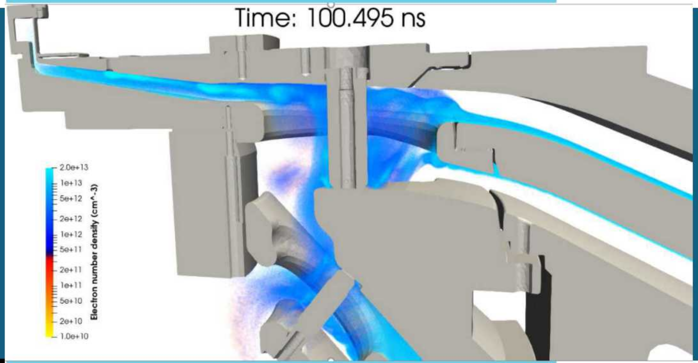
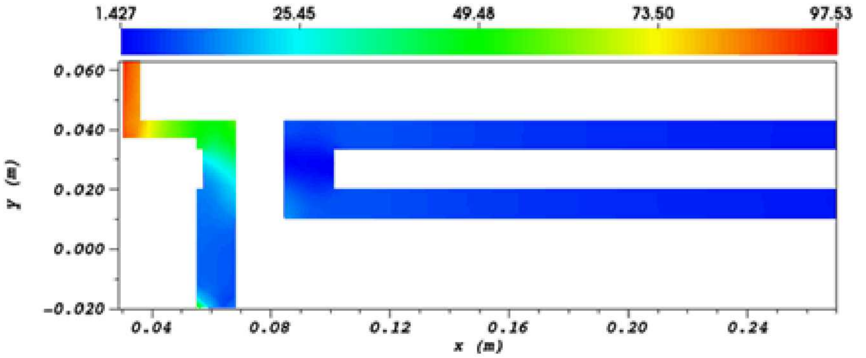
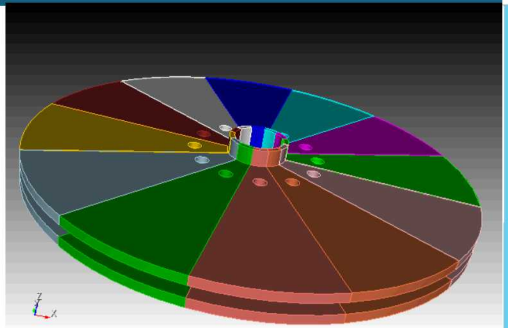
SAND2020-7978C

Powerflow modeling with EMPIRE







Presented by

D. Sirajuddin and M. Bettencourt

11th Workshop on Fundamental Science with Pulsed Power (ZFS) and User Meeting

August 3rd, 2020 at Sandia National Laboratories, Albuquerque, NM, USA

Requirements for full physics power flow simulations

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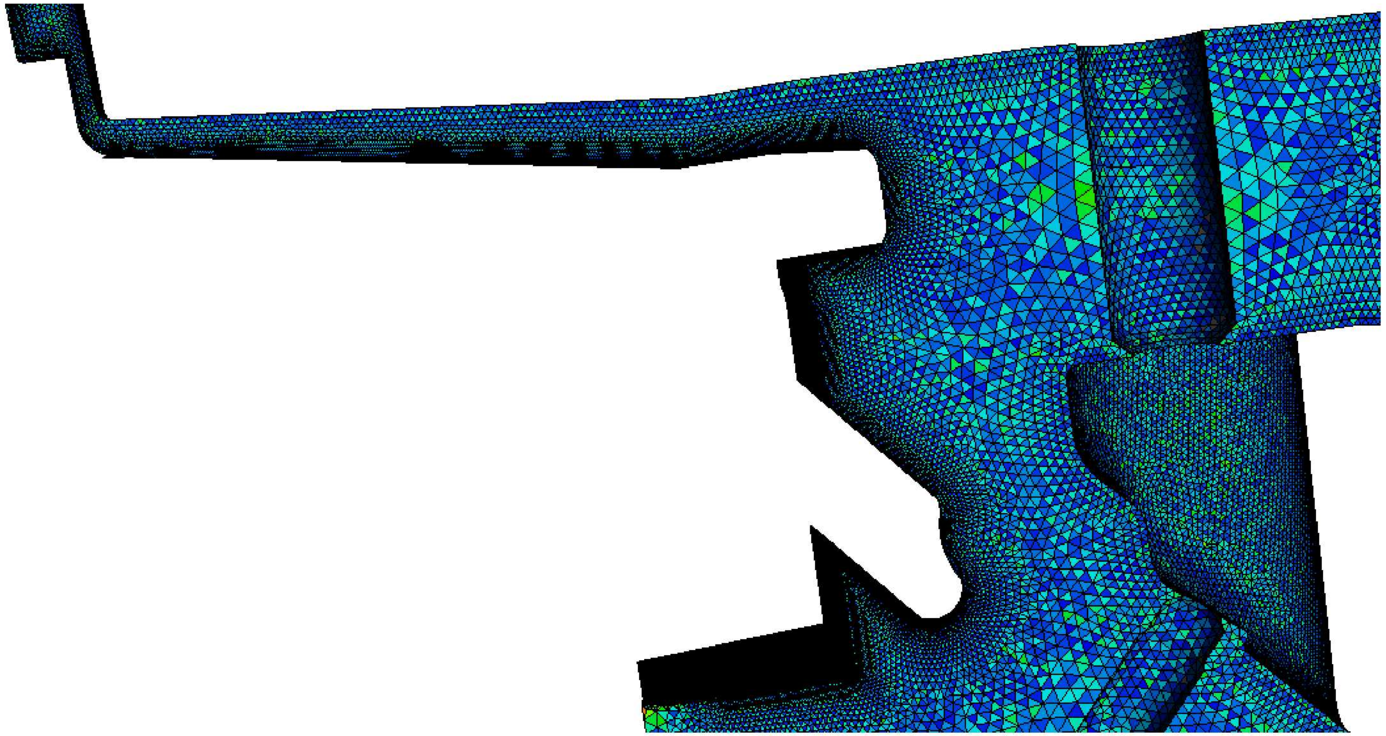
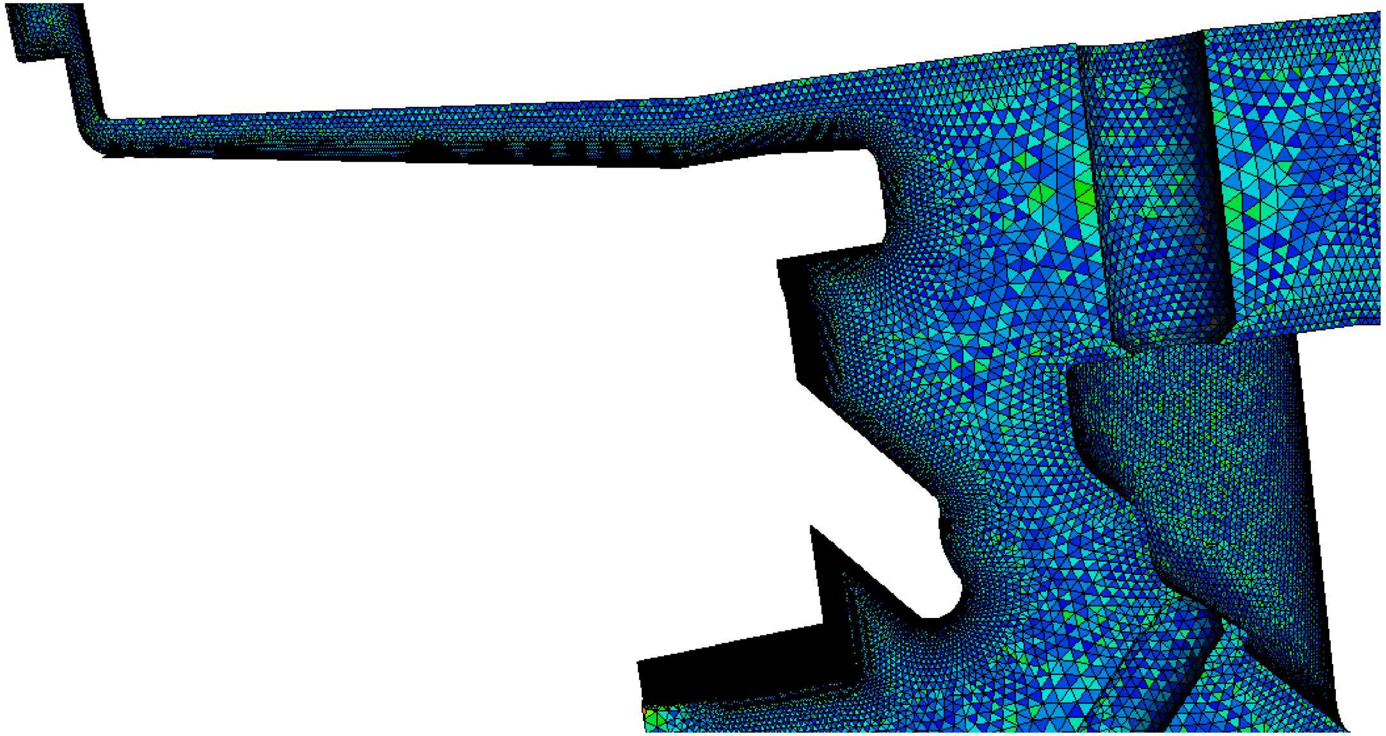
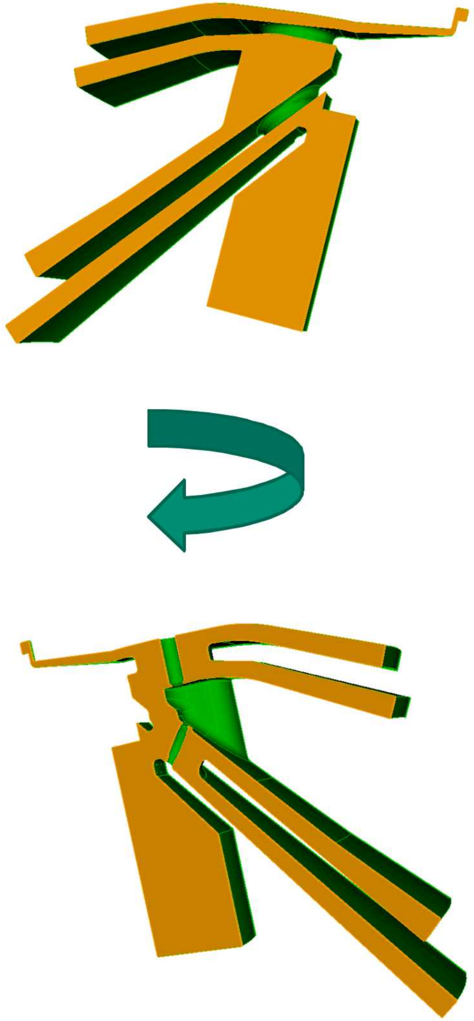
- Electromagnetics described on complex geometries



Requirements for full physics power flow simulations

- Electromagnetics described on complex geometries
- Symmetry boundary capabilities → reduced sim domain





Requirements for full physics power flow simulations

- Electromagnetics described on complex geometries
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- Relativistic particle dynamics

Requirements for full physics power flow simulations

- Electromagnetics described on complex geometries
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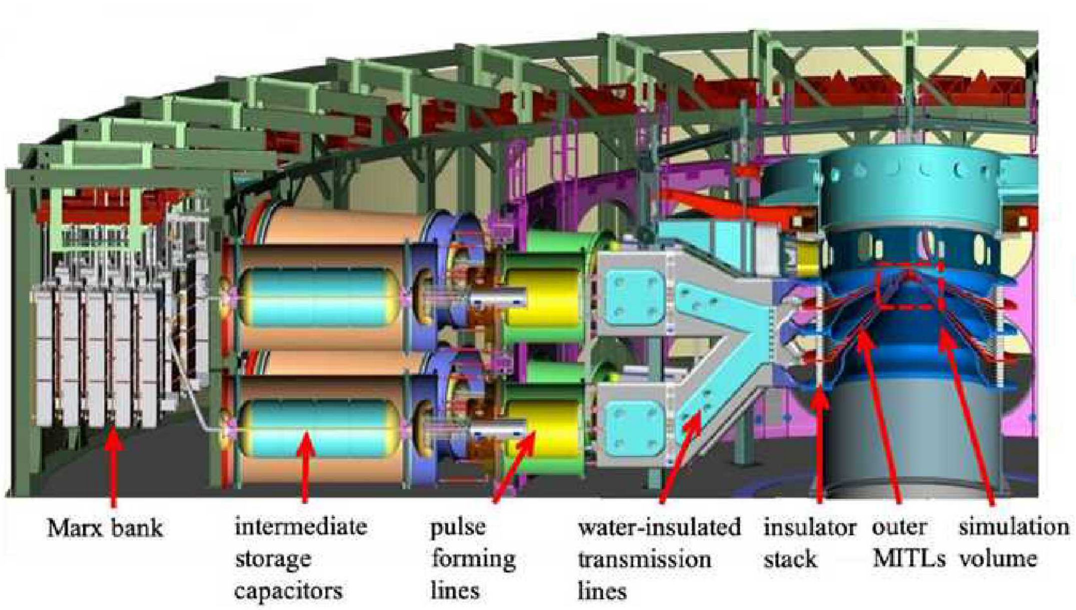
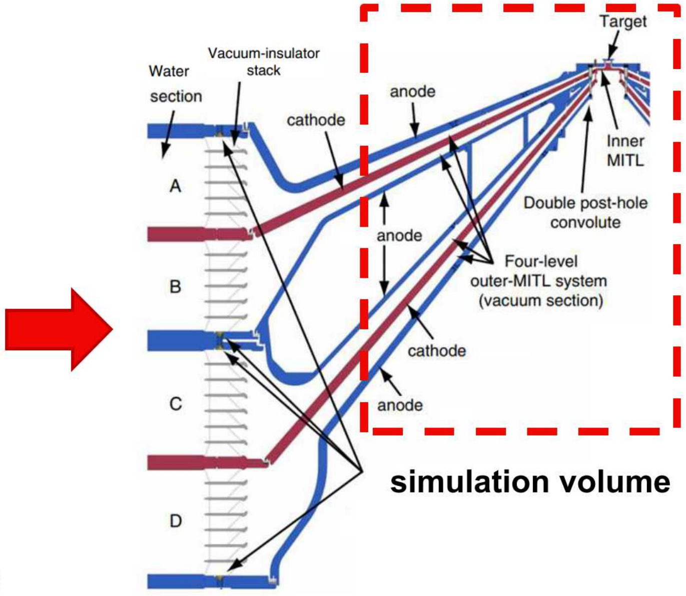
- Relativistic particle dynamics
- 1D Transmission line coupling for end-to-(almost)end simulations





Figures: E. Waisman et al., Phys. Rev. ST Accel. Beams, Vol. 17, 120401, (2014)

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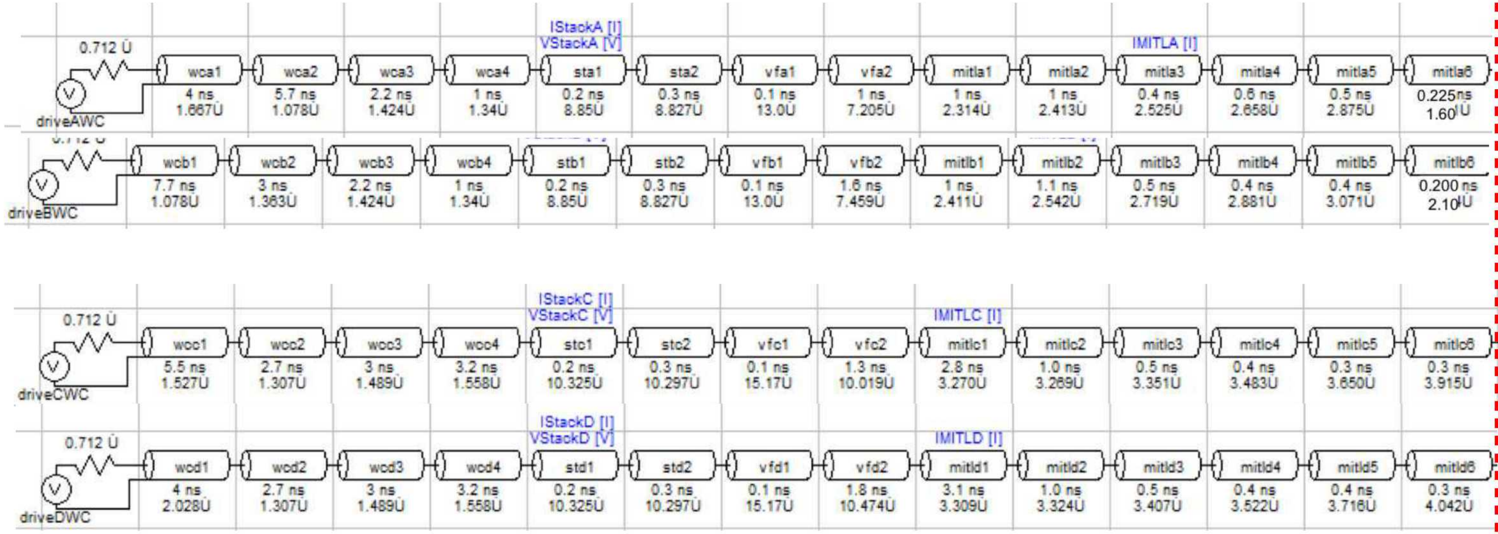
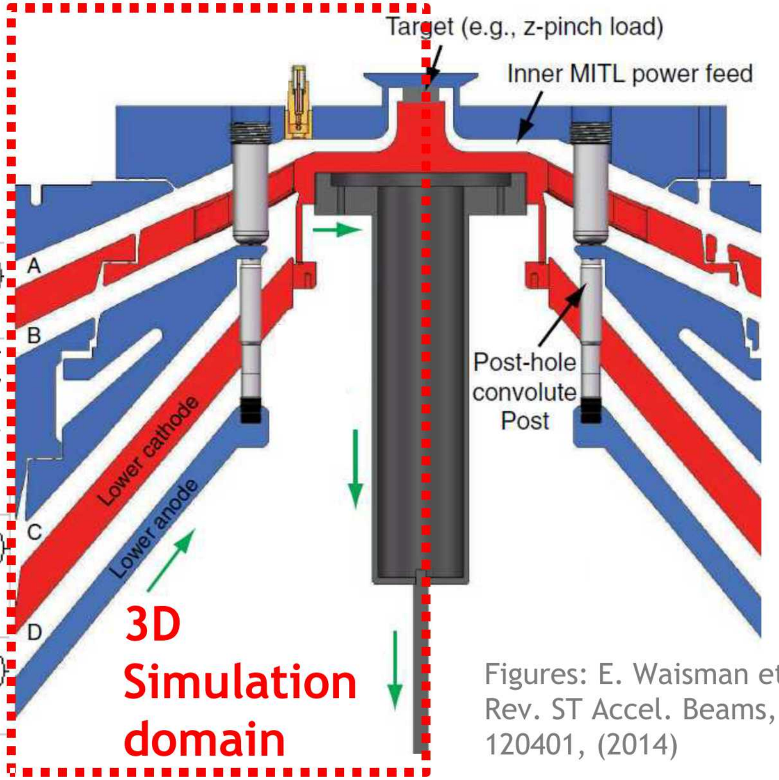
1D BERTHA circuit models (B. Hutsel)





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Requirements for full physics power flow simulations

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  - Emission:
    - Field-emitted electrons ~ 10^{13} cm^{-3} (> 200 kV/cm threshold)

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    - ❑ Field-emitted electrons ~ 10^{13} cm^{-3} (> 200 kV/cm threshold)
    - ❑ H_2O → $3e^-$ + $2H^+$ + O^+ plasma emission from cathodes and anodes

$$\frac{d\theta}{dt} = -k_0(T)\theta(t)e^{-\frac{E\prime}{k_B T}}$$

Polyani-Wigner rate

$$E'(\theta) = E_d(1 - \alpha\theta)$$

Temkin isotherm

Fitted parameters from TPD experiments (GCLDRD desorption thrust: S. Simpson et al)

Requirements for full physics power flow simulations

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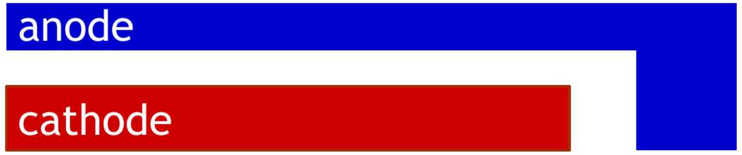
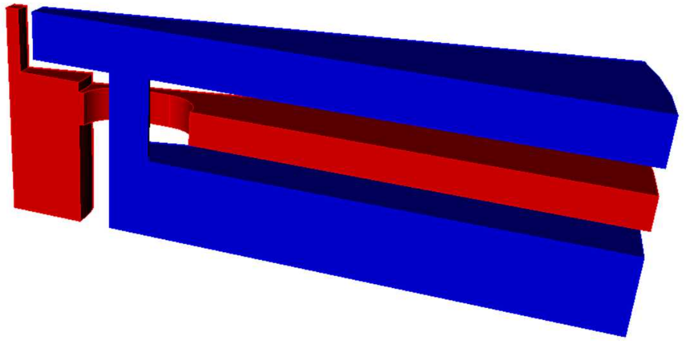
    - Field-emitted electrons ~ 10^{13} cm^{-3} (> 200 kV/cm threshold)
    - H_2O → $3e^- + 2H^+ + O^+$ plasma emission from cathodes and anodes
  - Heating:
    - Ohmic (EM wave propagation)
    - Particle fluxes impacting surfaces ("dE/dx" heating)

Powerflow model building has benefited from pushing tests for each physics module through a pipeline of increasingly complex MITL systems

