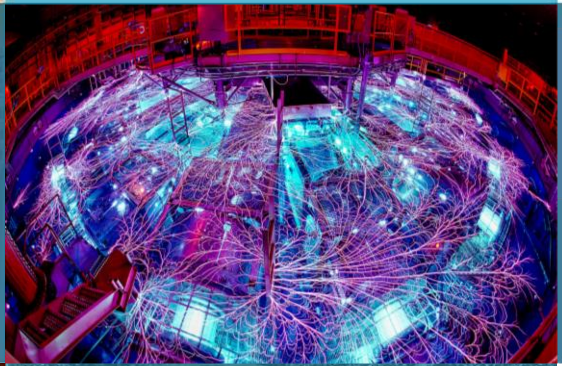
RAMSES impact on Sandia's pulsed power program



RAMSES

Charon CHEETAH EIGER EMPIRE Gemma
ITS NuGET Q SCEPTRE Xyce

Presented by

David Sirajuddin[1]

K. Cartwright[1], P. Christenson[1], R. DePriest[1], J. Douglas[1], M. Hess[1], B. Hutsel[1], C. Moore[1], R. Nicholas[1], N. Roberds[1], R. Pawlowski[1], T. Powell[1], M. Savage[1], R. Shapovalov[3], S. Shields[1], R. Spielman[3], B. Ulmen[1], B. Weber[2]

Trilinos User Group meeting (TUG24)
October 23, 2024, Albuquerque NM USA

[1]Sandia National Laboratories [2]Naval Research Laboratory, [3]University of Rochester

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SAND2024-14492C

Outline

- RAMSES' role in SNL's mission space
- Code overviews: ITS, Empire
- Pulsed power at Sandia
- RAMSES Simulation Results and Impact to Pulsed Power
- Outlook and Future Impacts

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"Stockpile Stewardship Ensuring the nation's nuclear weapons stockpile is safe, secure, and reliable". https://www.sandia.gov/missions/nuclear-weapons.

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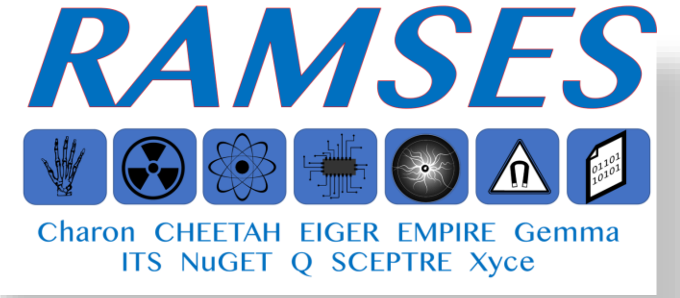
- The **R**adiation **A**nalysis, **M**odeling, and **S**imulation for **E**lectrical **S**ystems (RAMSES) code suite within Sandia's Advance Simulation & Computing (ASC) is an integral capability in supporting Sandia's nuclear deterrence (ND) work and are evolving to meet Sandia's broader Nuclear Deterrence strategy



