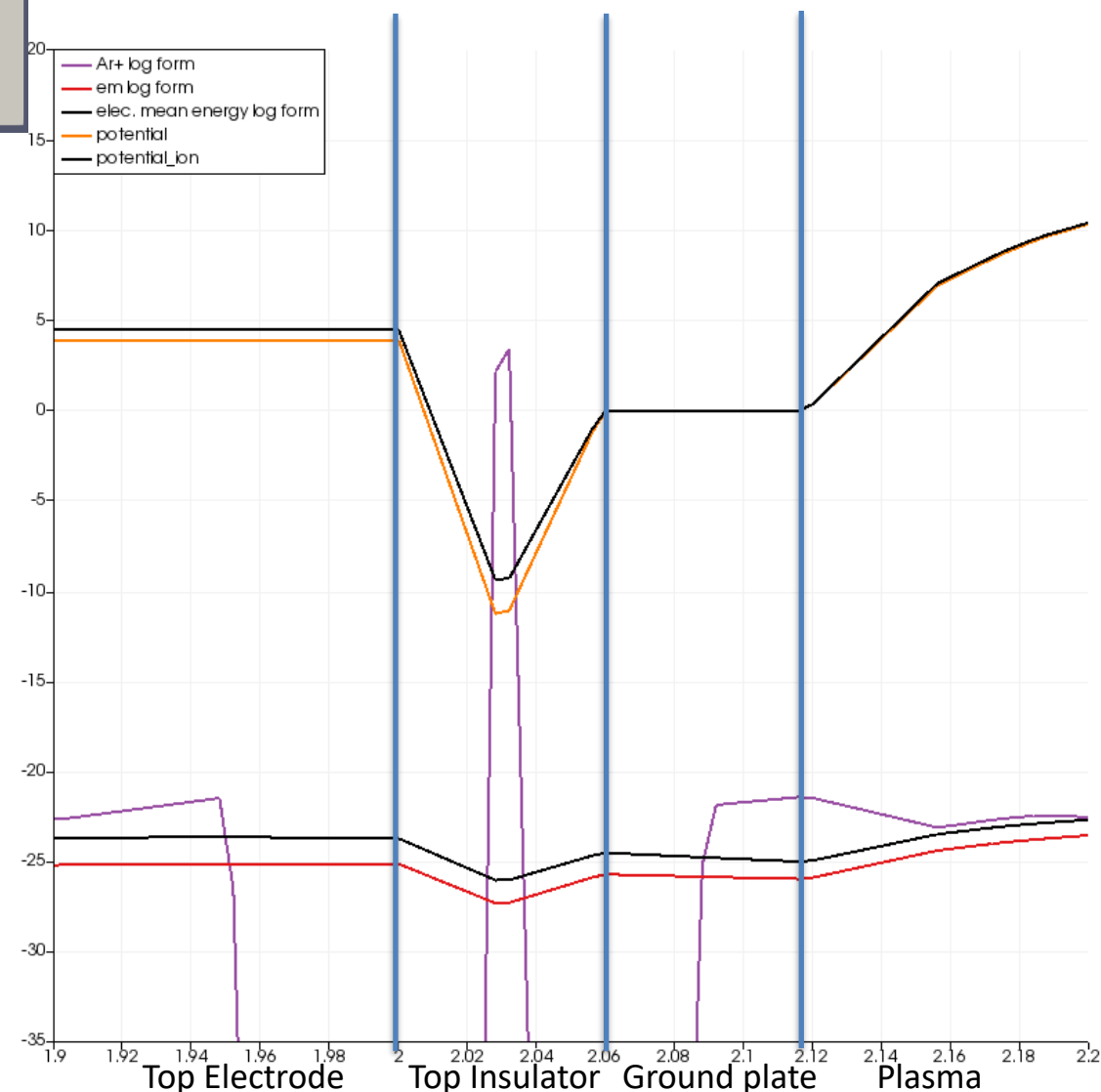


Ion Density [ $\text{m}^3$ ]Metastable Density [ $\text{m}^3$ ]