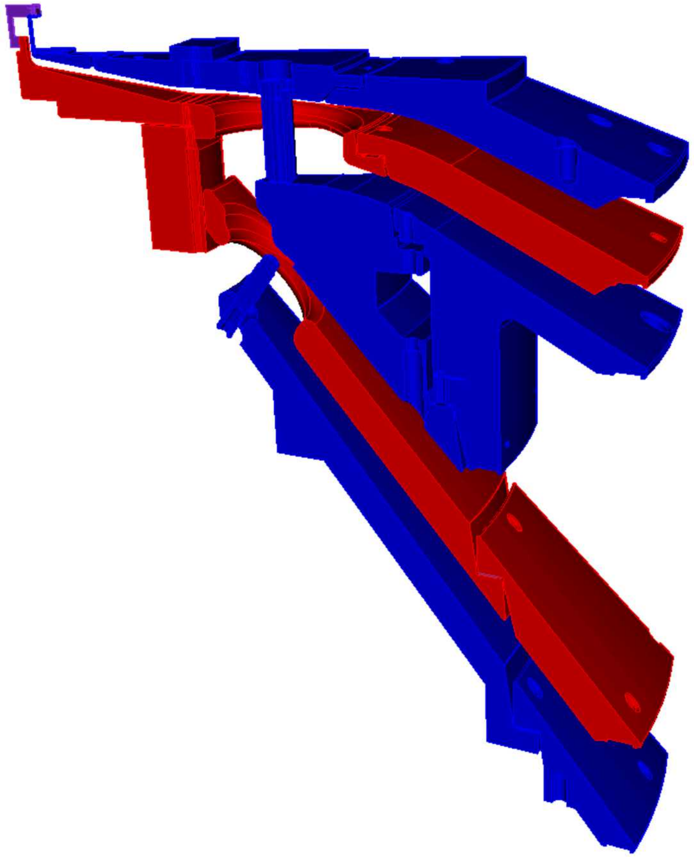
(2D) planar MITL



(3D) Half-o-lute



(3D) Powerflow 18a



Idealized single MITL geometry

"Half" of an idealized convolute geometry

Full geometry

Increasing complexity

Powerflow model building has benefited from pushing tests for each physics module through a pipeline of increasingly complex MITL systems

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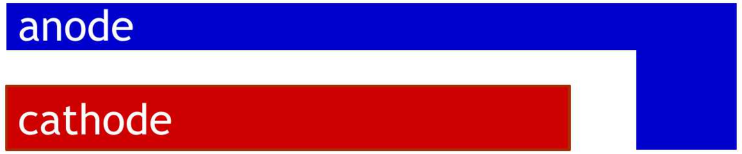

- Work by N. Hamlin, E. Evstati, K. Beckwith, A. Robinson, N. Bennett, N. Roberds

- **Verification successes:**
  - EM wave propagation: PECs, symmetry BCs
  - PIC SCL emission
  - Thermal desorption models
  - Combined physics: EM+SCL+desorp

UQ TPD: subject of following talk N. Hamlin

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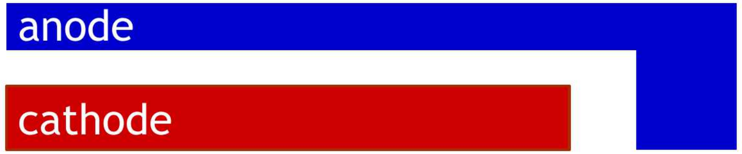

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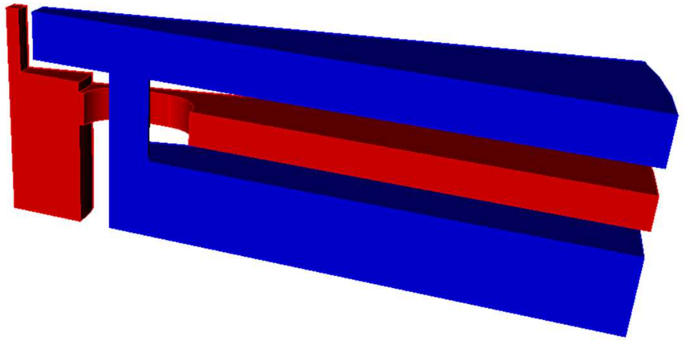

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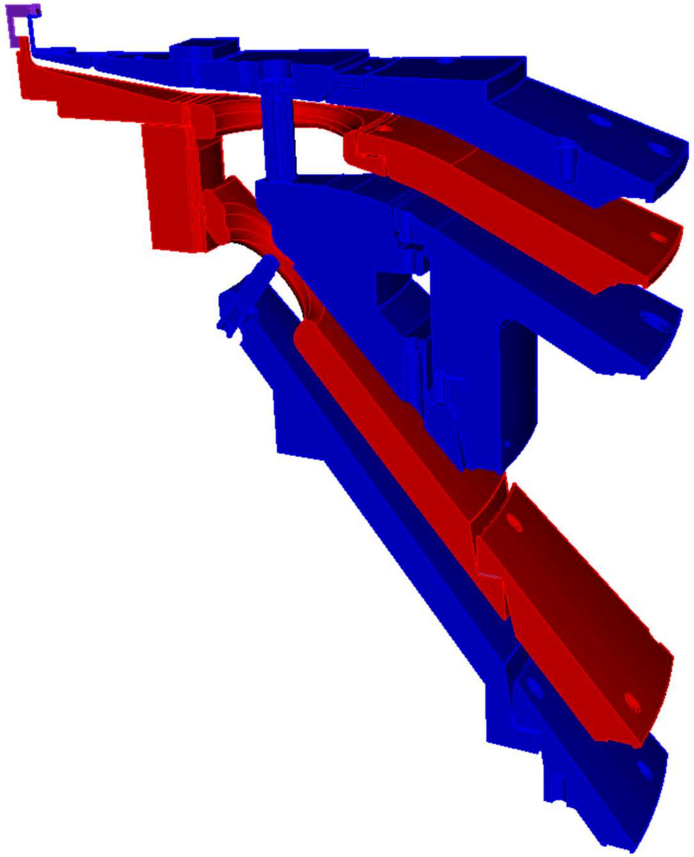

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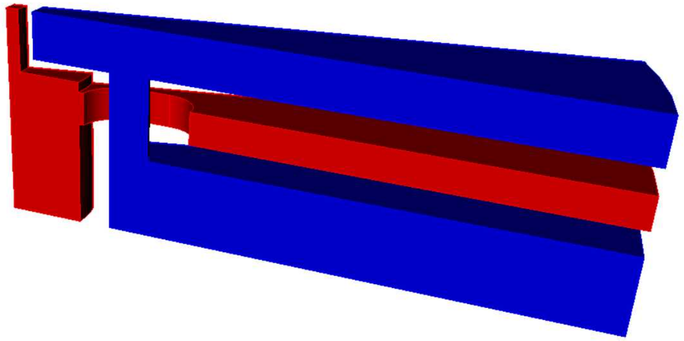


- EMPIRE and CHICAGO comparison work done by D. Sirajuddin, M. Bettencourt

- Full CHICAGO problem from D. Rose, D. Welch

- **Verification successes:**
  - EM wave propagation
  - Transmission line verification with static BERTHA model

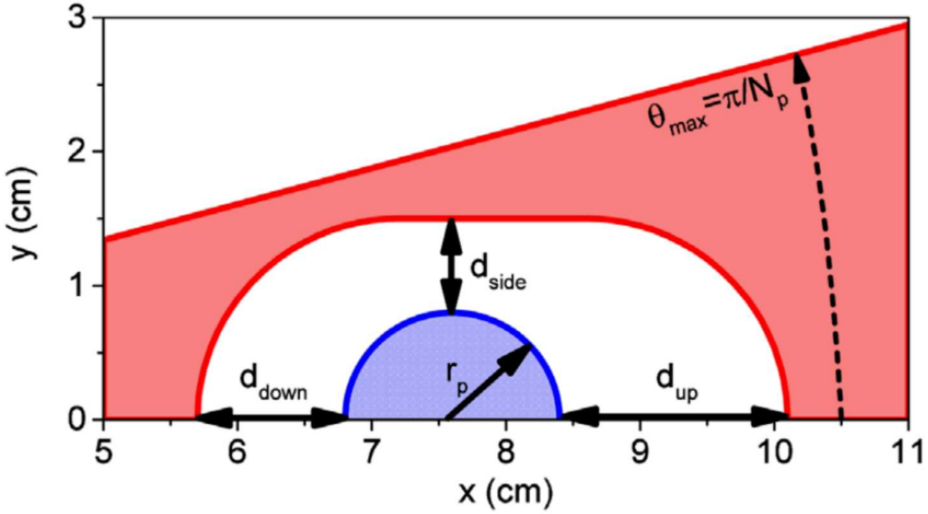
- **WIP**: SCL electron emission, UQ TPD

"Half" of an idealized convolute geometry

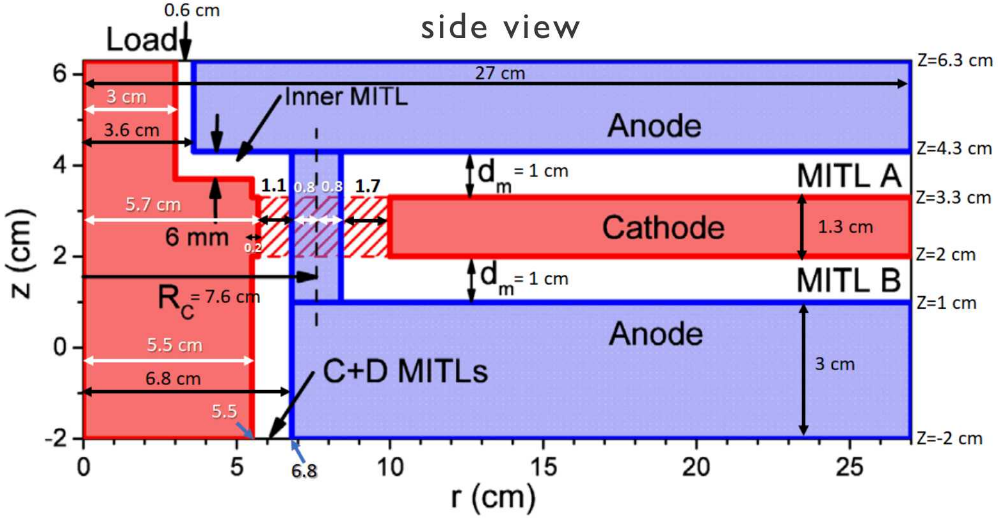
Increasing complexity

(Half-o-lute) geometry and tet mesh creation through cubit

top view



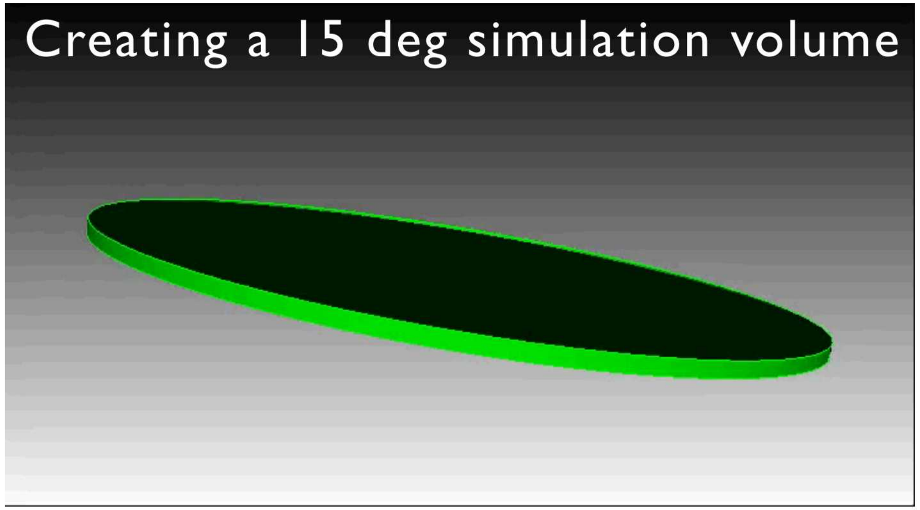
side view



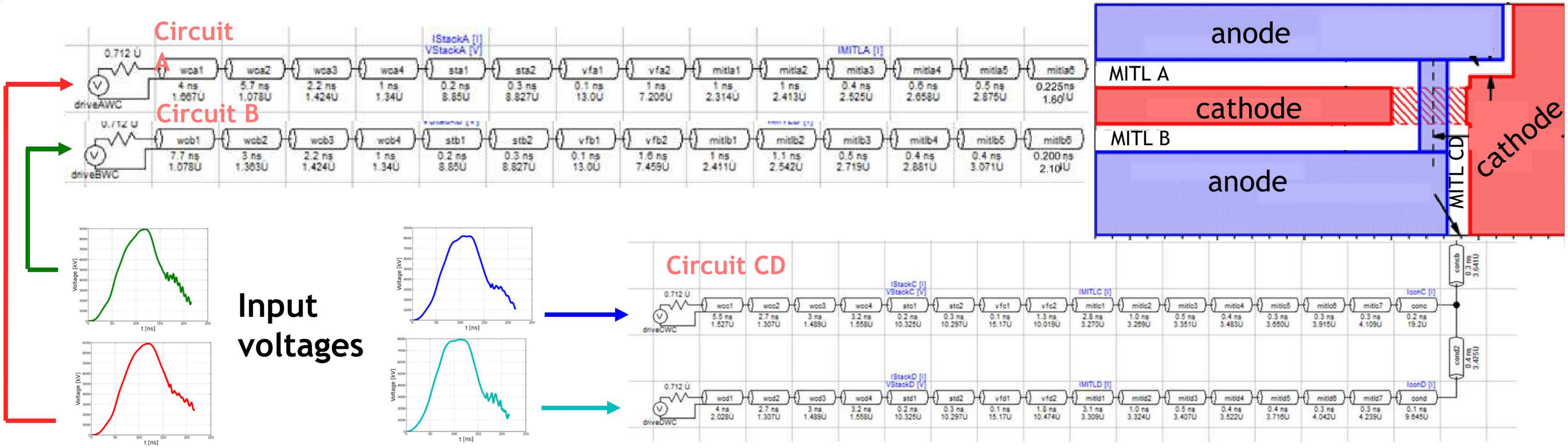
Figures: D. V. Rose, E. A. Madrid, D. R. Welch, R. E. Clark, C. B. Mostrom, W. A. Stygar, and M. E. Cuneo Phys. Rev. ST Accel. Beams 18, 030402

Meshing parameterized with vvtest and aprepro

```
# import geometry (cub) file
open "halfolute-EM_--_geometry_in_mm.cub"

# -- Mesh settings
# -- -- scheme
vol all scheme tetmesh

# -- -- element size adaption (value of 1.0 is ~ uniform mesh)
vol all tetmesh growth_factor 1.0

# -- -- what "effort level" should the mesher strive to revaluate
#       connectivity to improve element quality during mesh generation?
#       (0 = none, 6 = maximum)
set tetmesher optimize level 6

# -- Run meshing algorithm in same units as cub file (mm)
vol all size {mesh_size * 1.0e3}
mesh vol all

# -- export genesis file in units of meters
transform mesh output scale 1e-3
set exodus netcdf4 off
set large exodus on
export mesh "halfolute-EM_--_{mesh_size}m-mesh.gen" dimension 3 block 1 overwrite
```



(Half-o-lute) Verifying EM+branched transmission line coupling



About Chicago-pic sim:

0.98 hours on cee-pp-ldrd01, 14 cpus

Mesh: 64,260 elements

Time: 180 ns at 6 ps steps

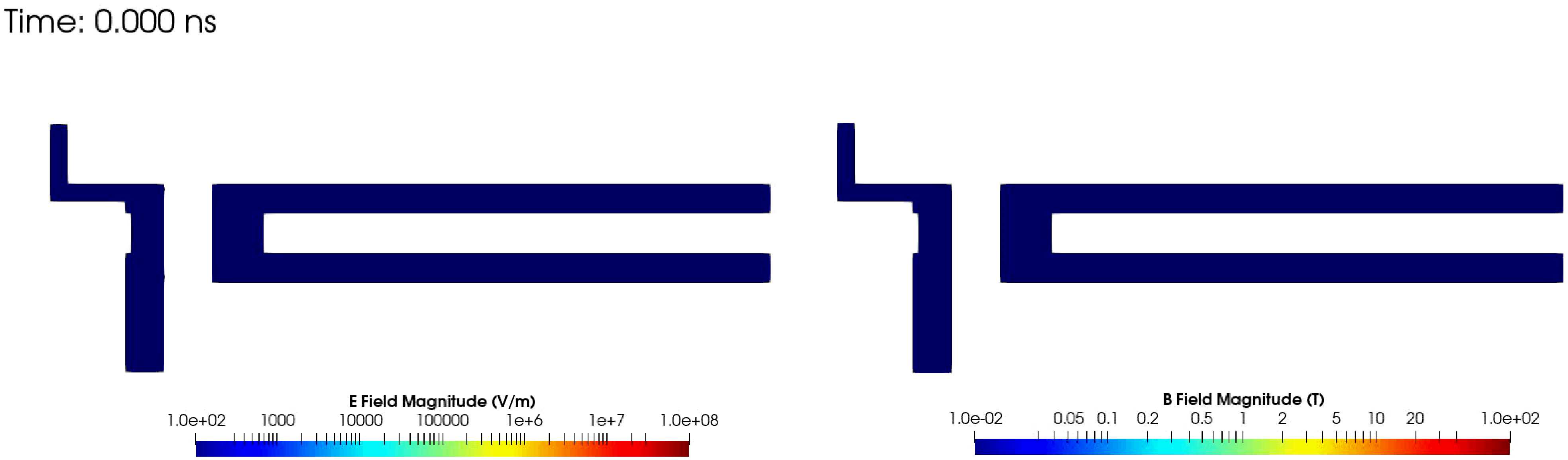
About empire-pic sim:

1.76 hours on cee-pp-ldrd01, 26 cpus

Mesh: 221,180 elements

Time: 180 ns at 6 ps steps

(Half-o-lute) Verifying EM+branched transmission line coupling



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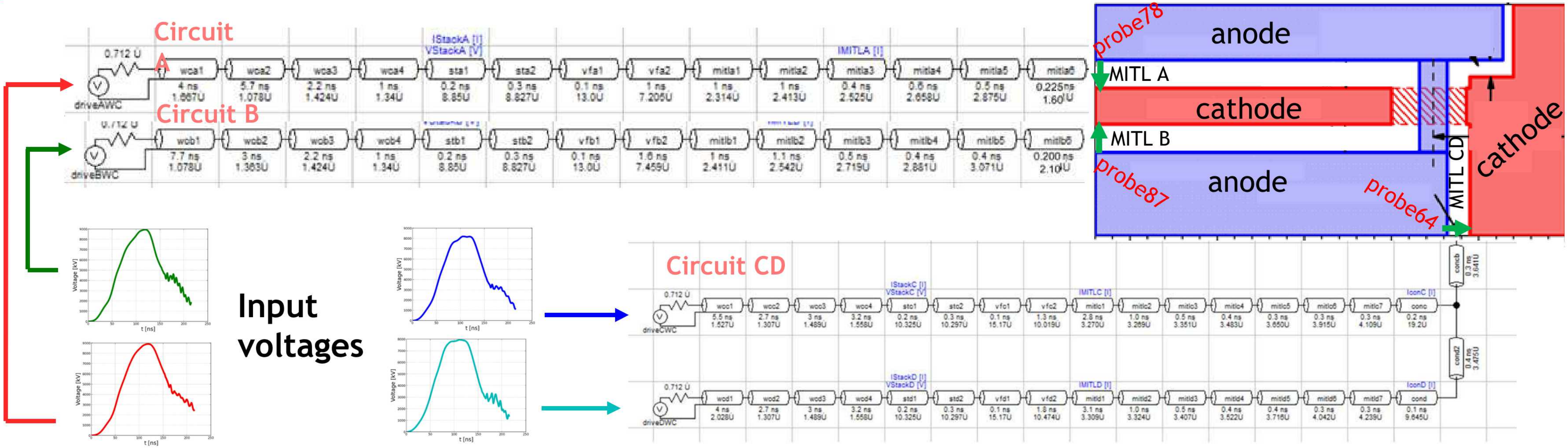
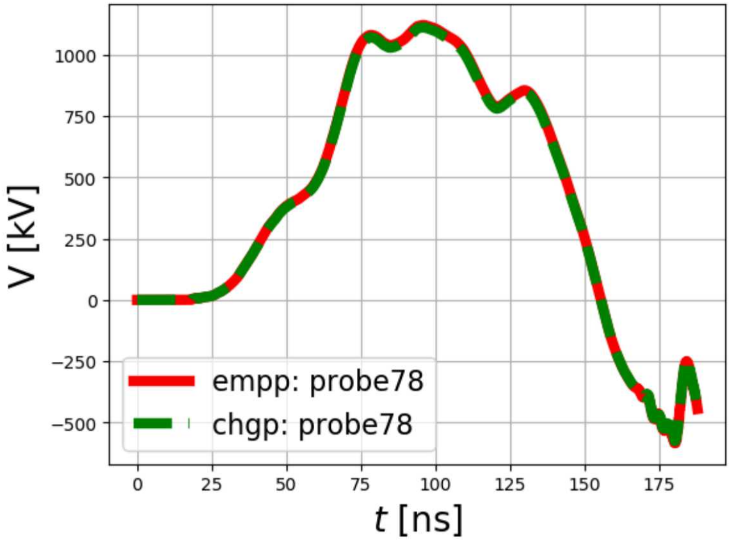
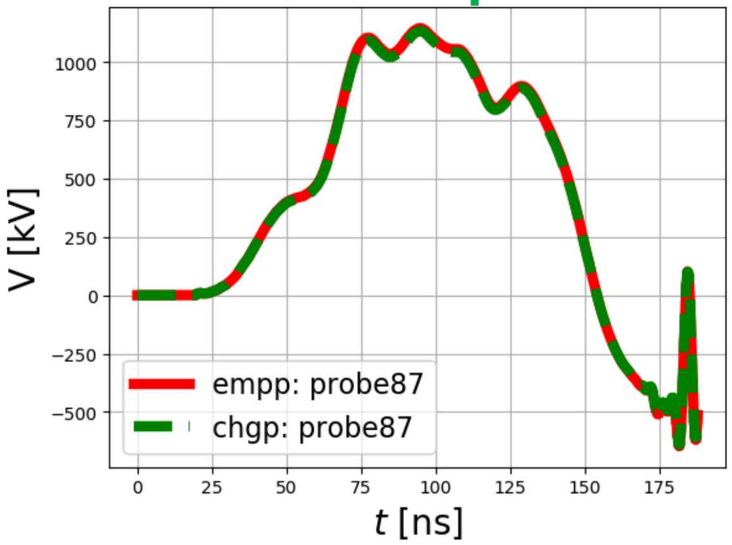