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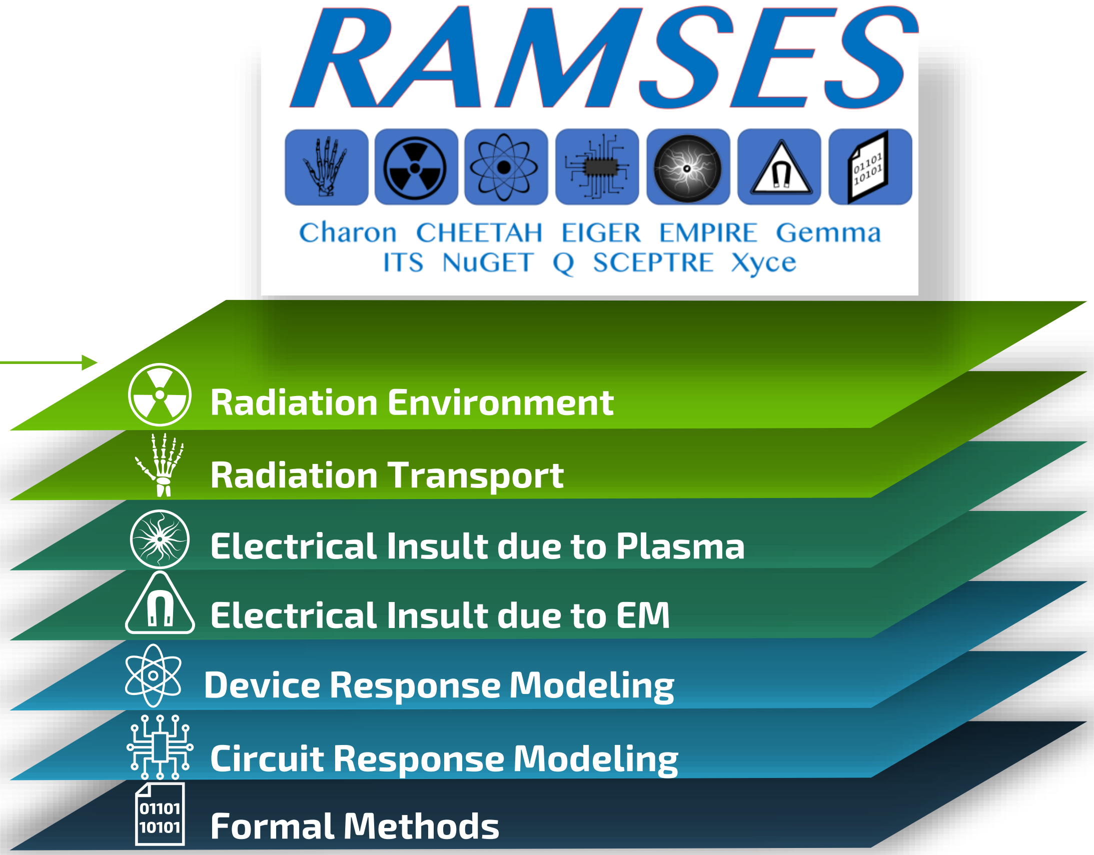

Figure: we envision RAMSES as a "vertical stack" of environment, transport, coupling, and response physics applications wherein each use-case traverses some-or-all of this stack to provide answers.

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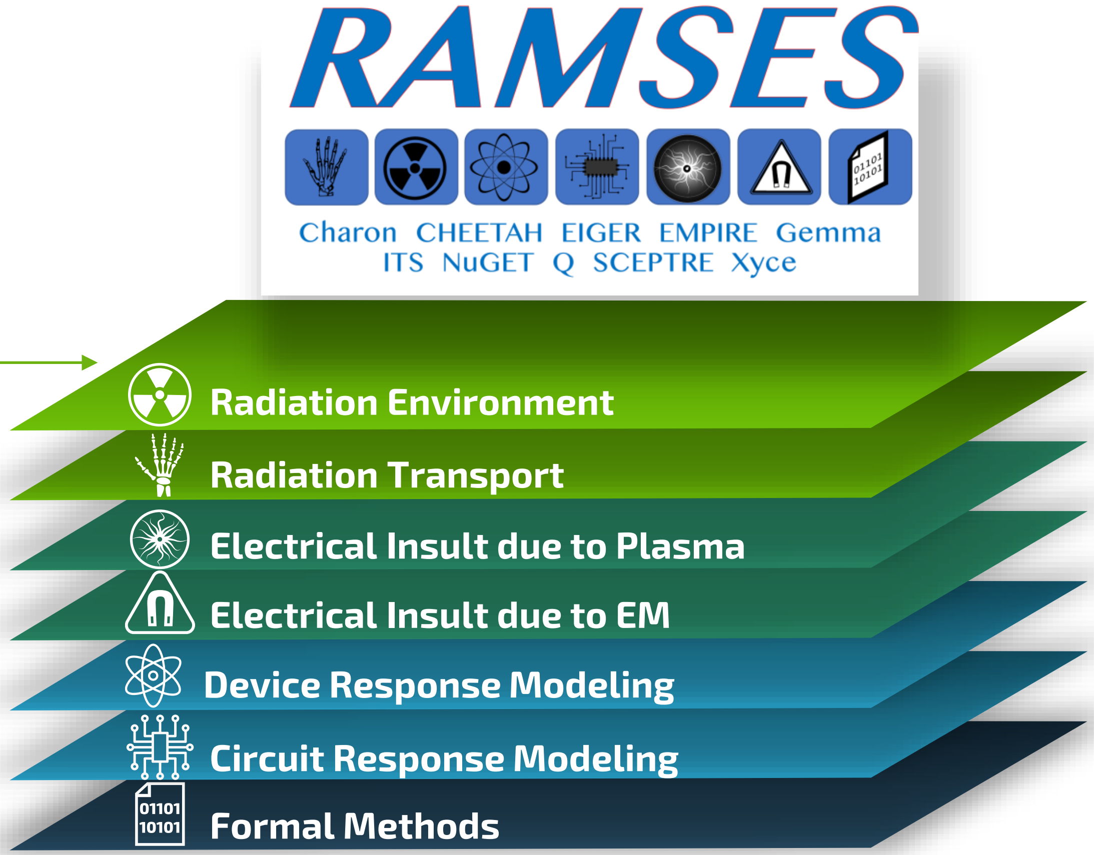