## Bottom Boundary



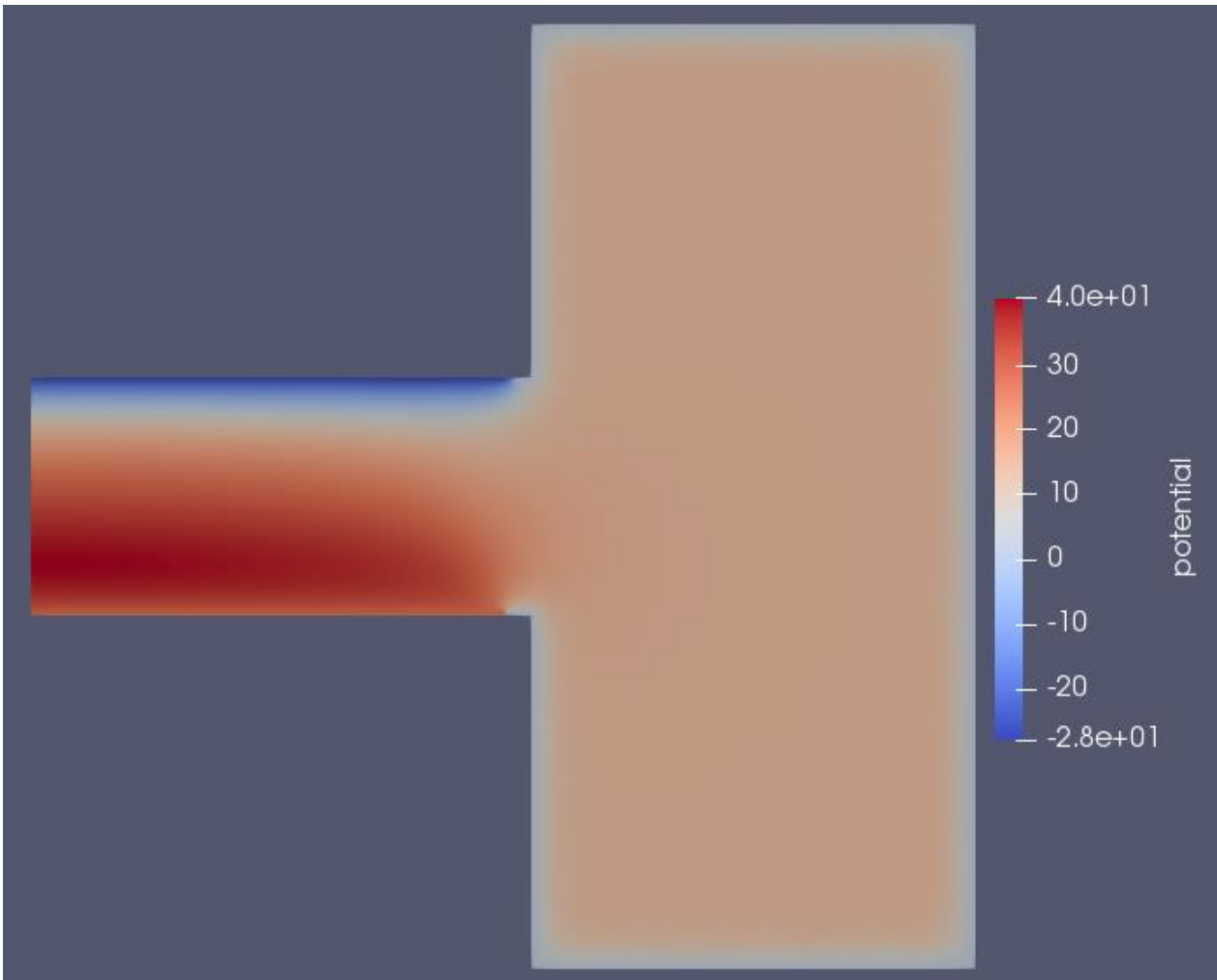
## Top Boundary