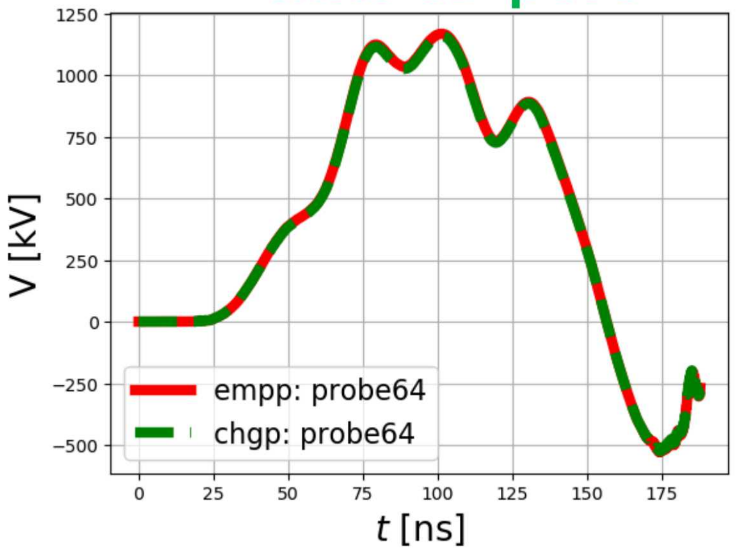
mitl A port



mitl B port



mitl CD port



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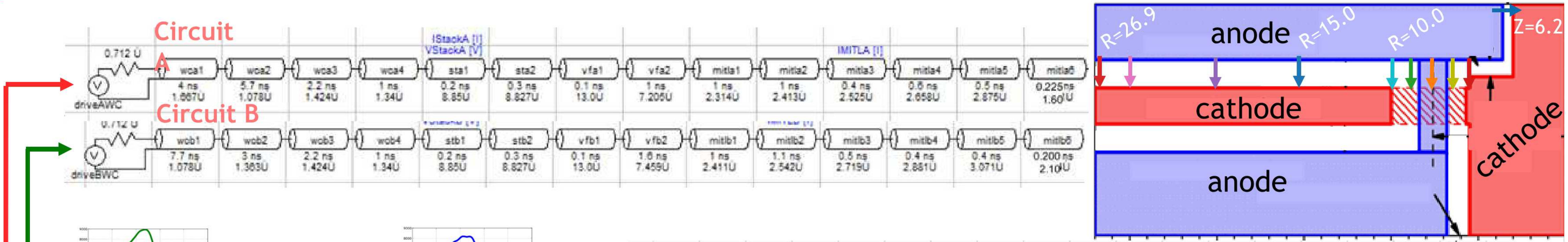
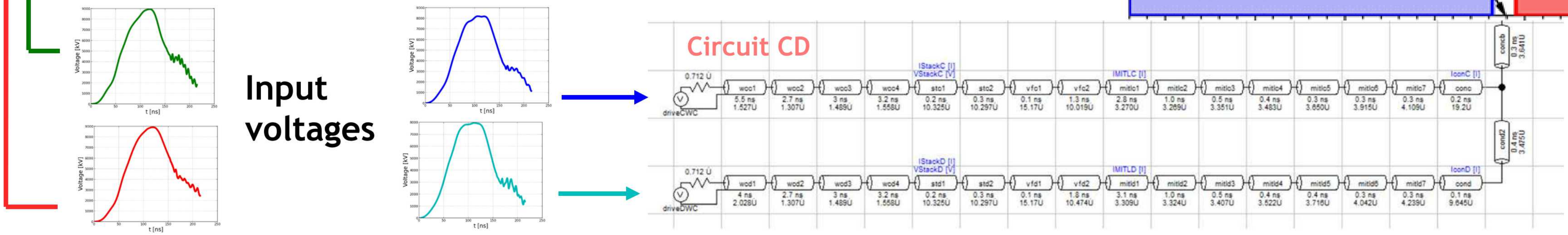
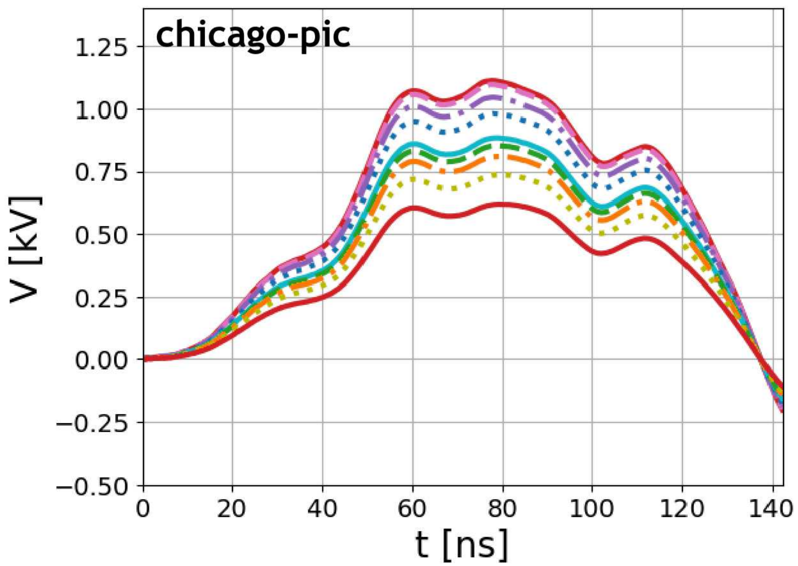
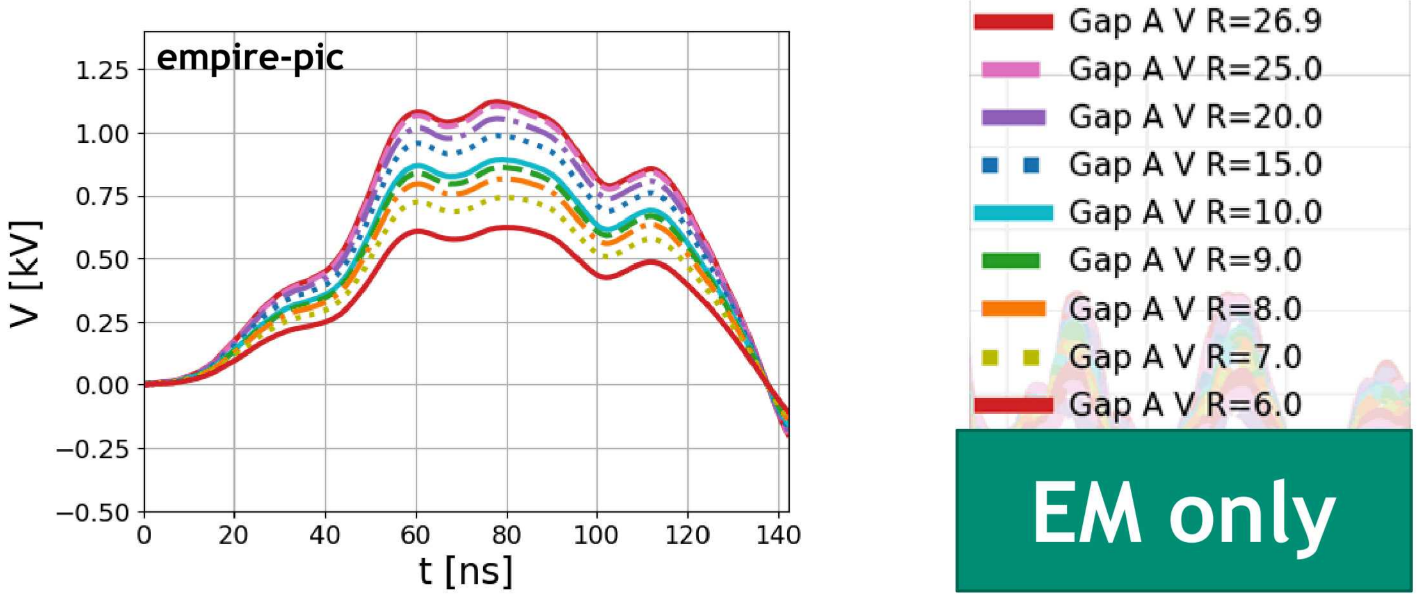


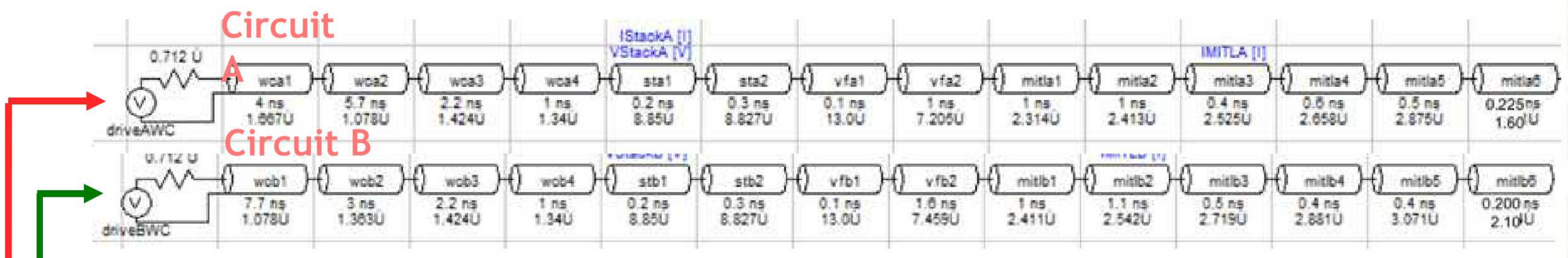


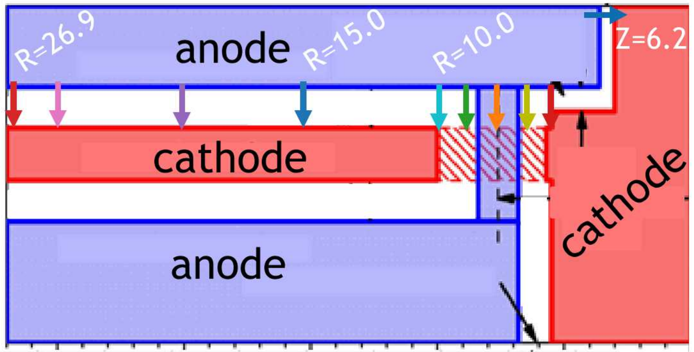


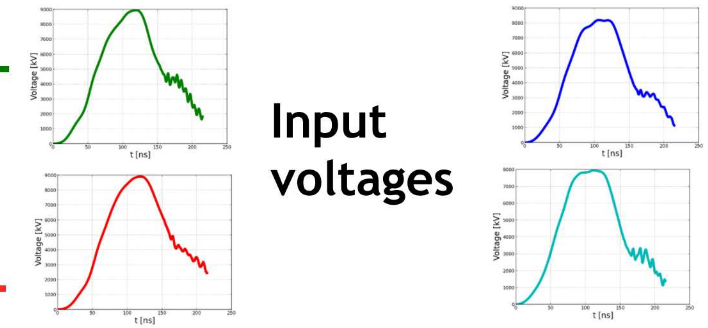


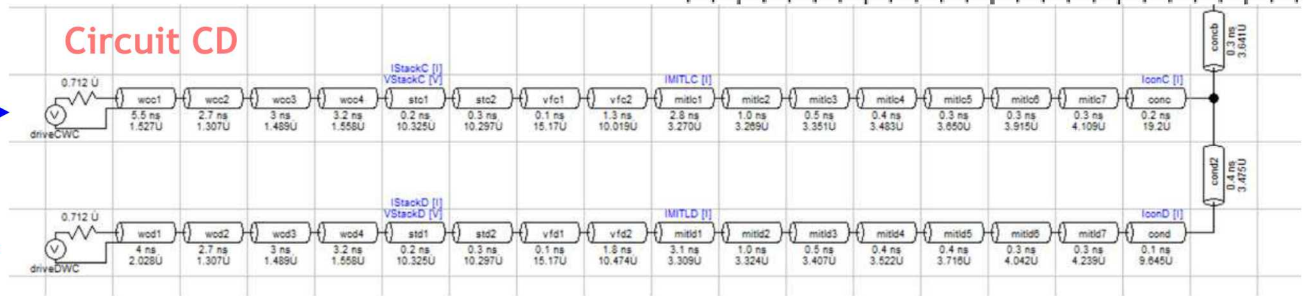
EM only

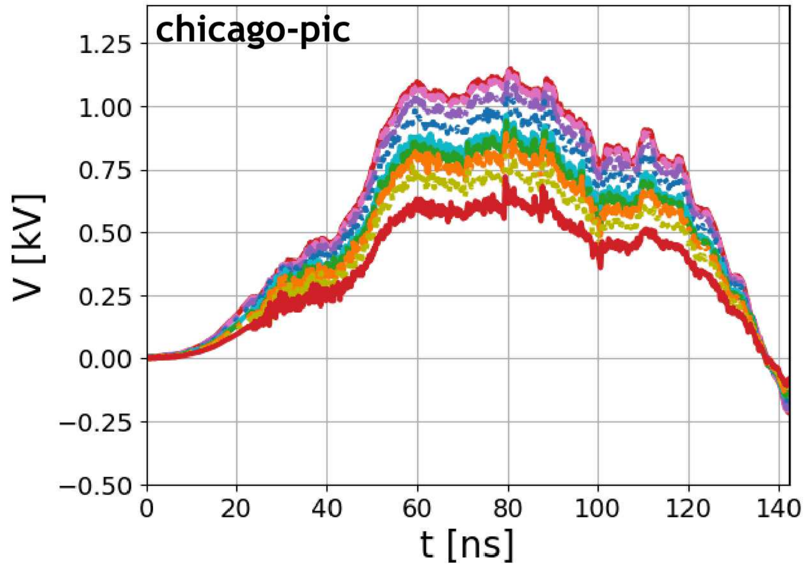
(Half-o-lute) Work-in-progress: SCL electrons, initial comparisons

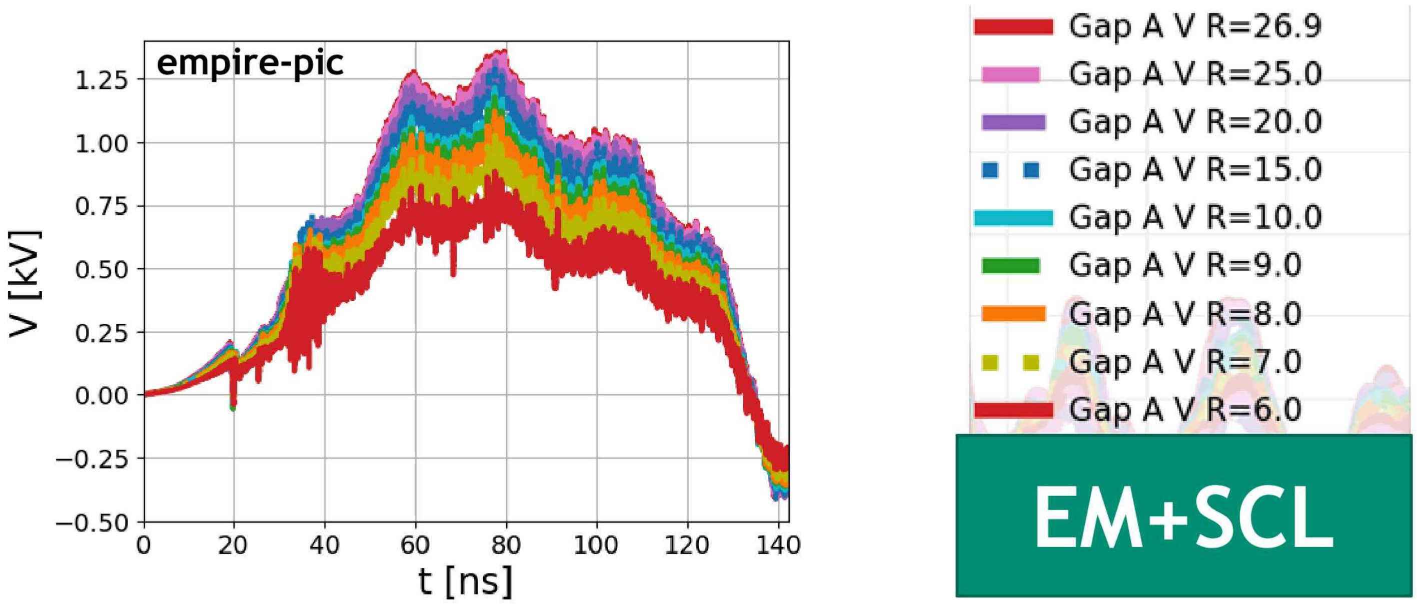












EM+SCL

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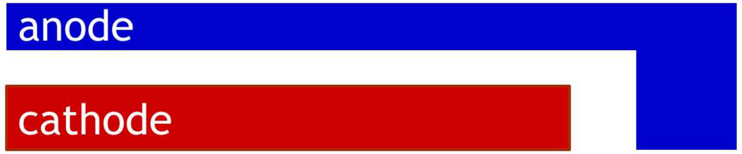
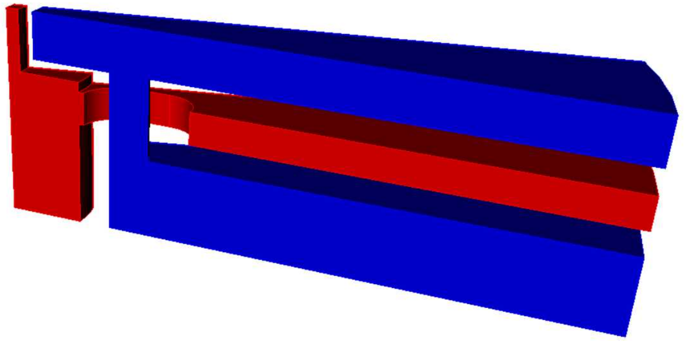
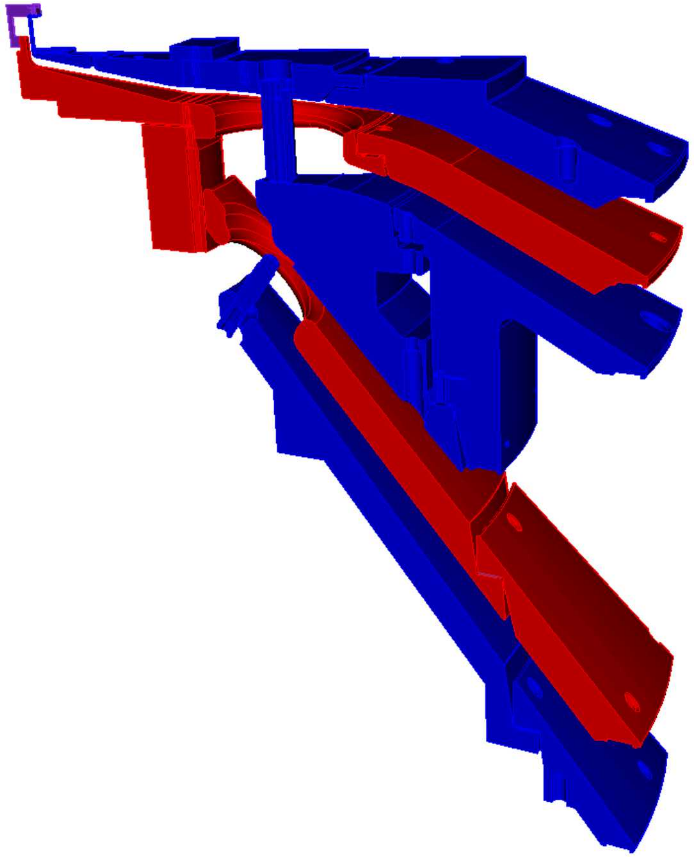


(3D) Half-o-lute



(3D) Powerflow 18a



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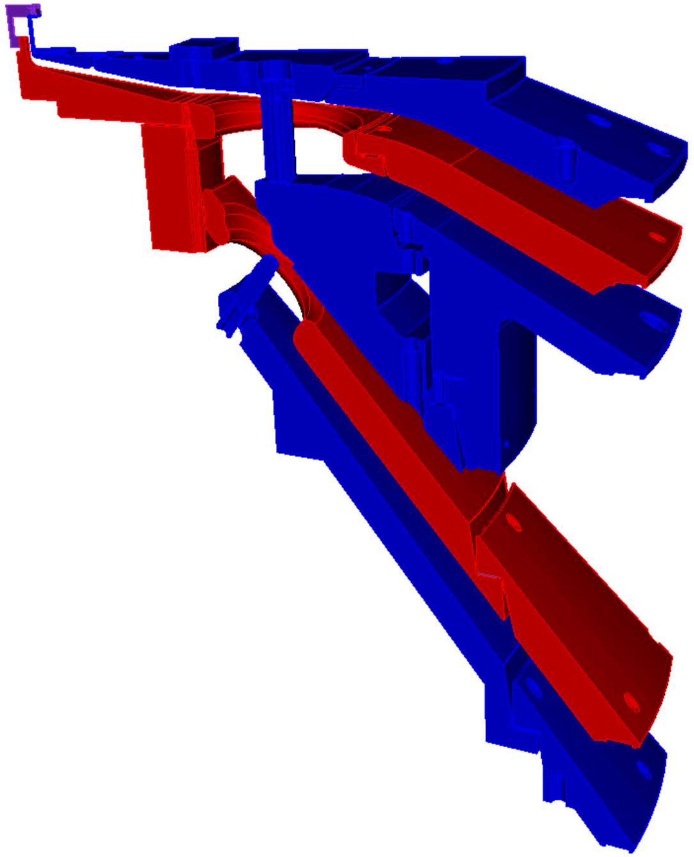
- EMPIRE work by D. Sirajuddin, M. Bettencourt
- CHICAGO work by N. Bennett