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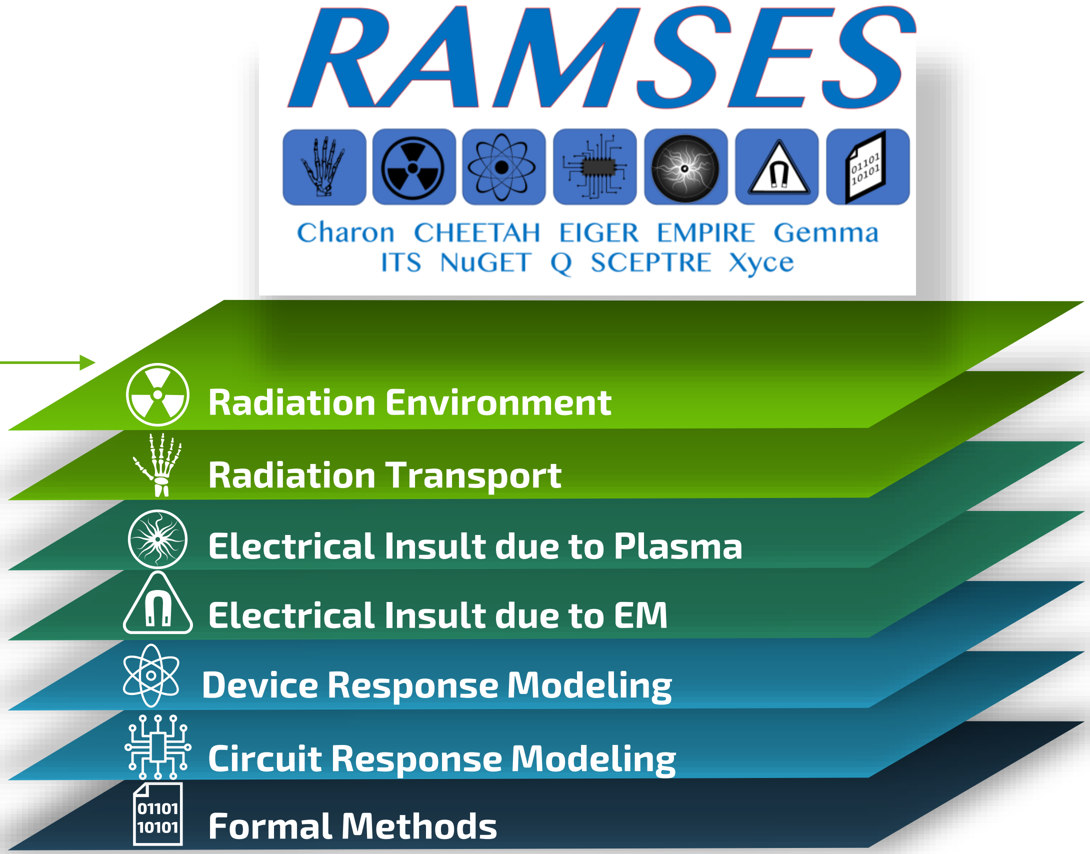
- Scalable solvers, discretization packages, I/O libraries, among others from **Trilinos** are **heavily leveraged and critical to Empire's continued success in simulating these larger problems at feasible computational cost**



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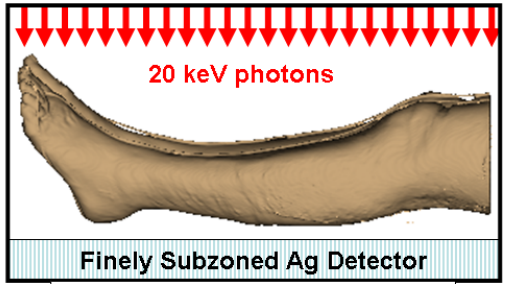
The radiation transport code