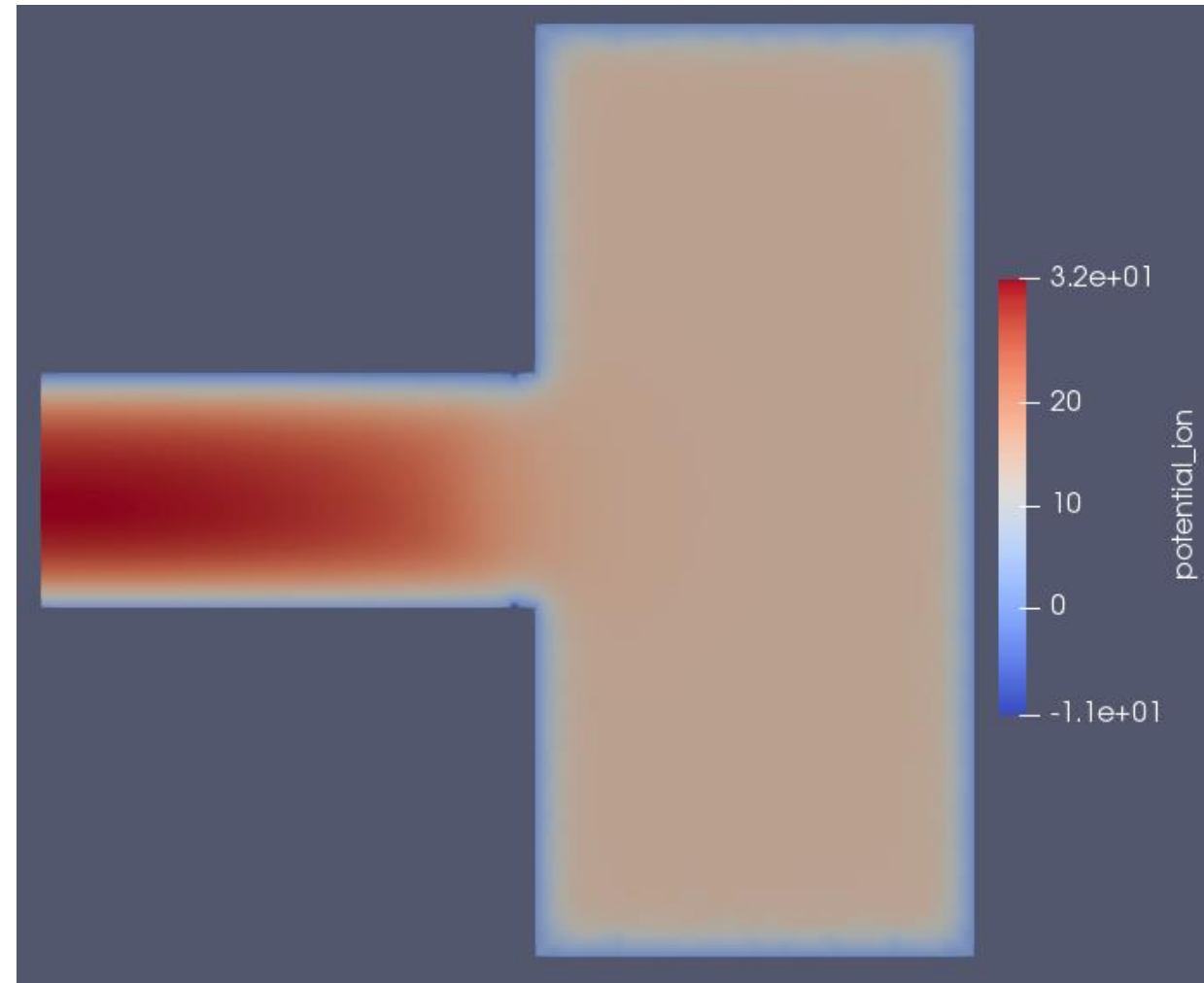


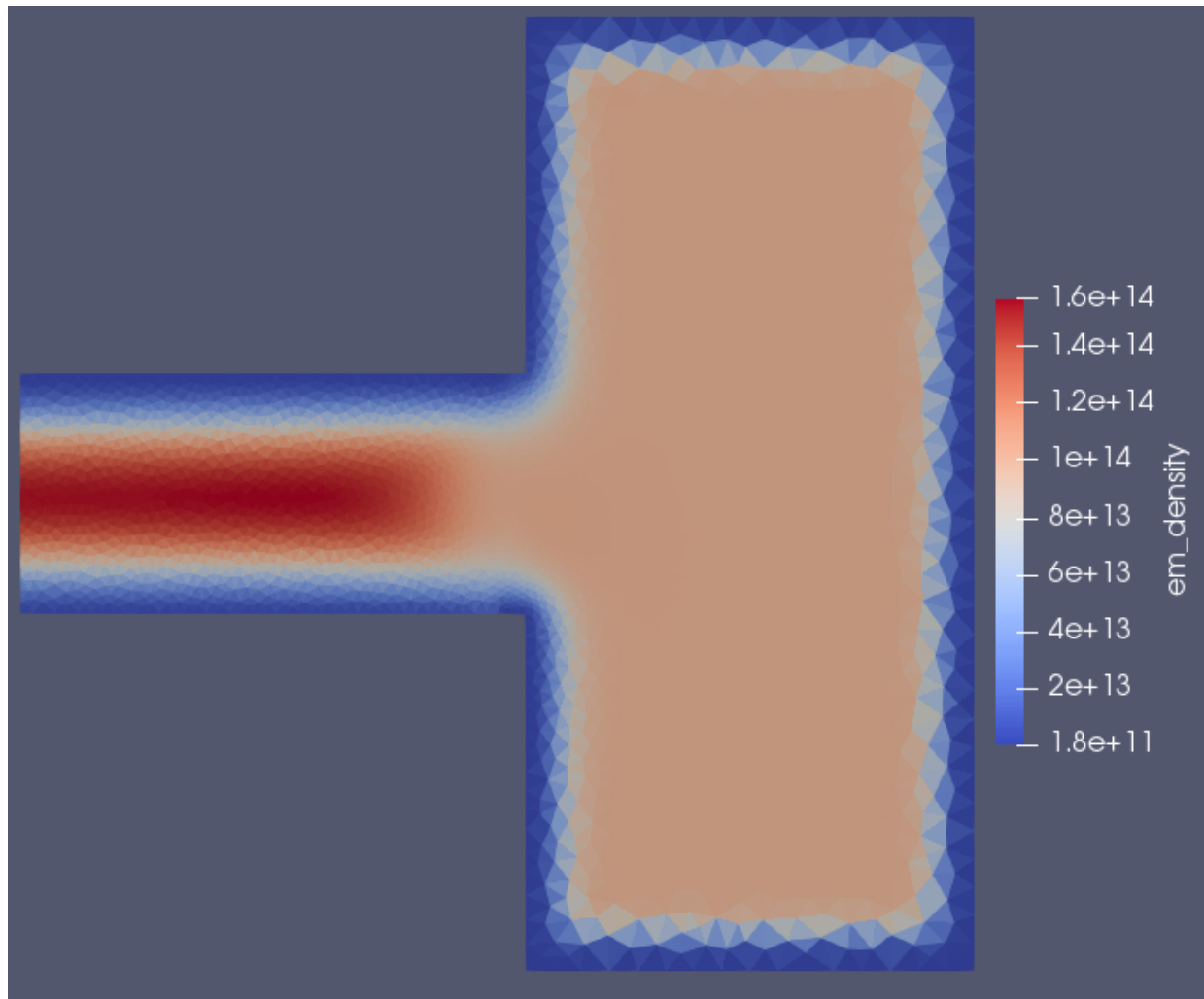
# **Results for Rearranged BC / Actions / No Dimensional Scaling Coarse Mesh**

Potential [V]