- Verification successes:
  - EM wave propagation
  - Transmission line verification
  - SCL electron emission

WIP: H_2O → plasma desorption from electrodes

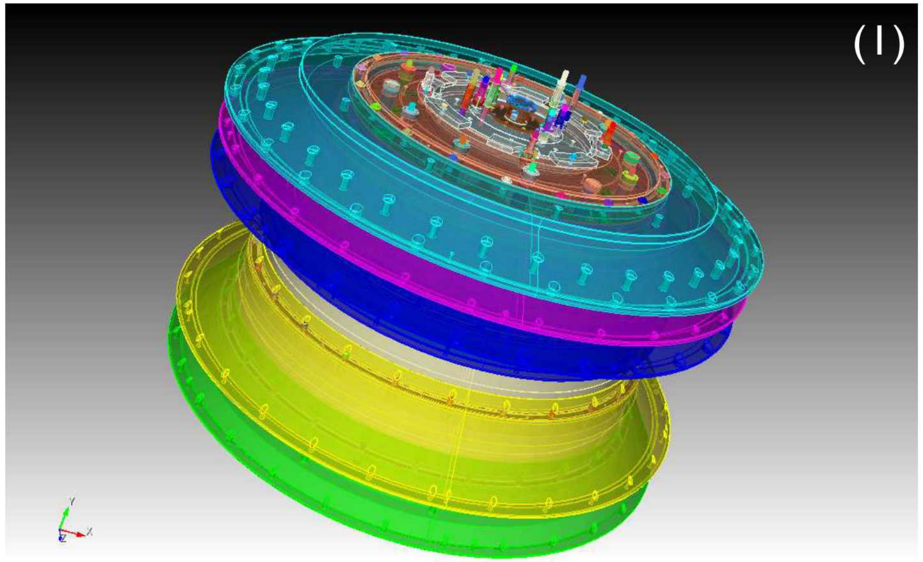
(3D) Powerflow 18a



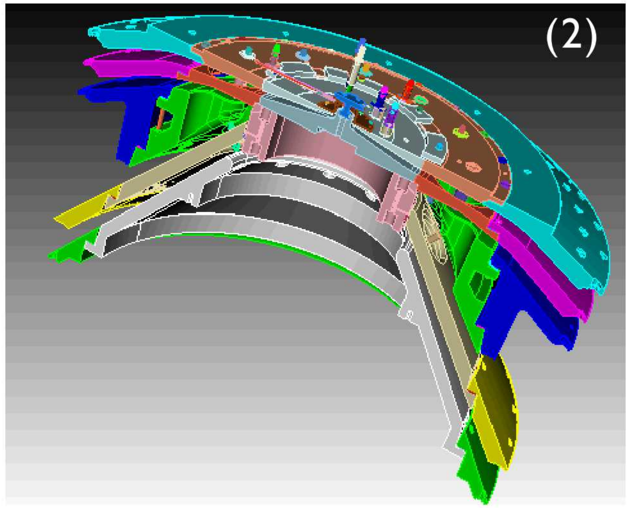
Full geometry

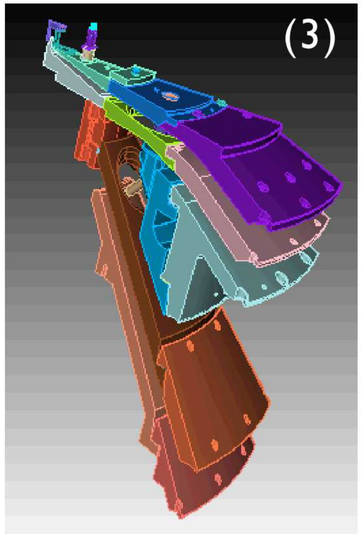
Increasing complexity

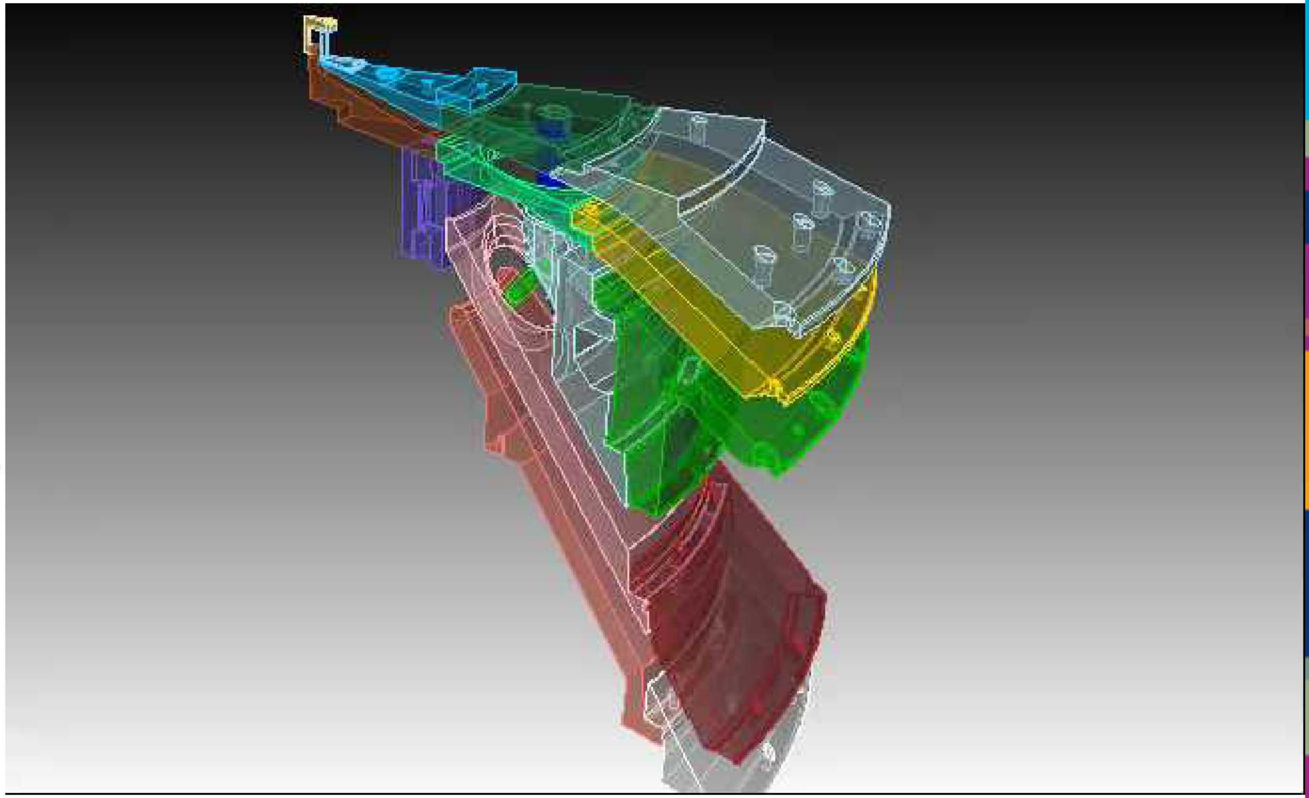
(Powerflow18a) geometry and tet mesh creation through cubit



Cut out a 15 deg. symmetric wedge

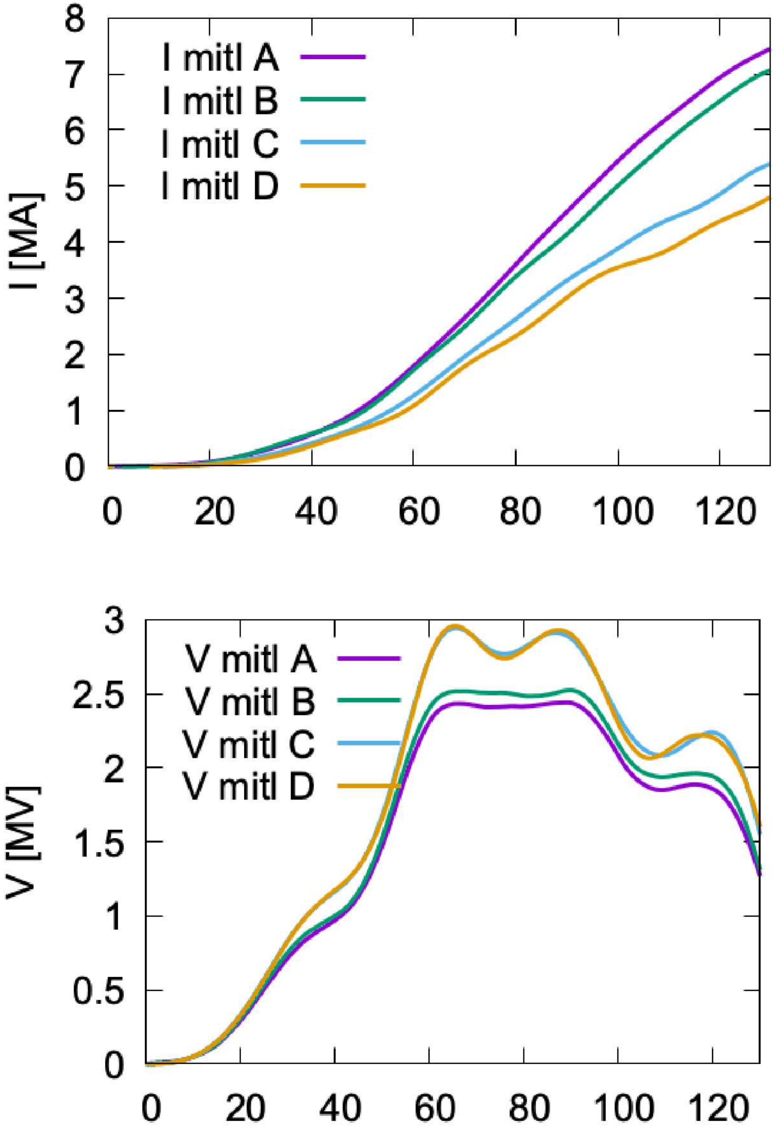






(Power flow 18a): Verifying EM – measurements at ports

CHICAGO-PIC



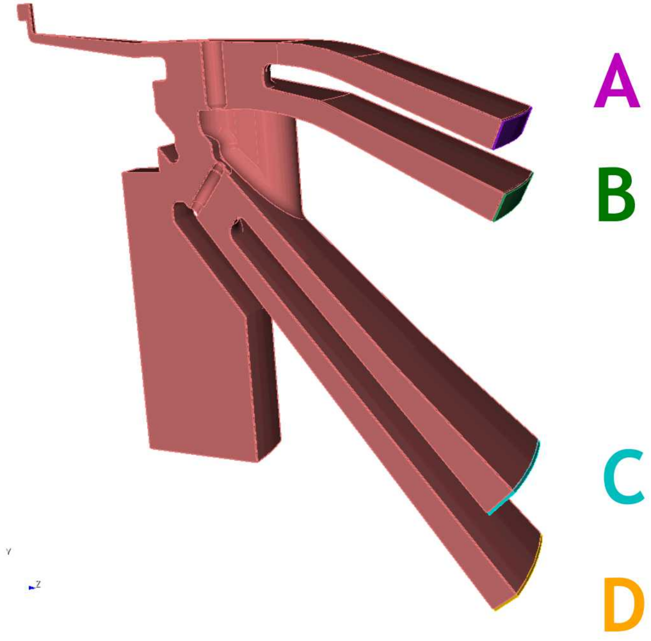
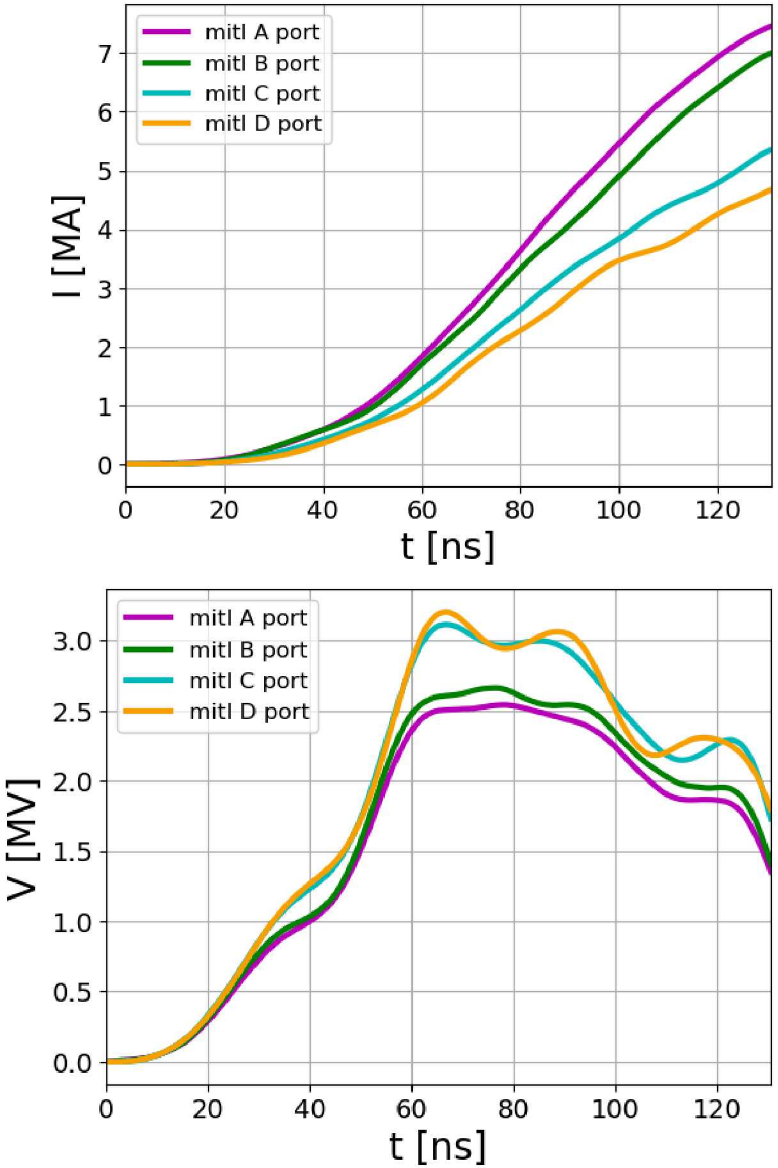


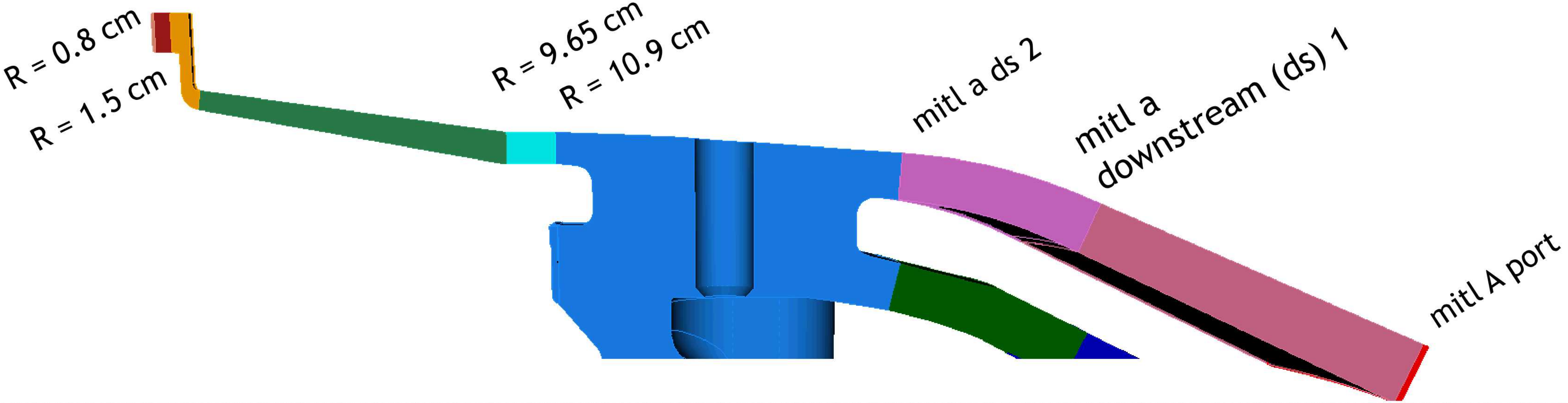
Figure: EMPIRE-PIC simulation volume

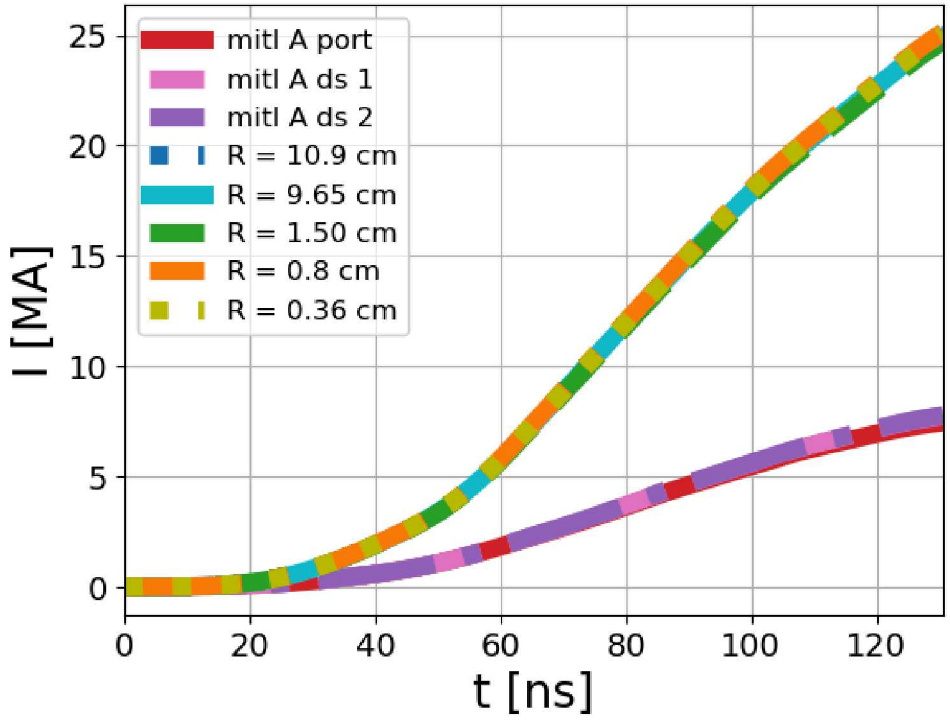
EMPIRE

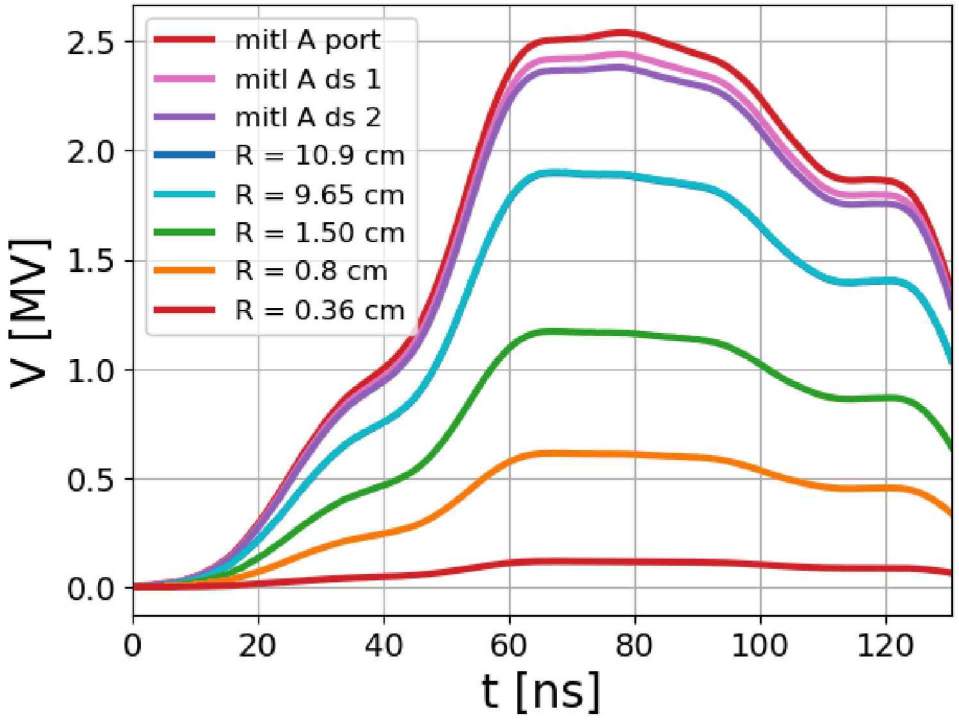


N. Bennett, D. R. Welch, C. A. Jennings, E. Yu, M. H. Hess, B. T. Hutsel, G. Laity, J. K. Moore, D. V. Rose, K. Peterson, and M. E. Cuneo Phys. Rev. Accel. Beams 22, 120401