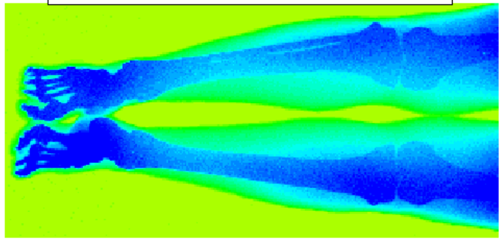
A set of 1D (TIGER), 2D (CYLTRAN), and 3D (ACCEPT) Monte Carlo coupled electron/photon radiation transport codes

Written in Fortran (with CAD and facet geometry capabilities enabled using C++)

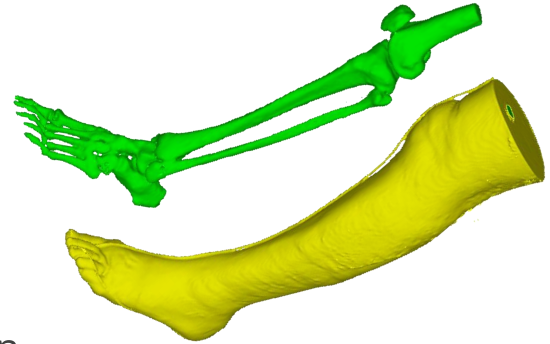
Continuous-energy/multigroup cross sections available through XGEN/CEPXS



Above Bone/Tissue Facet Model Has Over One Million Facets From Visible Human Project®

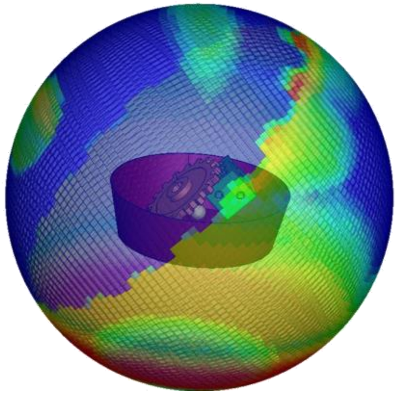


ITS-Simulated Dose(Ag) Distribution



Traditional (Forward) Transport

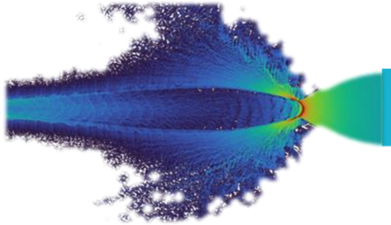
- Tallies for energy and charge deposition (Figures: *right*), photon and electron flux, photon and electron escape, electron surface emission, pulse-height, ….
- Magnetic fields (in materials and voids) and Electric Fields (voids only)



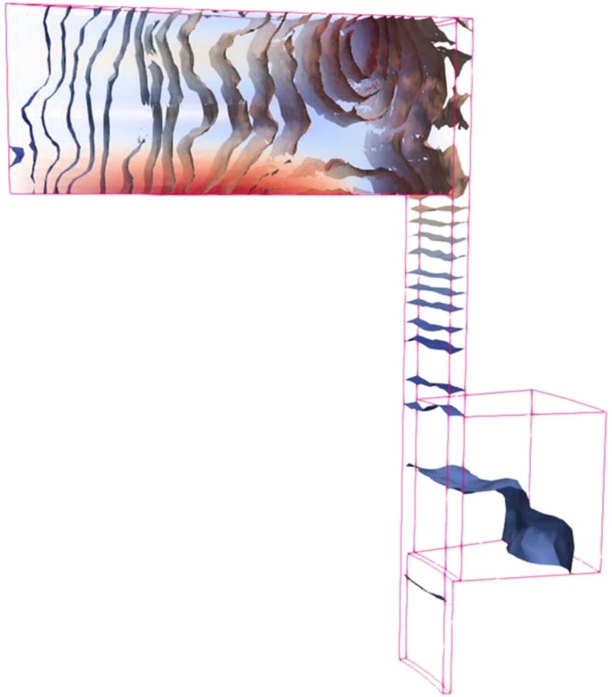
Adjoint mode calculations available in 1D and 3D codes