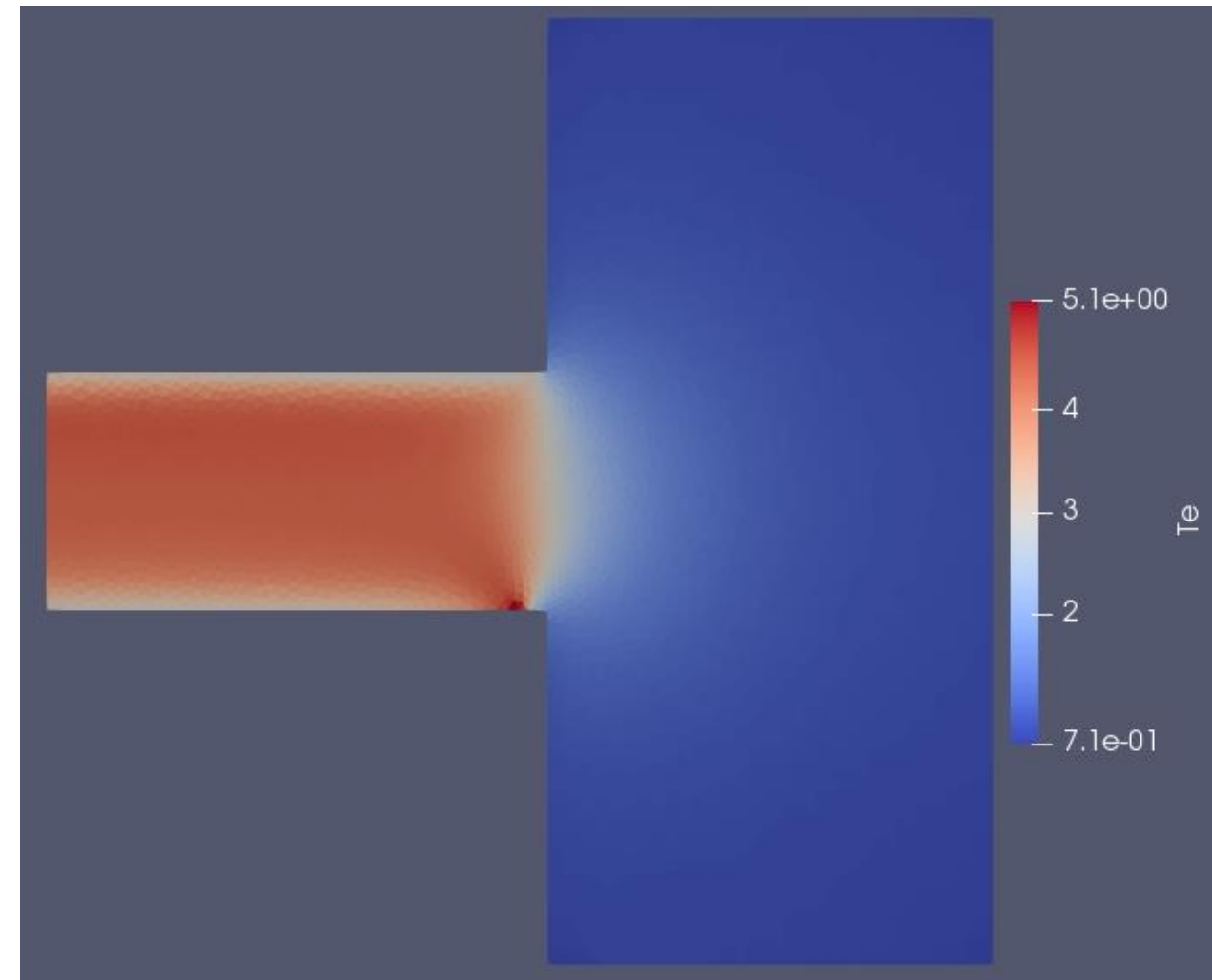


Ion Potential [V]