(Power flow 18a): Verifying EM – measurements across top level



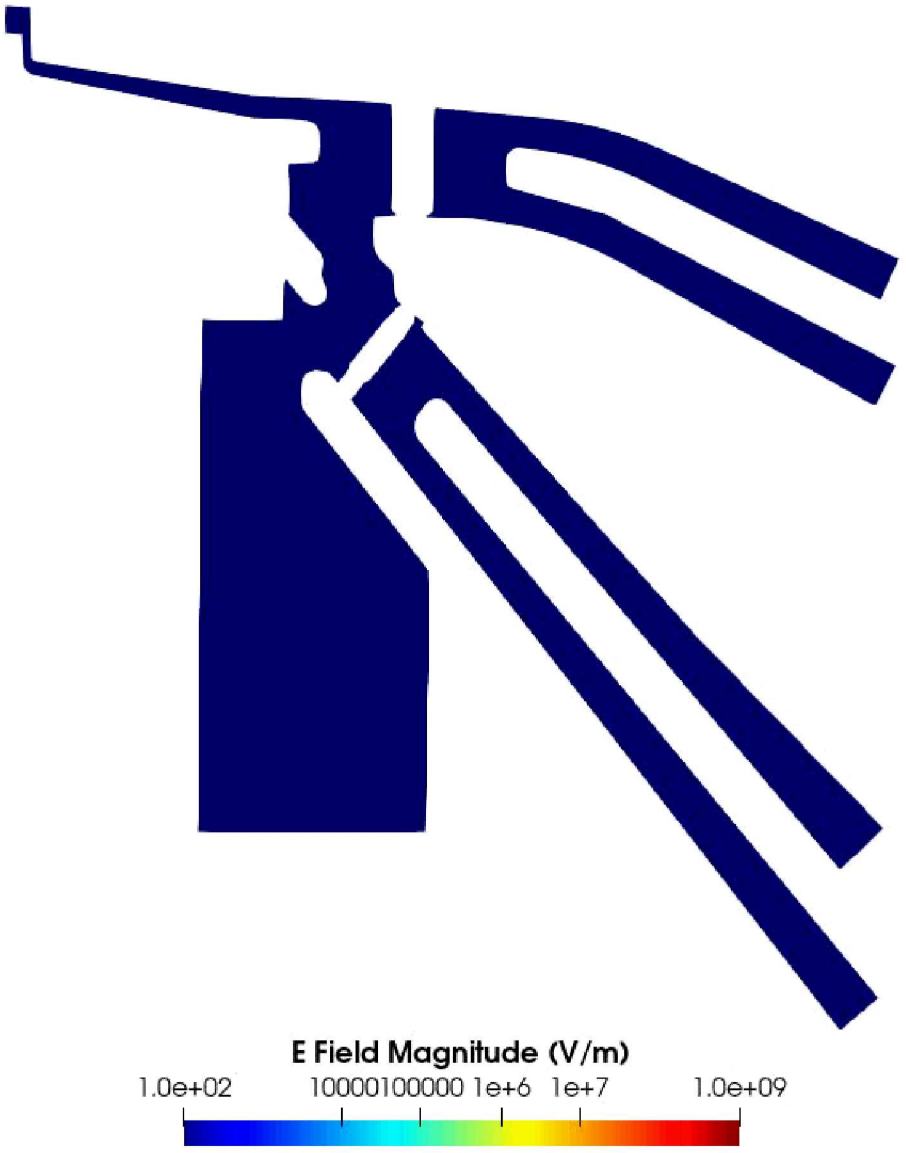


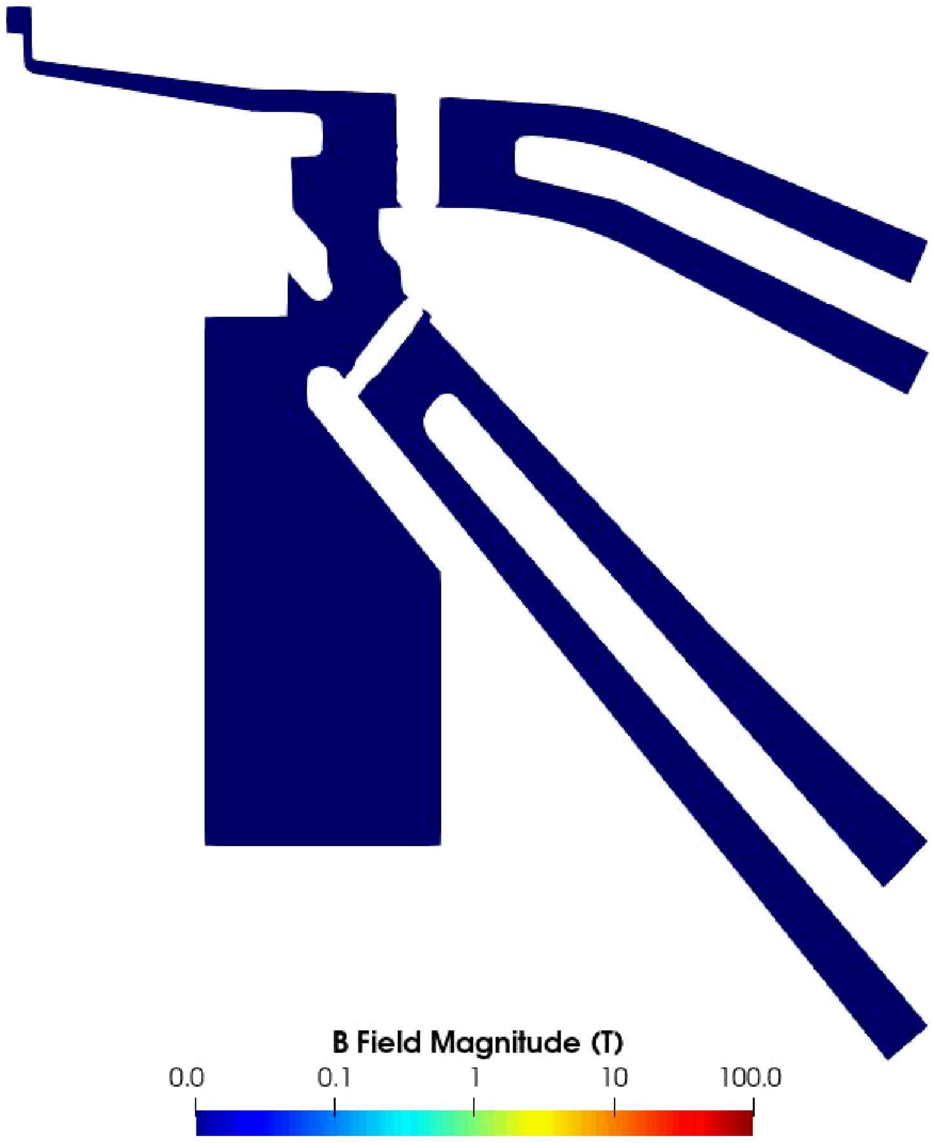


(Power flow 18a): Verifying EM+SCL electrons

EMPIRE-PIC

Time: 0.000 ns





(Power flow 18a): Verifying EM+SCL electrons

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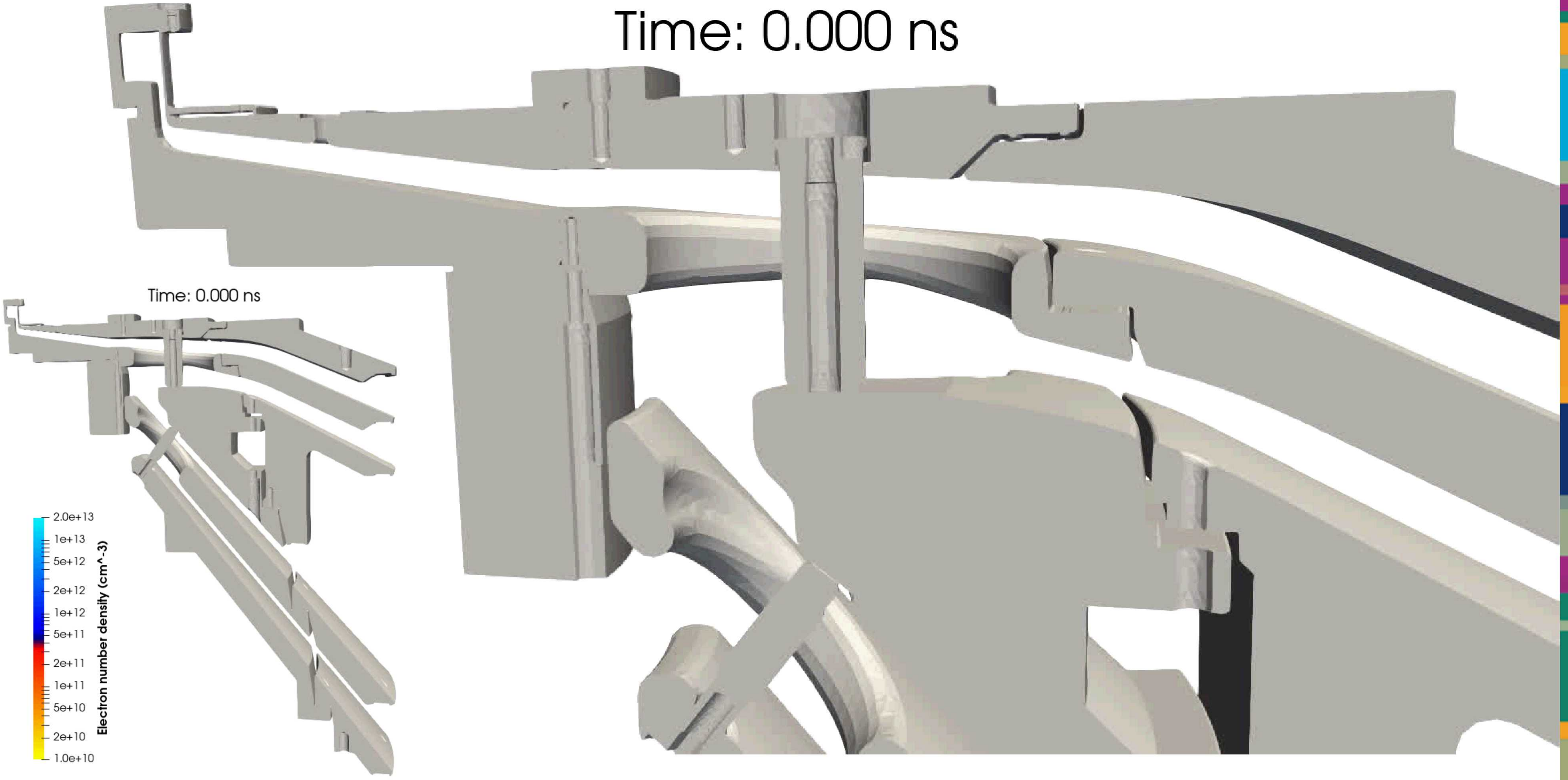

(Power flow 18a): Verifying EM+SCL electrons

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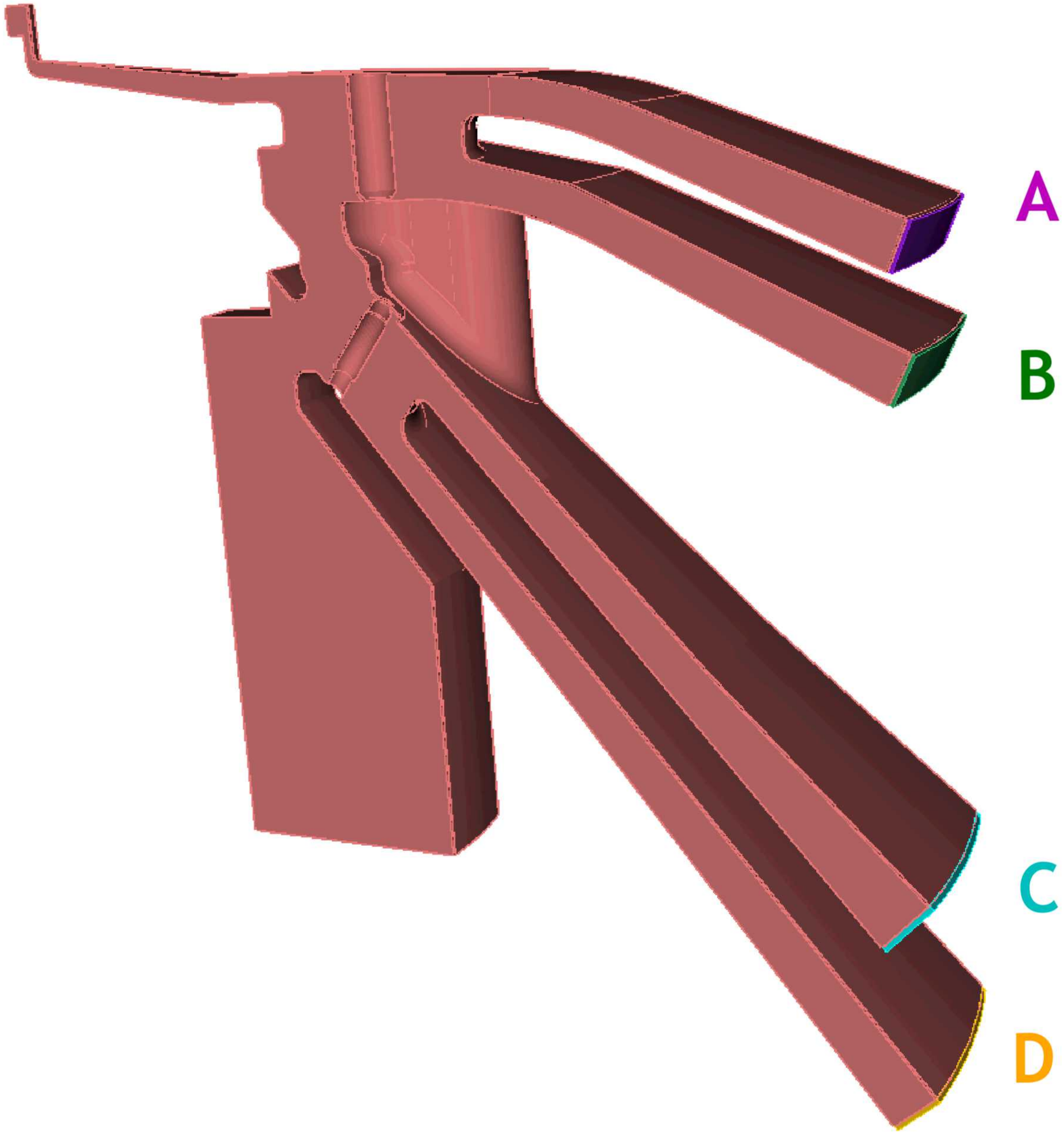
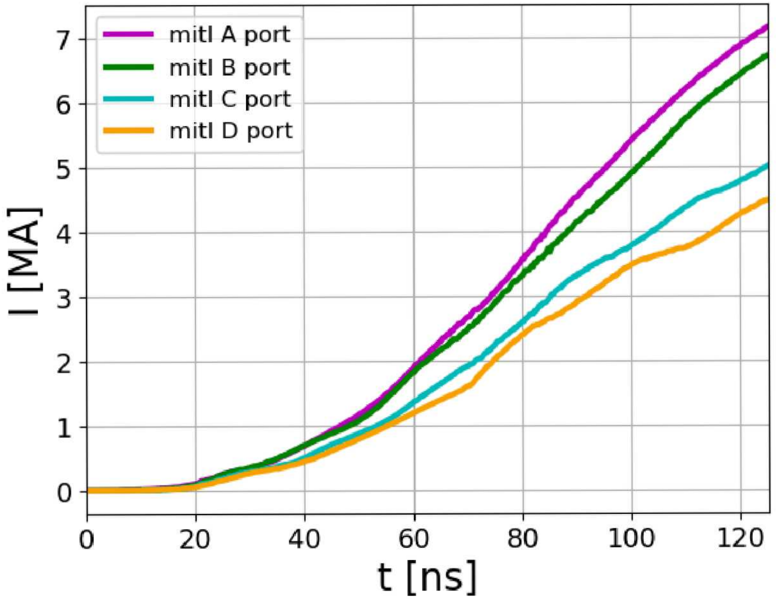
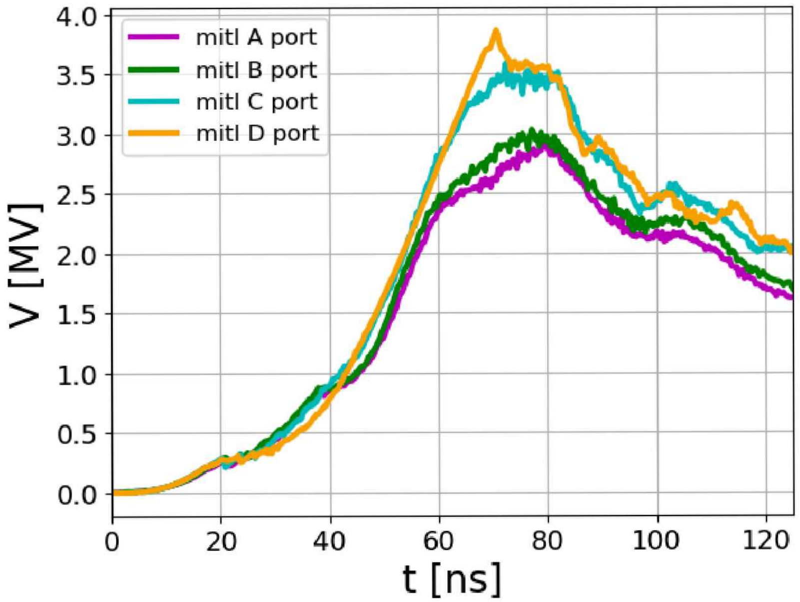
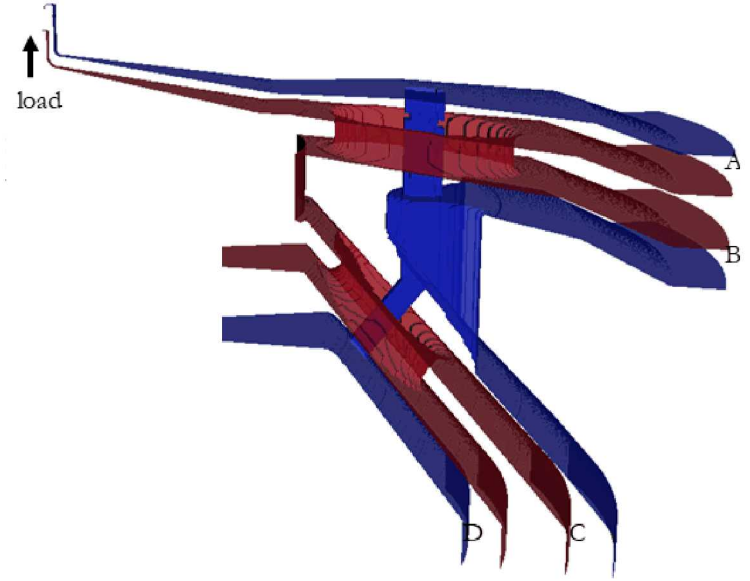


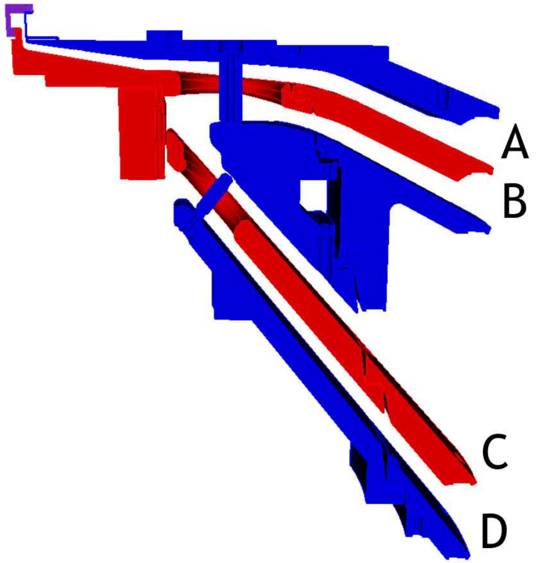




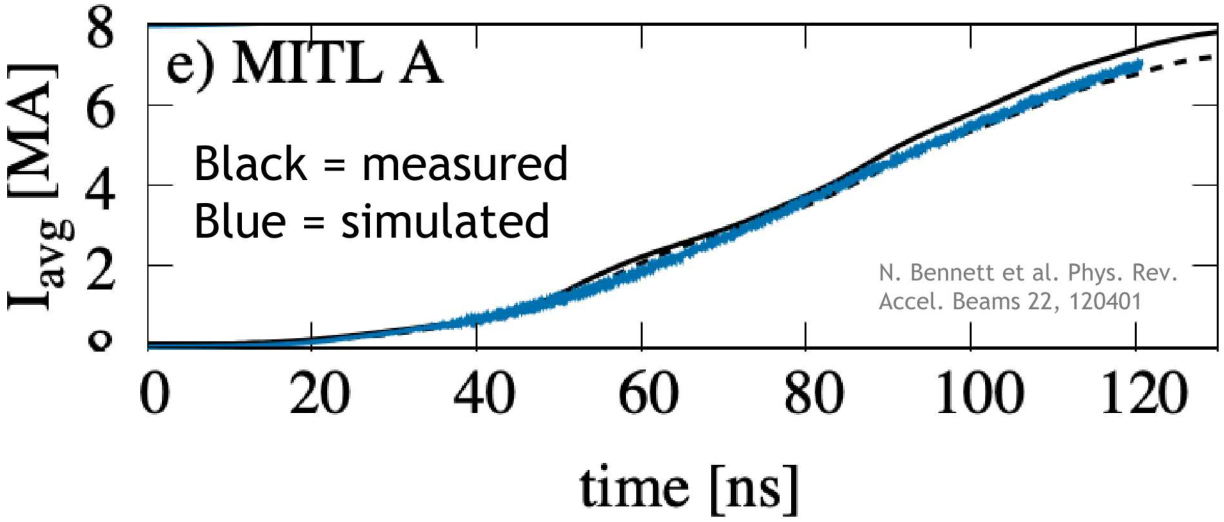
(Power flow 18a): Verifying EM+SCL electrons