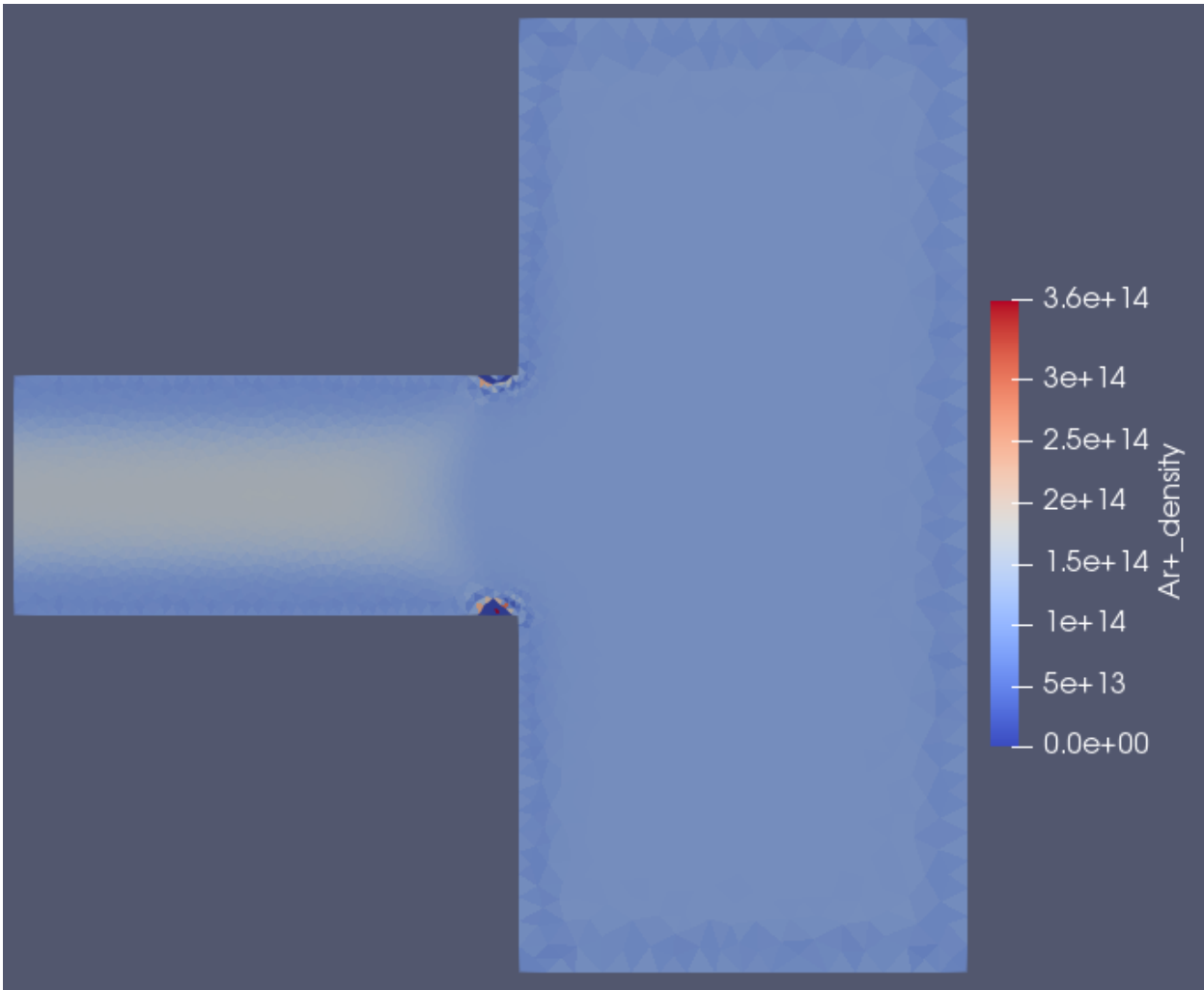


Electron Density [ $\text{m}^3$ ]