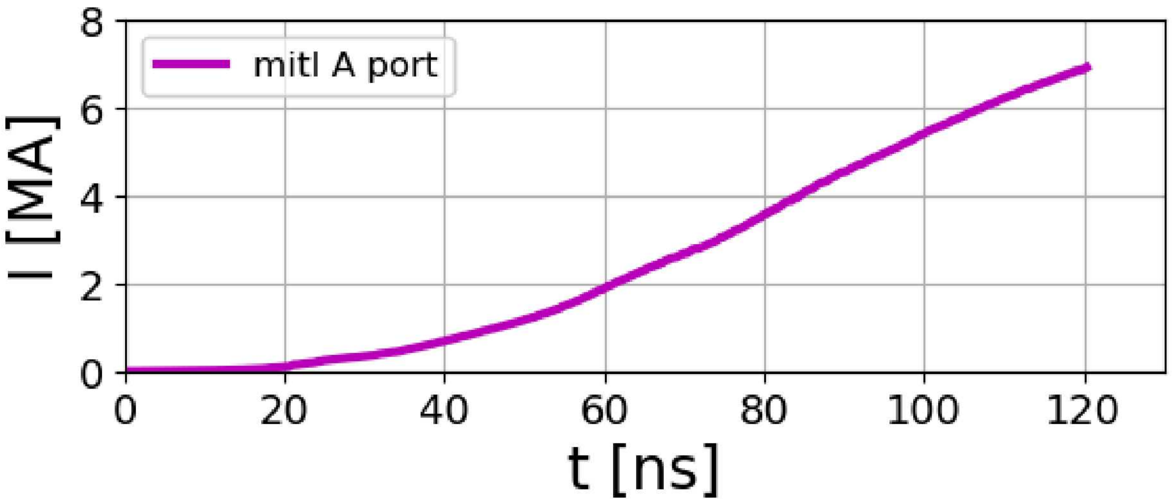


SCL + desorption
Chicago-pic

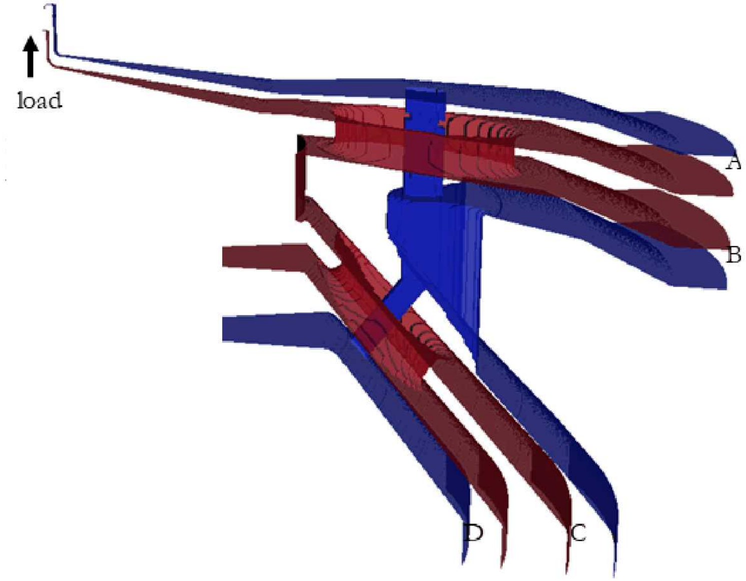


SCL only
Empire-pic (results from M.Bettencourt)

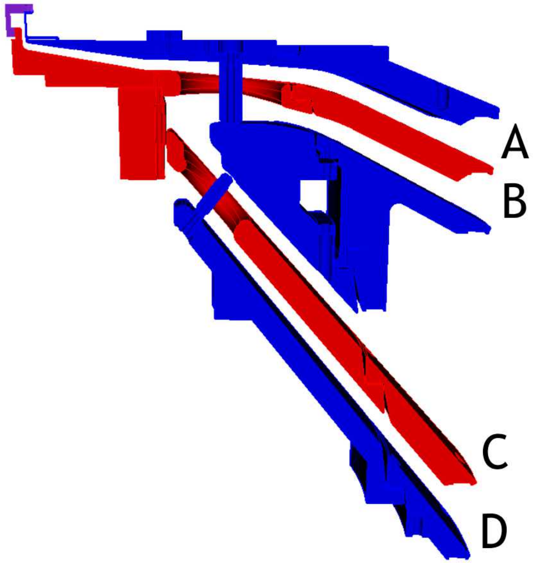




(Power flow 18a): Verifying EM+SCL electrons



SCL + desorption
Chicago-pic



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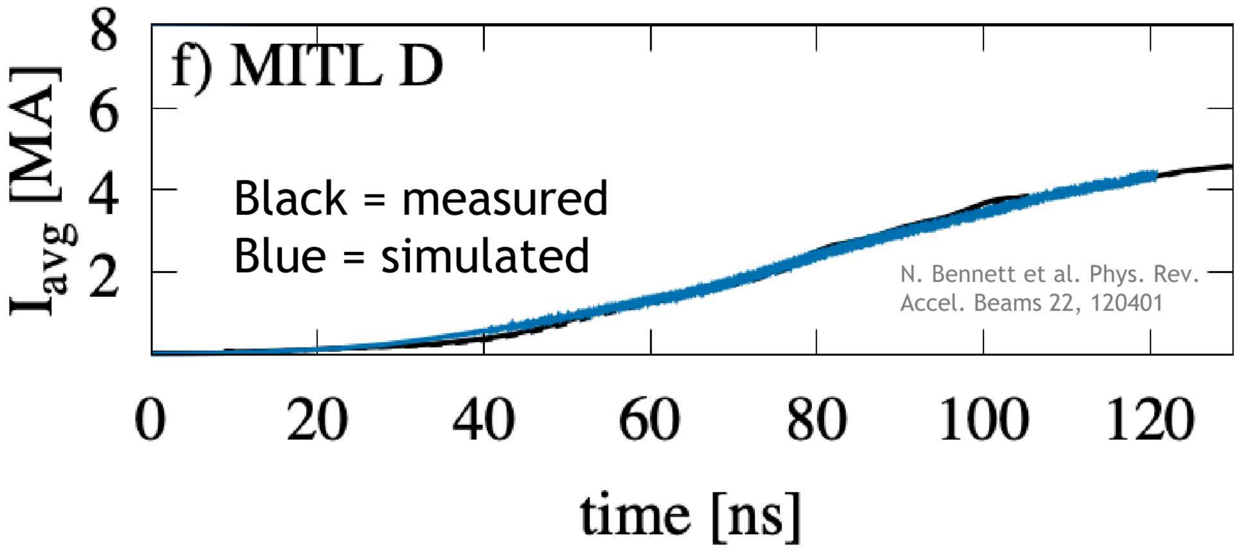
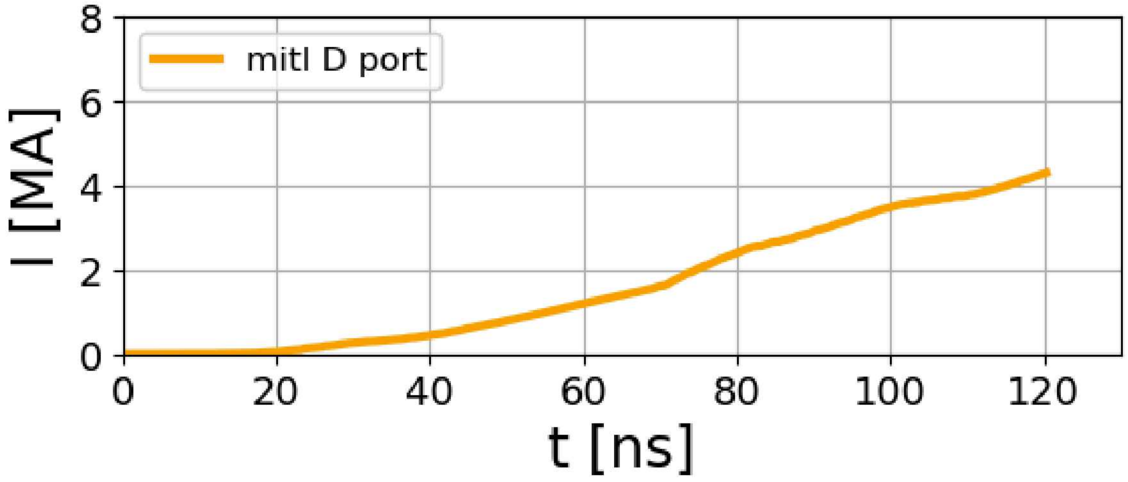
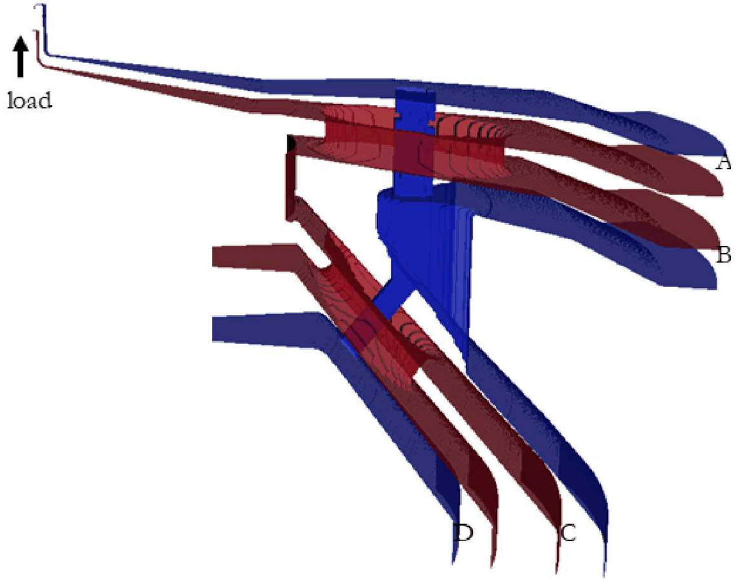
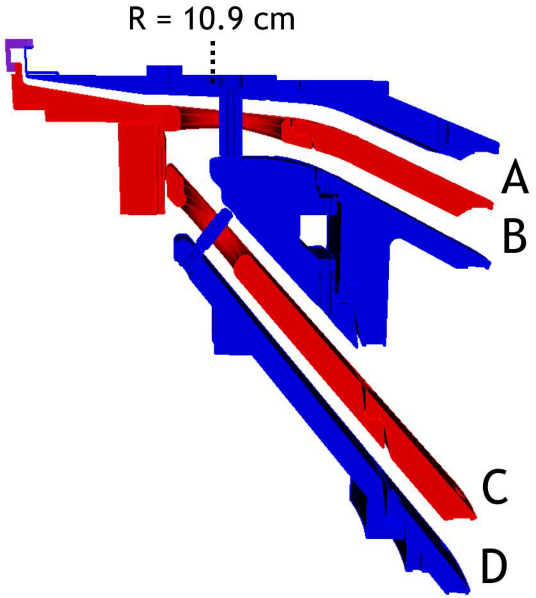




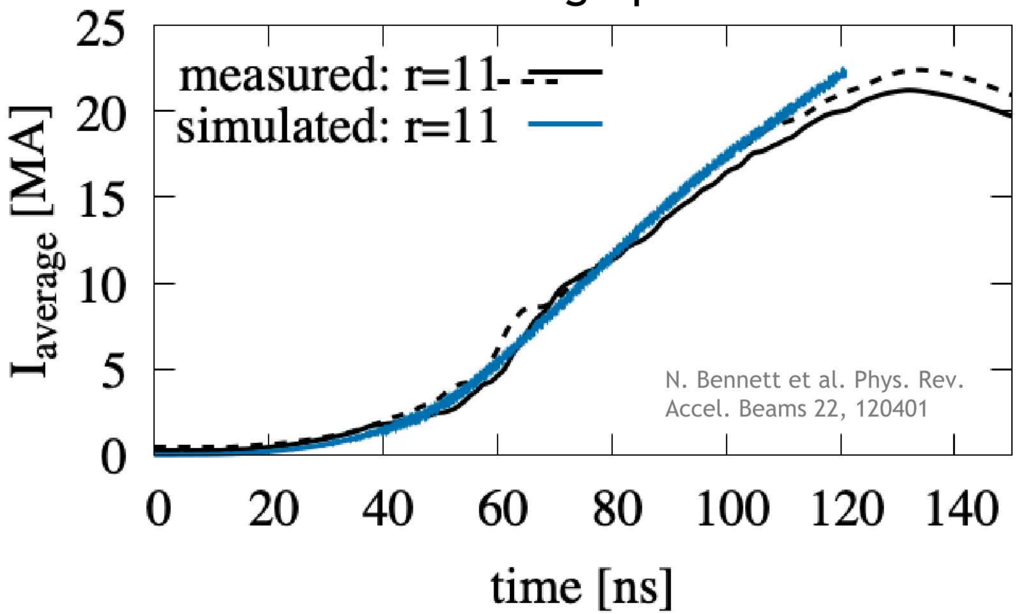
(Power flow 18a): Verifying EM+SCL electrons

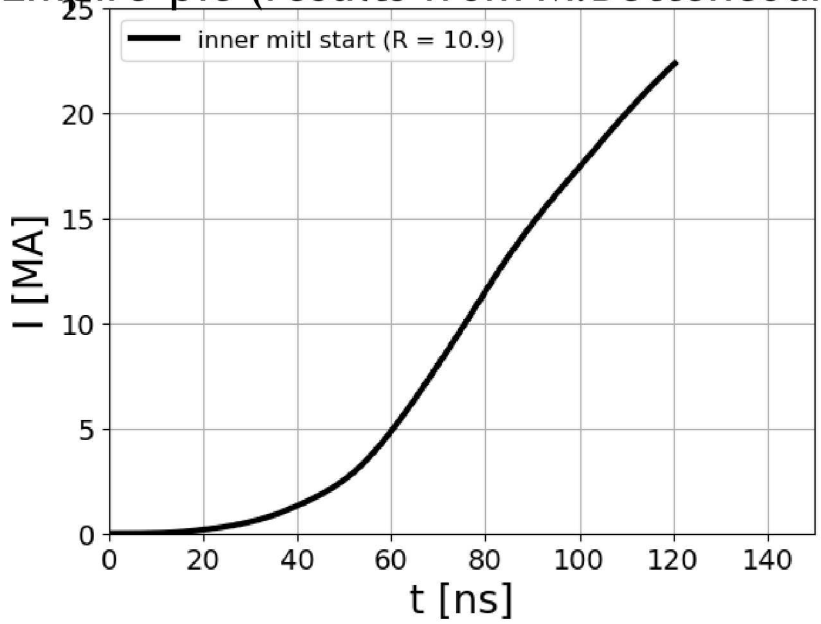


SCL + desorption
Chicago-pic

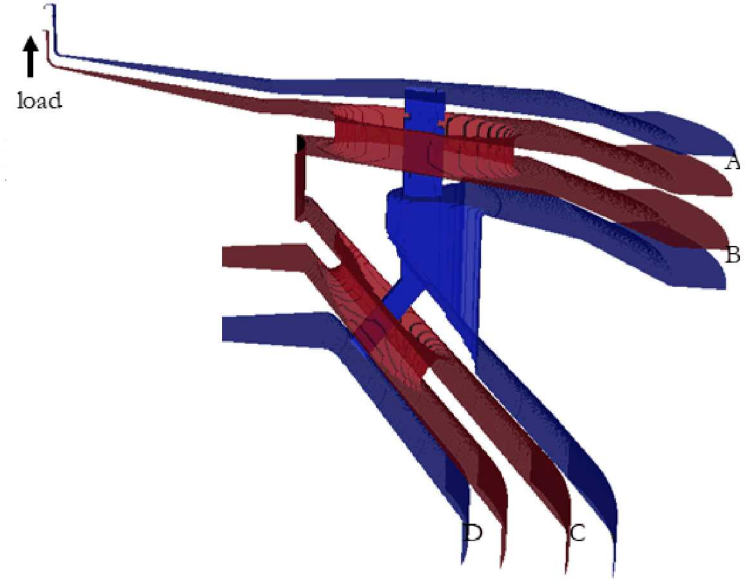


SCL only
Empire-pic (results from M.Bettencourt)

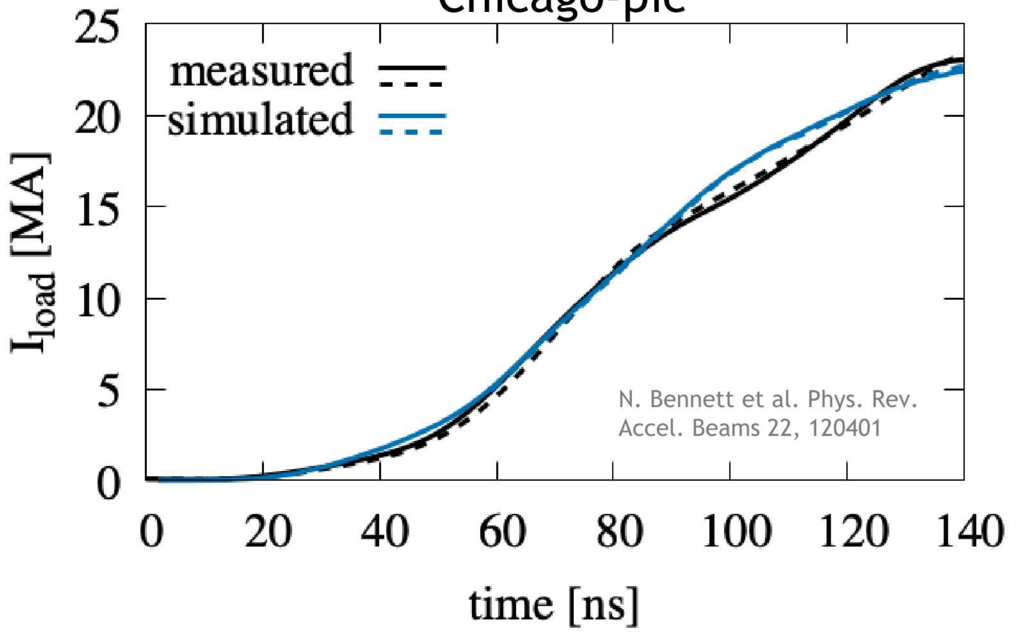


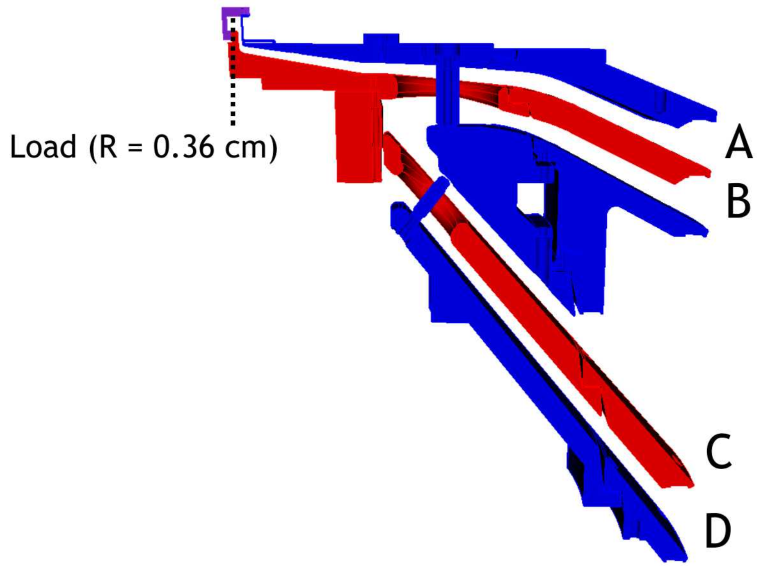


(Power flow 18a): Verifying EM+SCL electrons

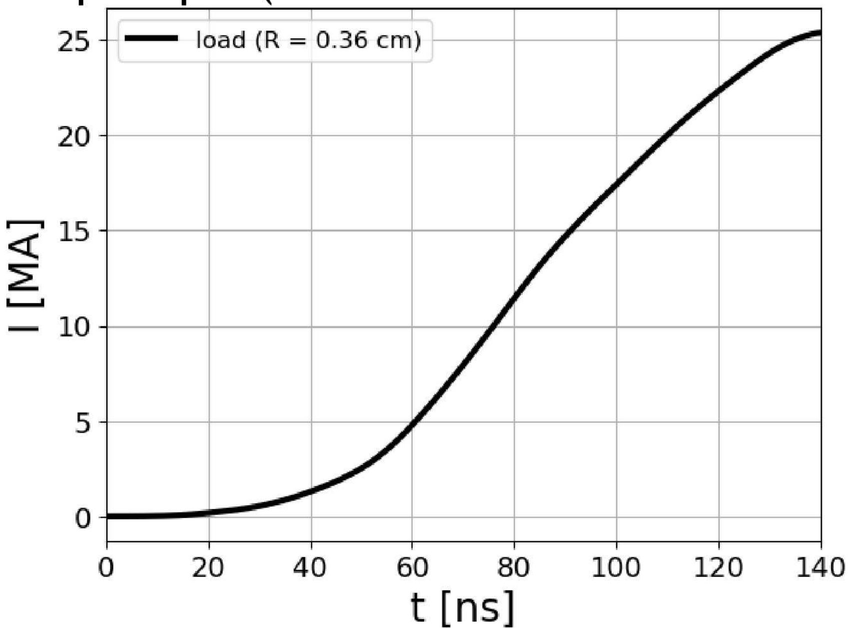


SCL + desorption
Chicago-pic





SCL only
Empire-pic (results from M.Bettencourt)



Conclusions

- Two exemplar problems (Half-o-Lute and Powerflow 18a) are being developed for the grand challenge LDRD
- Half-o-lute
  - EM and branching transmission line coupling has been ~ verified
  - Currently working on verifying SCL electrons between CHICAGO and EMPIRE implementations
- Powerflow18a
  - EM and transmission line coupling verified
  - SCL electron emissions shows good agreement between CHICAGO and EMPIRE results
  - Currently working on implementing and verifying plasma desorption models for the next step