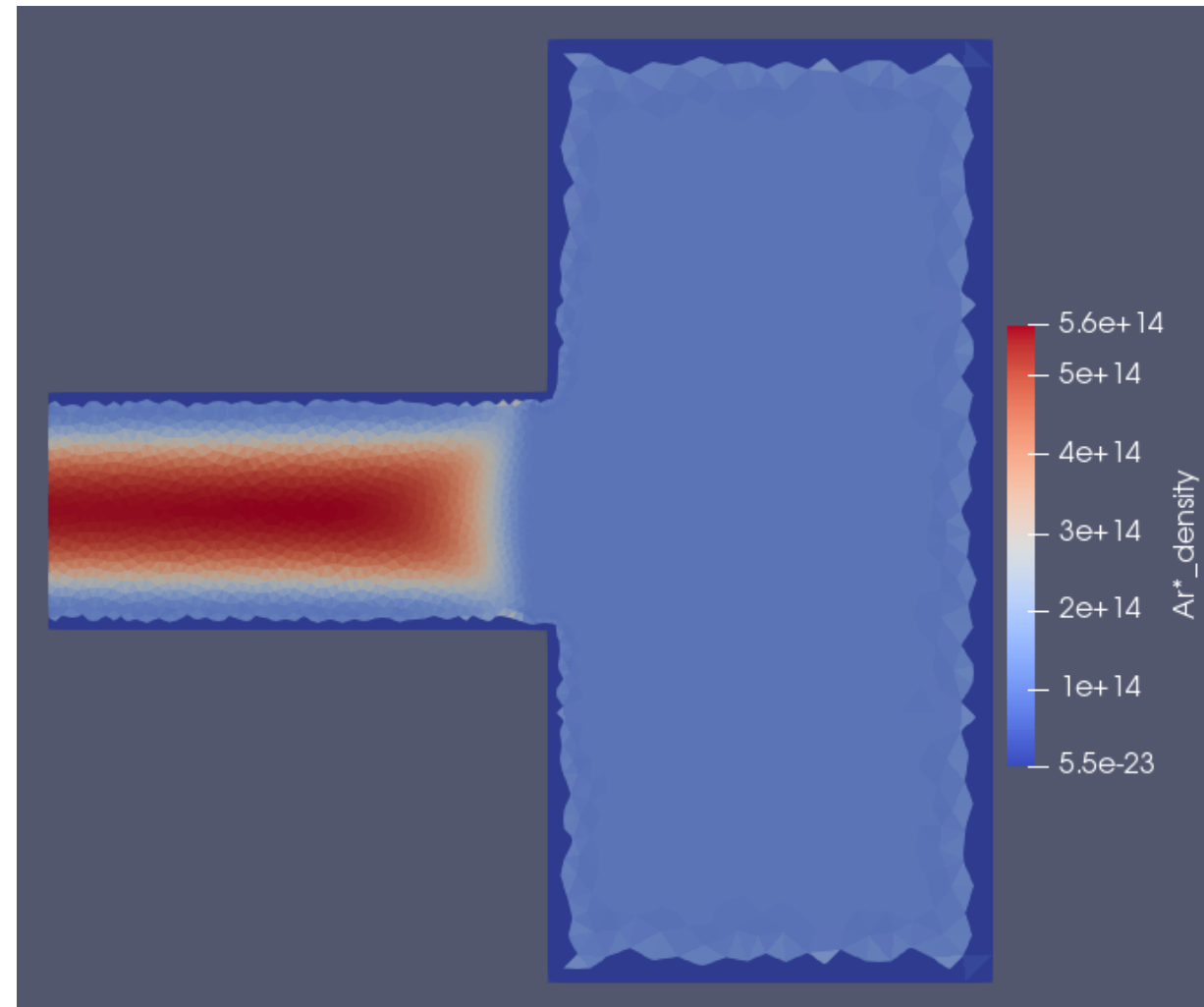
Electron Temperature [V]