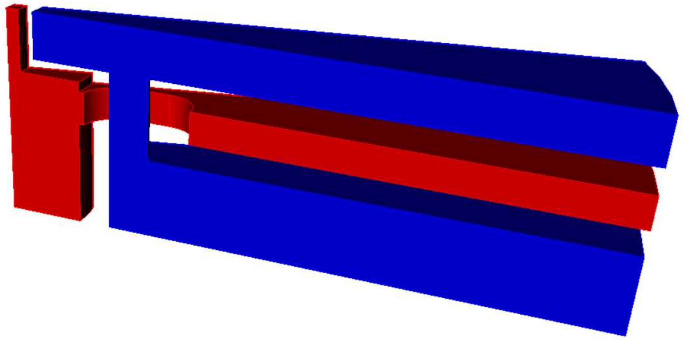
Extras

powerflow model building has benefited from vetting and fine-tuning developing code capabilities by pushing tests through a pipeline of increasingly complex MITL systems

(2D) planar MITL

Idealized single MITL geometry
(to be covered in next talk by N. Hamlin)

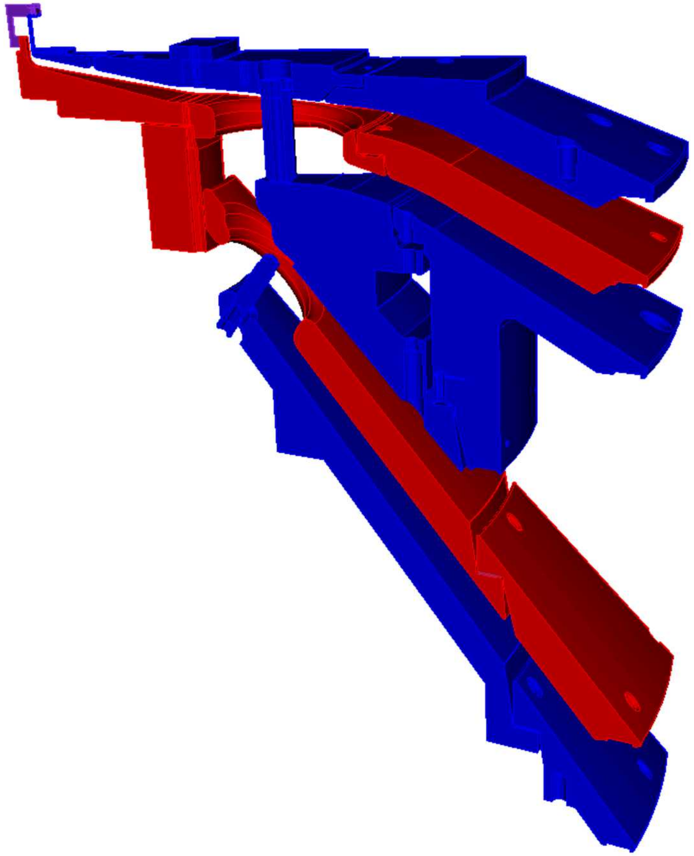
(3D) Half-o-lute



"Half" of an idealized convolute geometry

3 simplified MITLs → single post-hold convolute → load

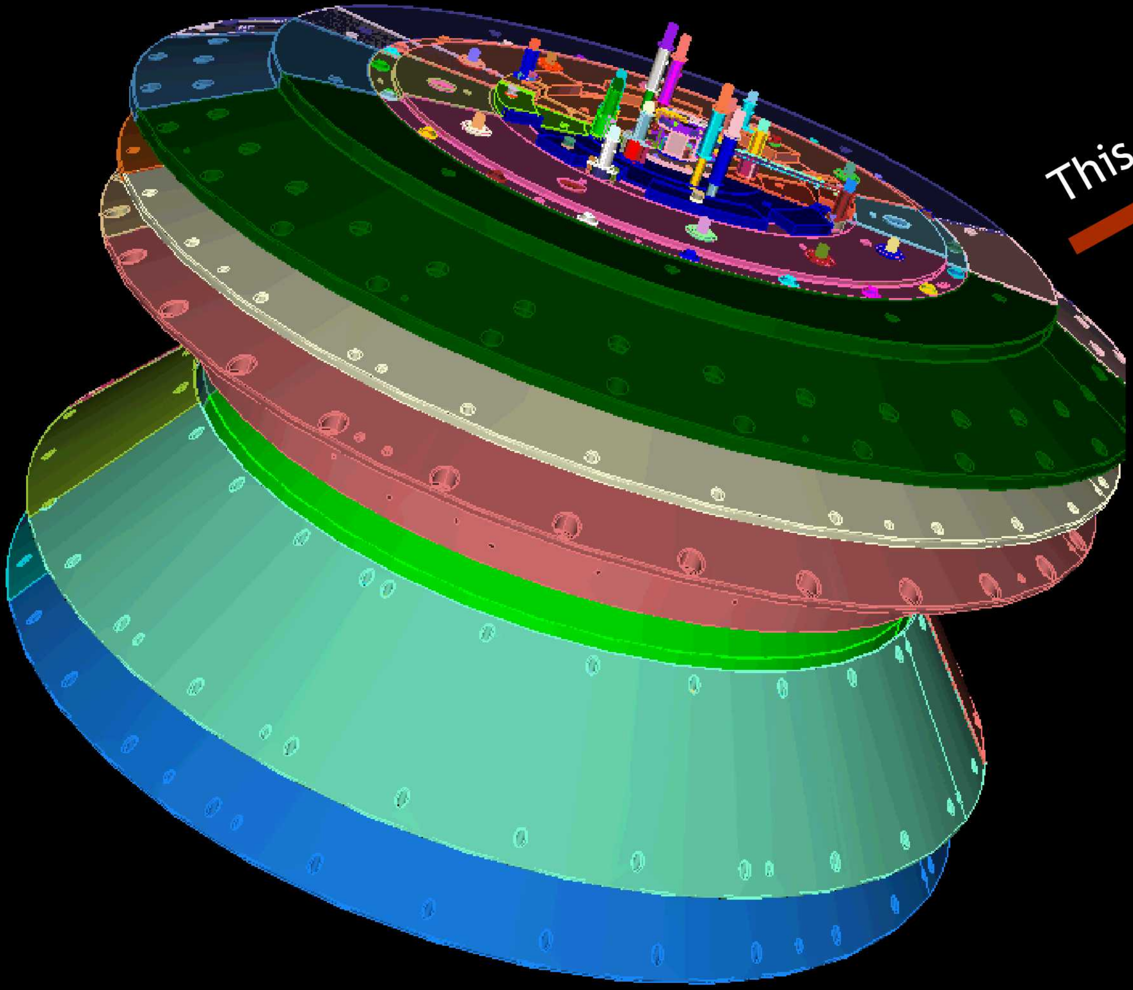
(3D) Powerflow 18a

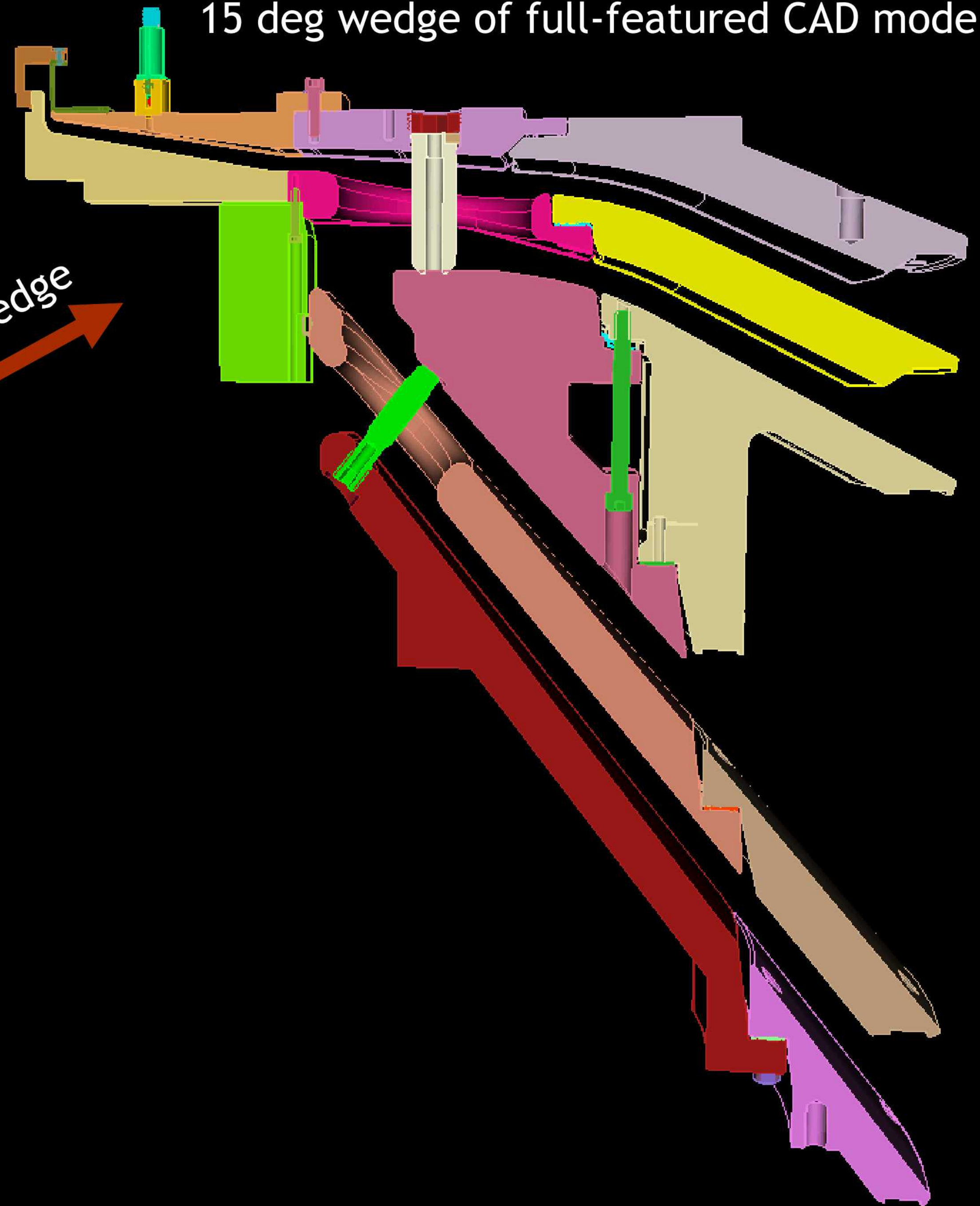


Full geometry (CAD)

4 tapered MITLs → double post-hole convolute → load

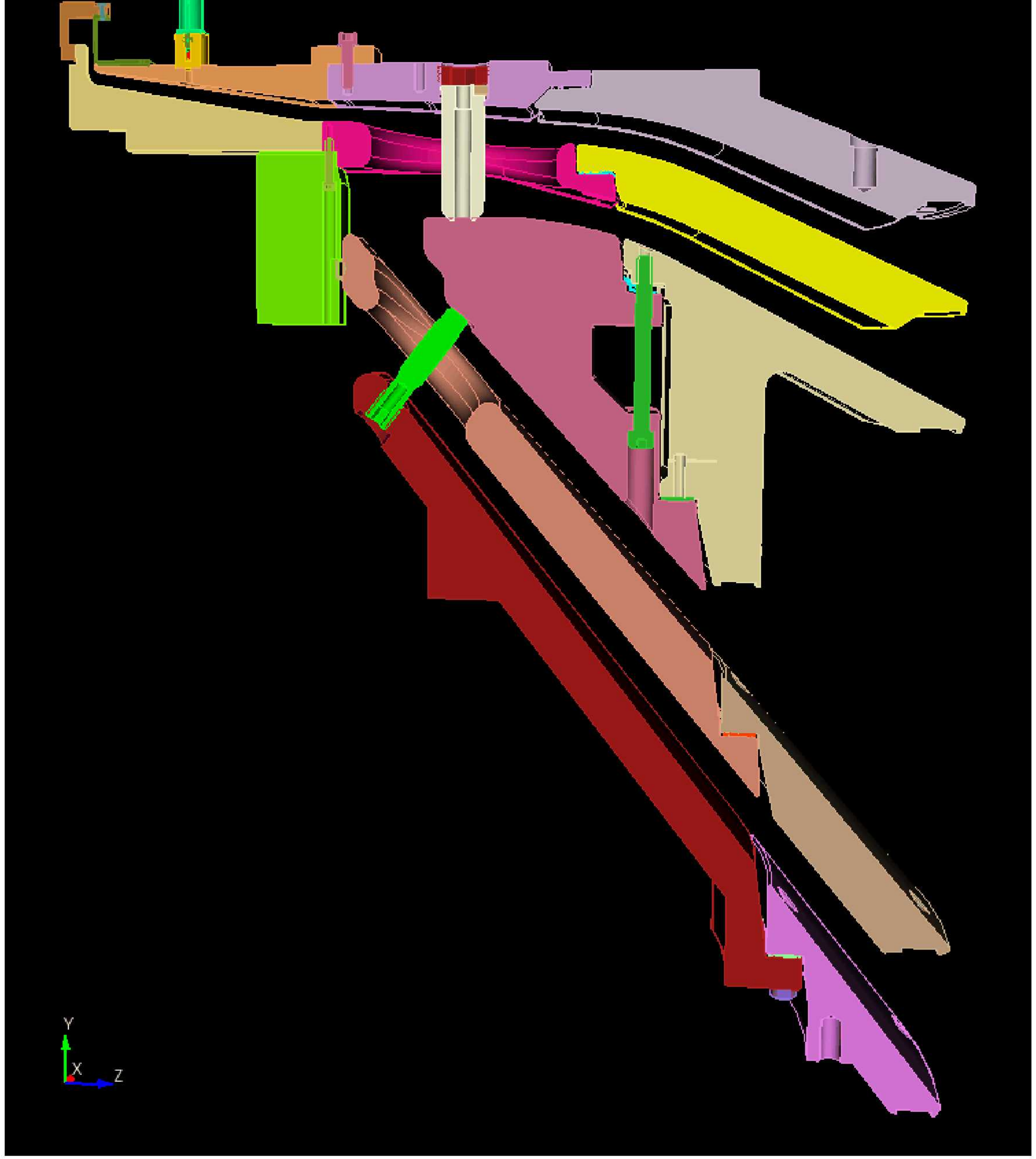
Full-featured CAD model
(imported into cubit)



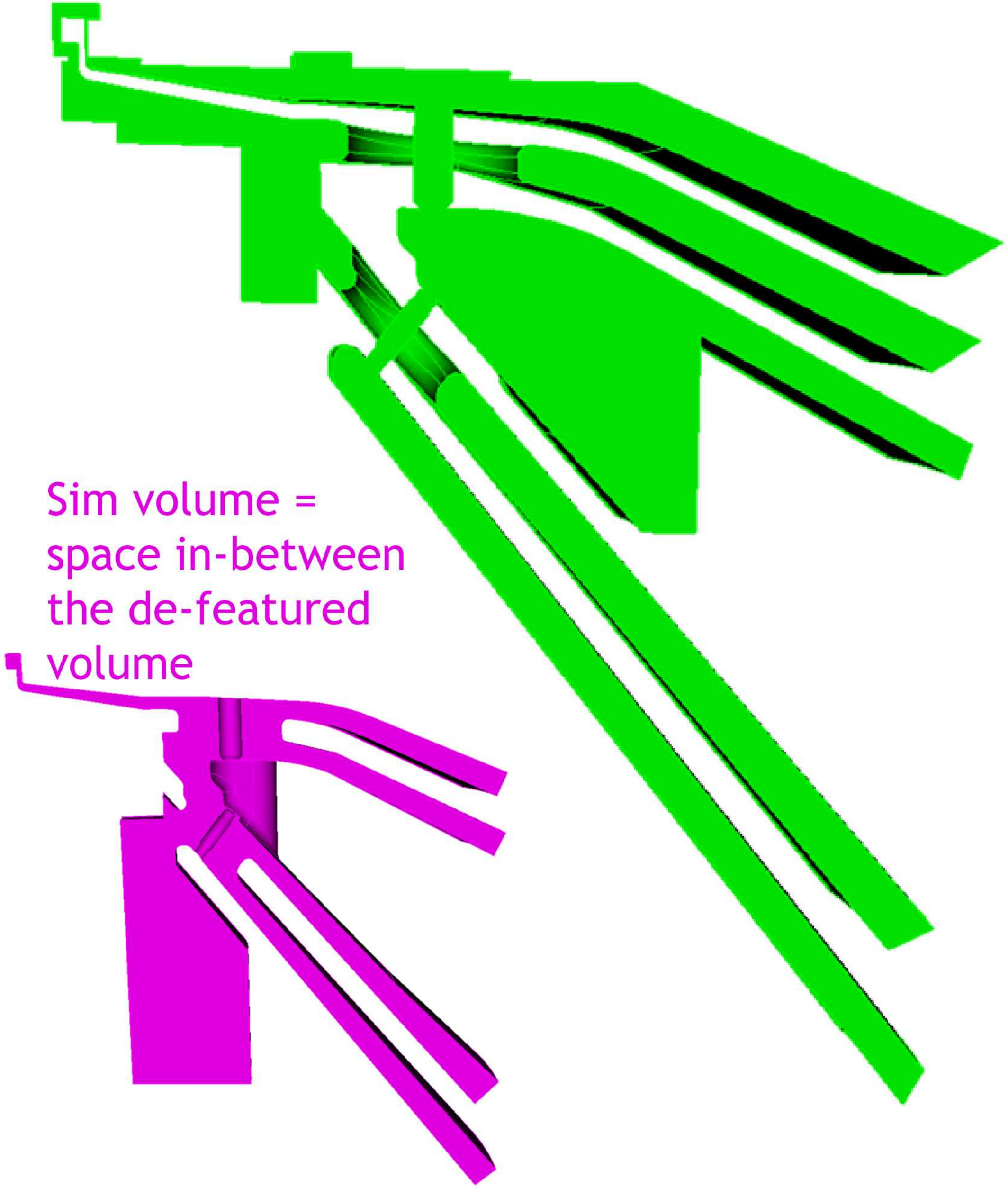


15 deg wedge of full-featured CAD mode

full-featured hardware



De-featured hardware



Sim volume = space in-between the de-featured volume

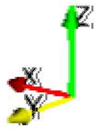
(Power flow 18a): Work-in progress – plasma desorption model

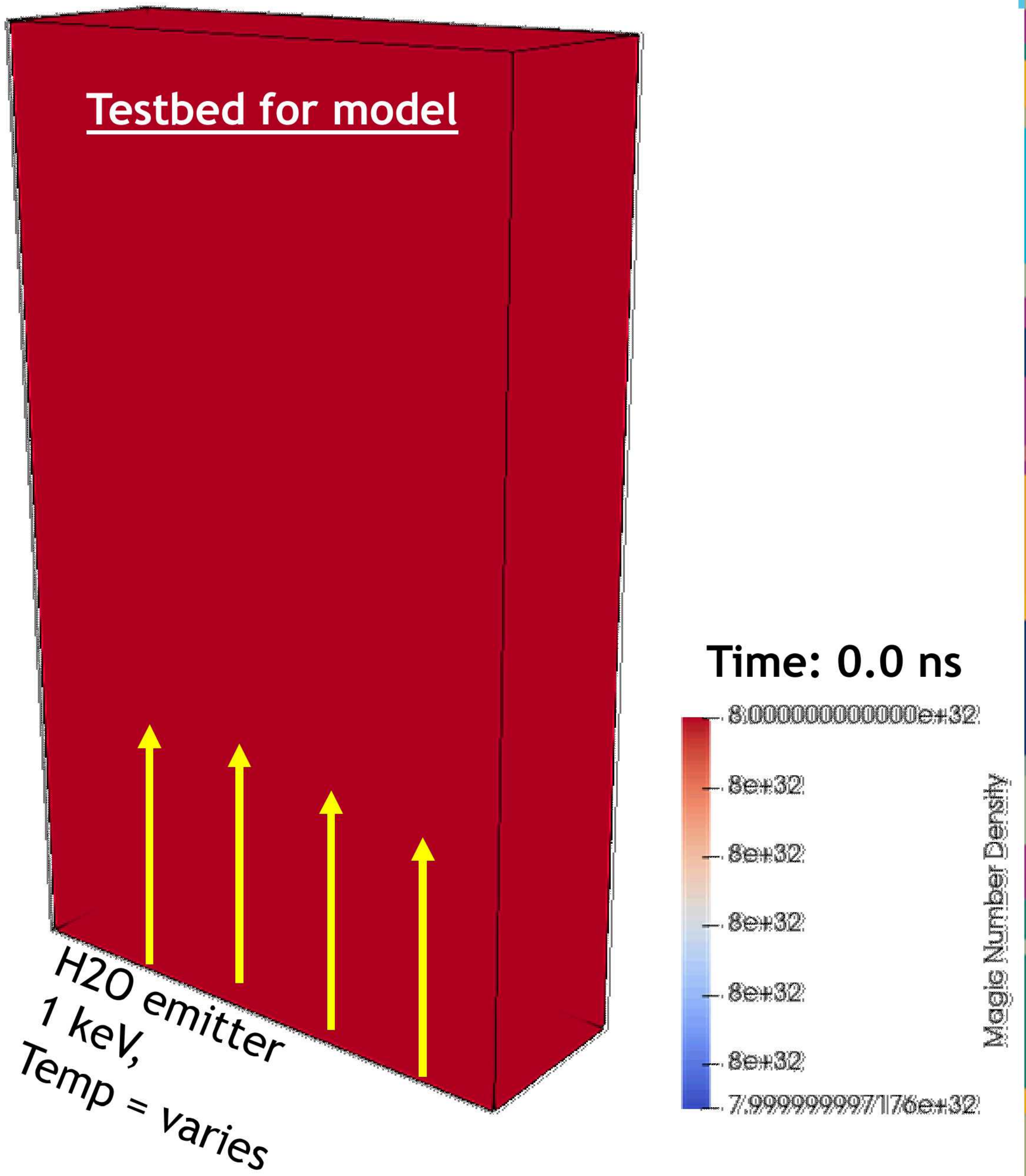
Developing a fragmentation model via SPIN

$$H_2O \rightarrow 3e^- + (O^+) + 2(H^+)$$

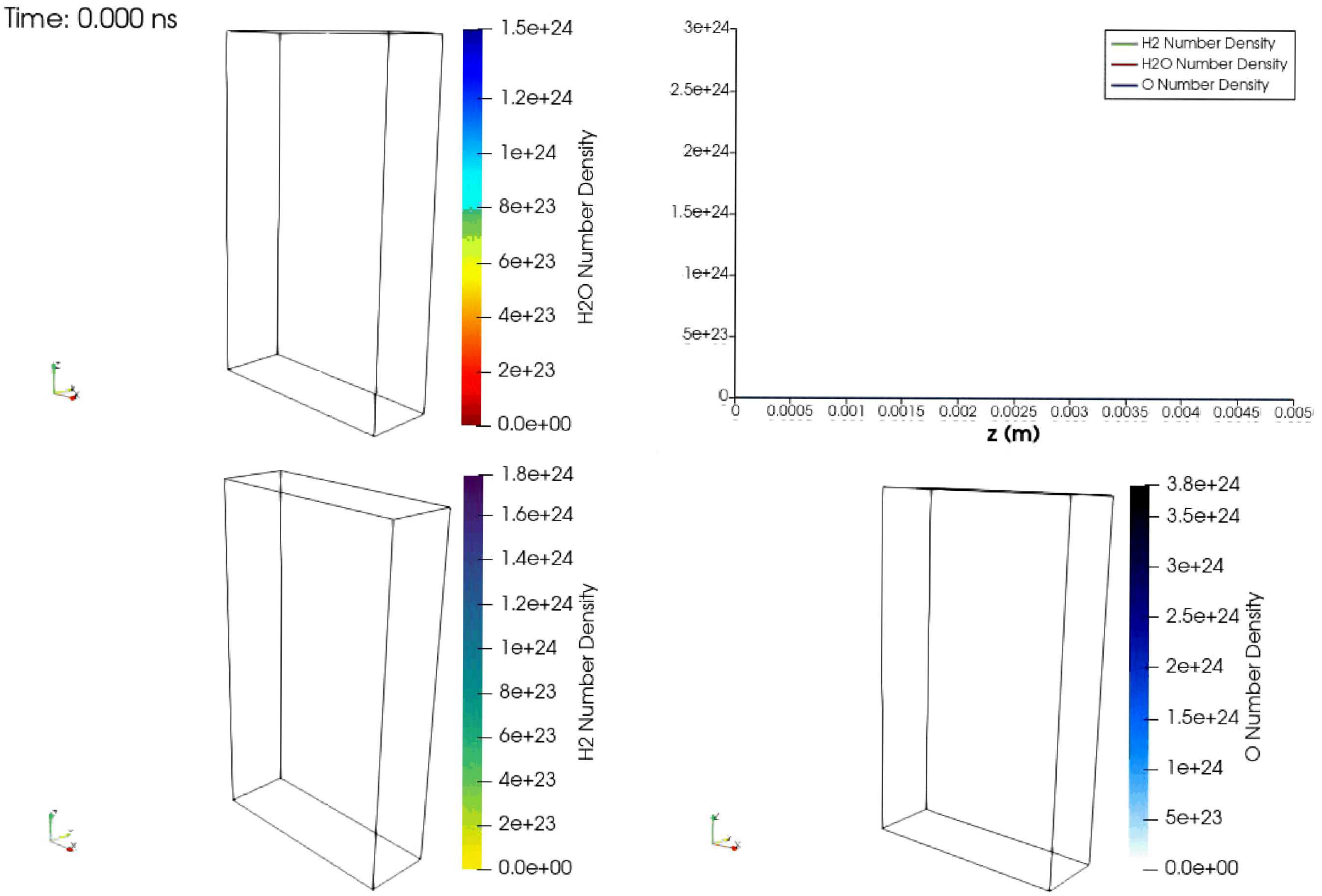
- **Magic particles** fill the domain:
  - count = 1 per cell
  - mass = 1 kg (so mom. transfer is small → stationary)
  - n*sigma chosen to give desired 1 / mfp

- **Use SPIN module**:
  - DSMC collisions of desorbing H2O interact with magic particles with chosen mfp



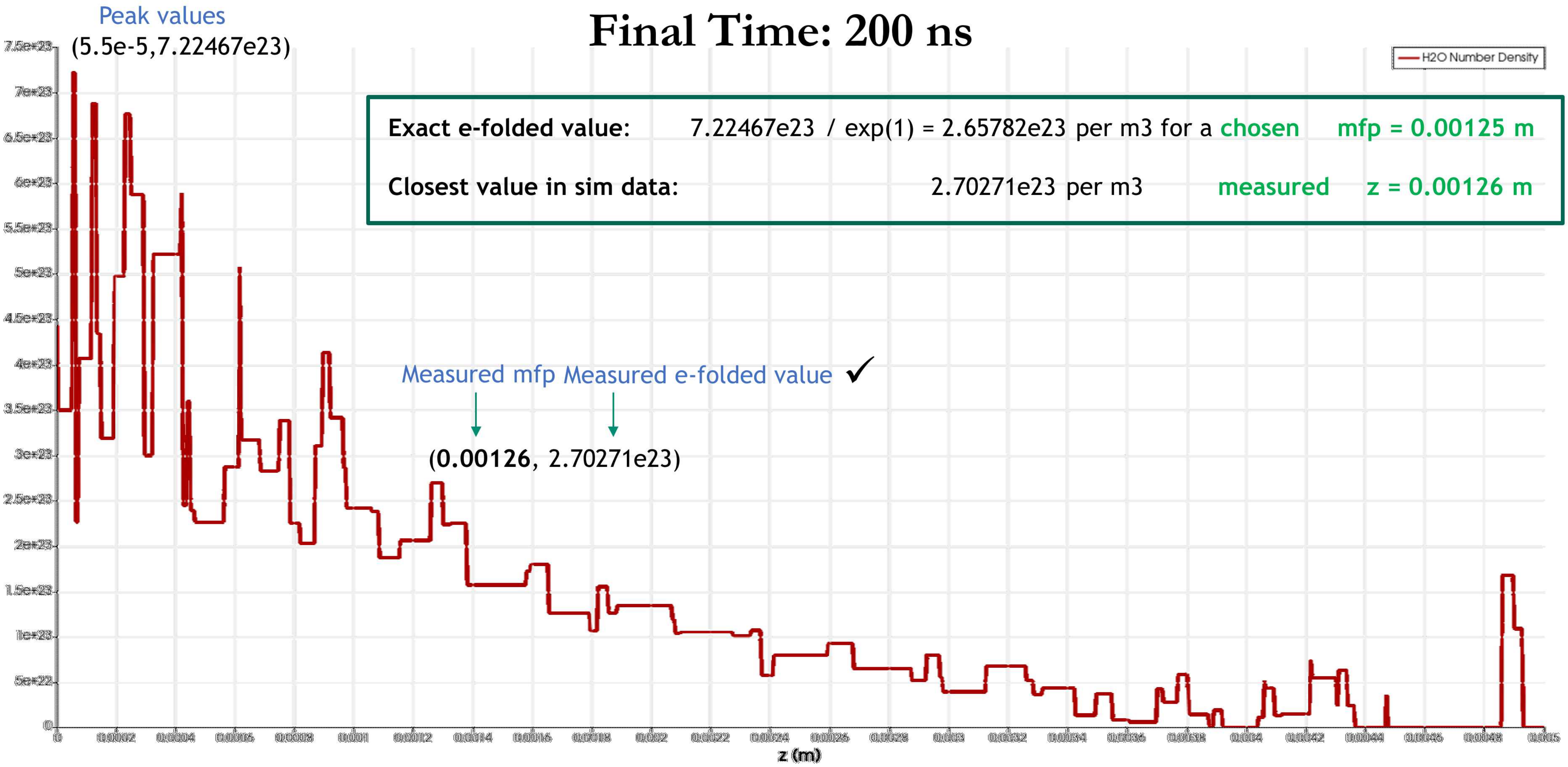


(Power flow 18a): Work-in-progress – plasma desorption model

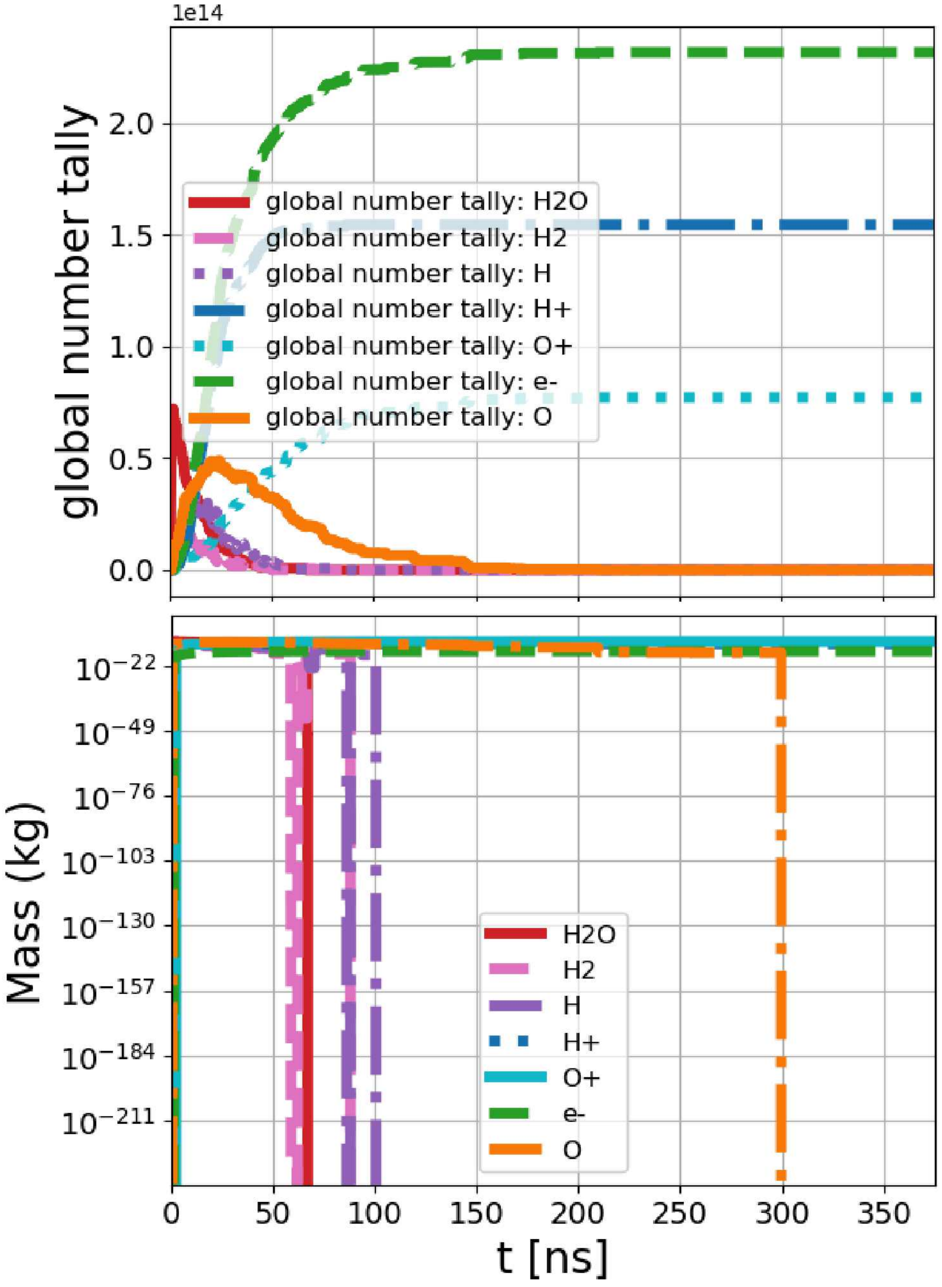


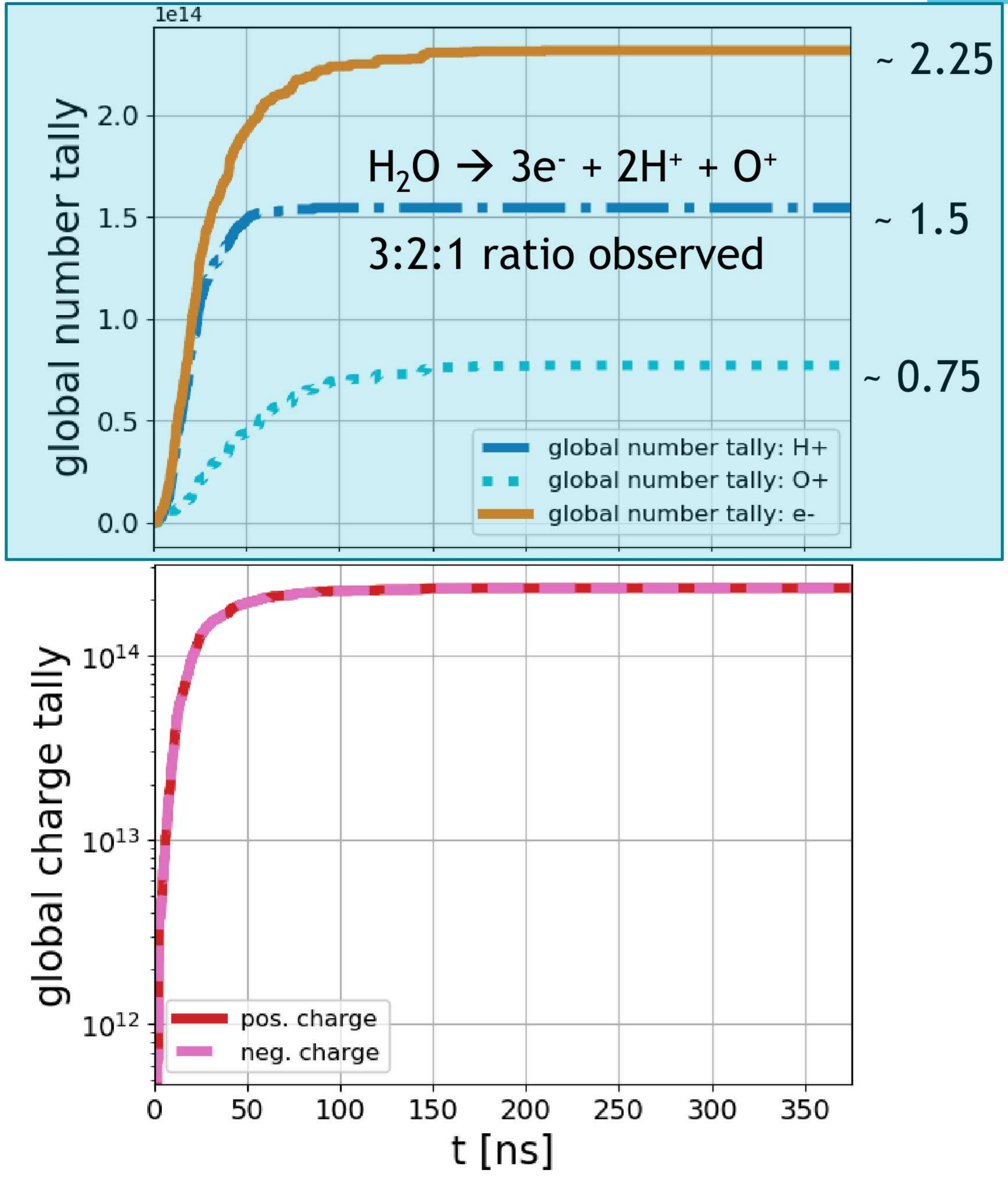
(Power flow 18a): Work-in-progress – plasma desorption model

Final Time: 200 ns

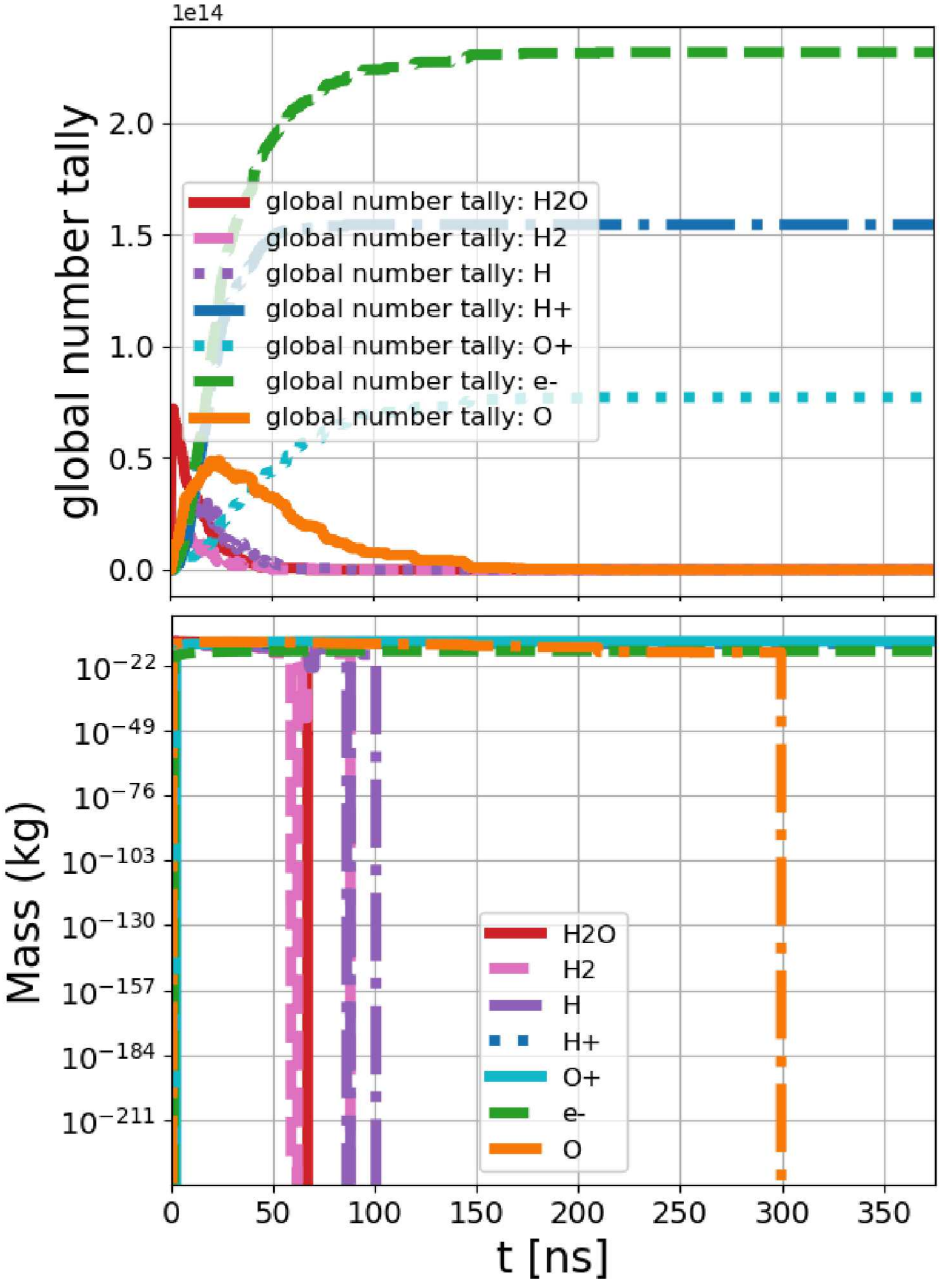


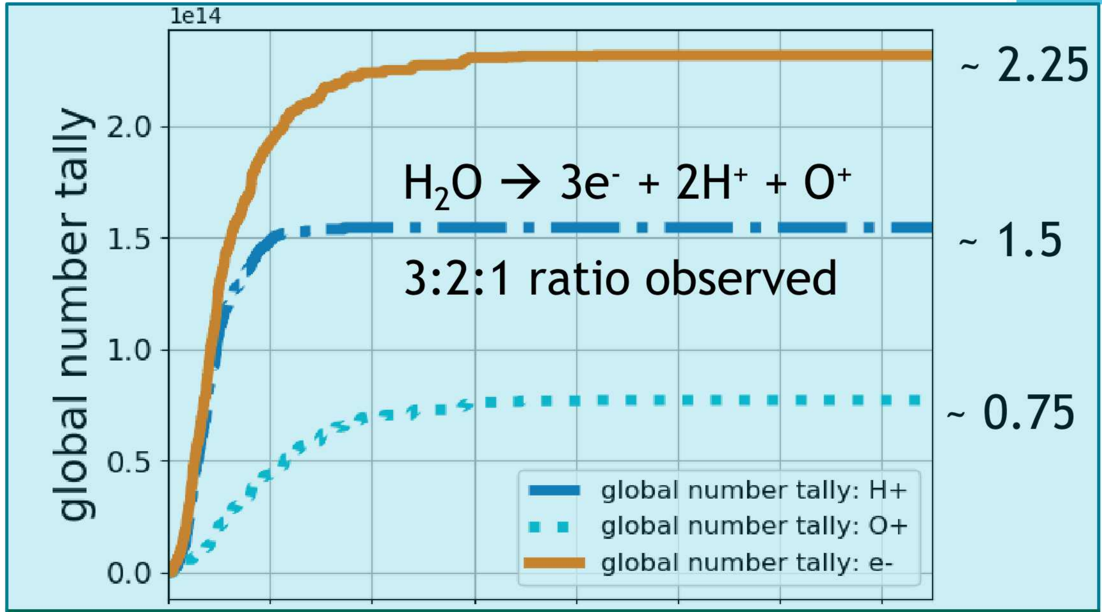
(Power flow 18a): Work-in-progress – plasma desorption model





(Power flow 18a): Work-in-progress – plasma desorption model





Next step: incorporate into EMPIRE-PIC model and troublesooot