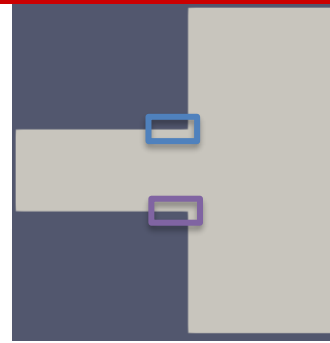
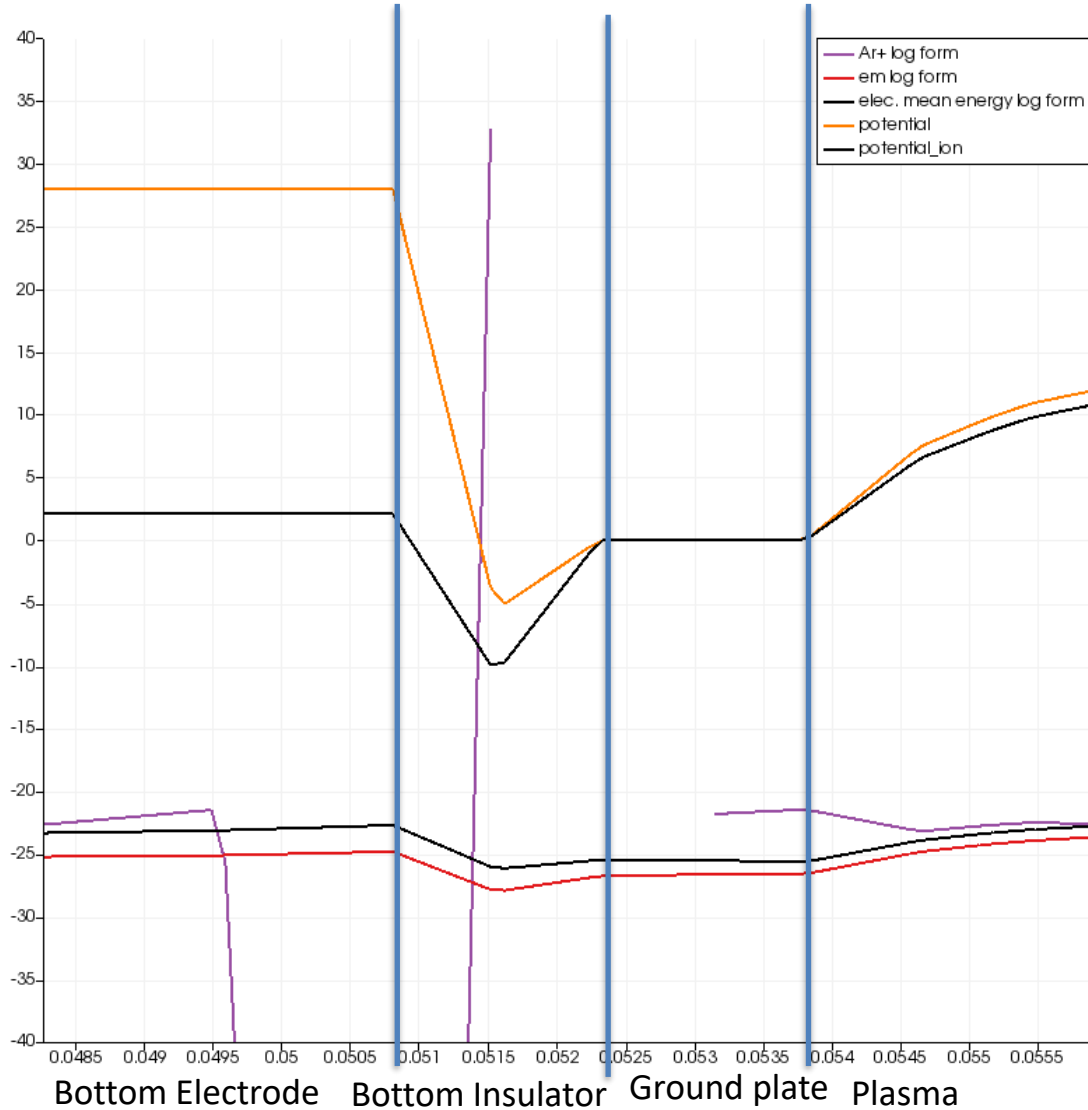
**Ion Density [ $m^3$ ]**



**Metastable Density [ $m^3$ ]**



## Bottom Boundary



## Top Boundary