- Assessing dose from multiple source spectra in a single calculation
- Generating dose response functions that can be used long after the initial calculation.
- A direction-sphere output capability to display a dose-direction map (Figure: left), and associated ray-tracing capability
- Facilitates mass-sectoring calculations, Allows fast scoping of complex geometries

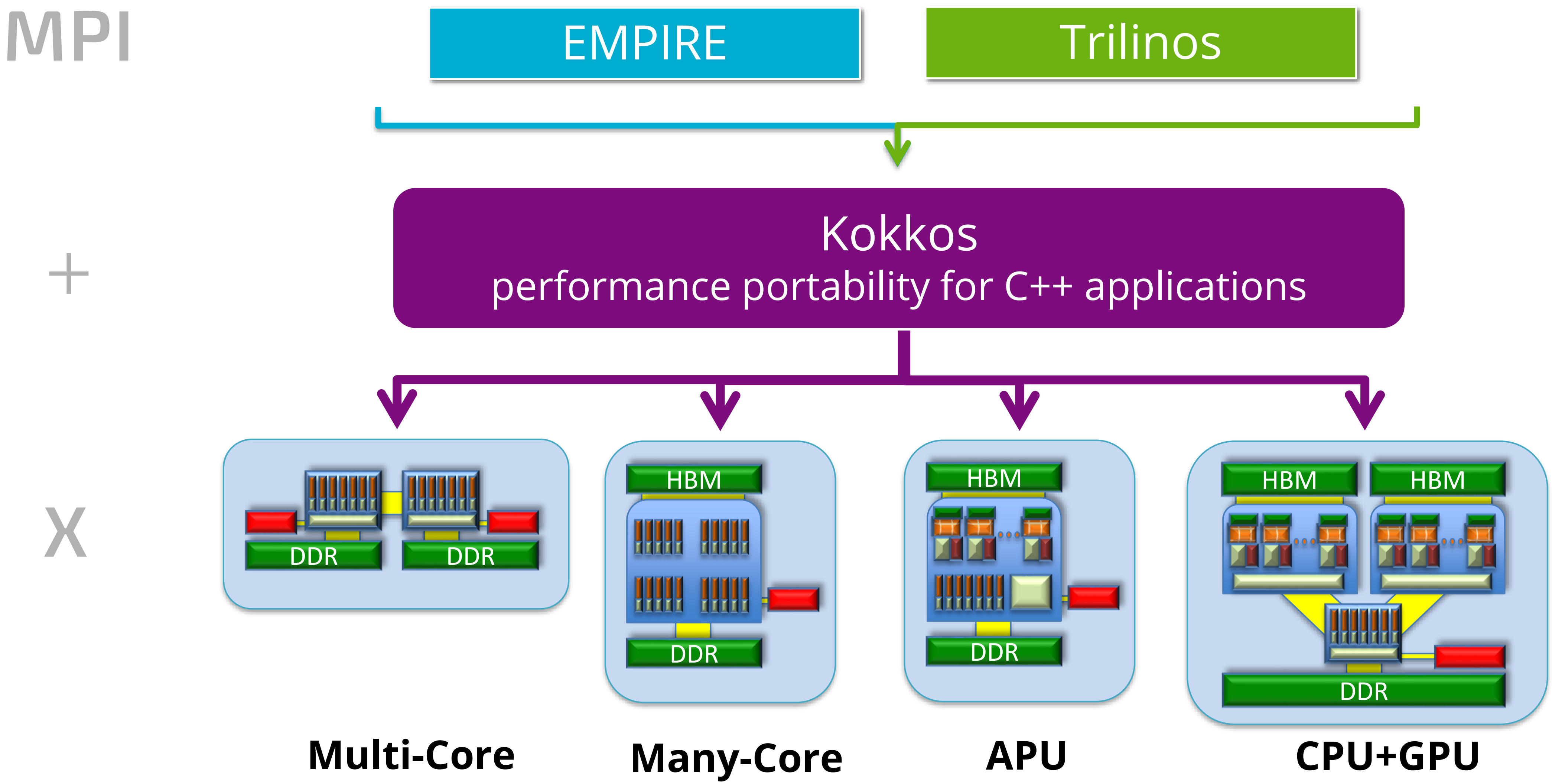
The EMPIRE Plasma Simulation Code



- **Fields** — **Electrostatics** (ES), **Electromagnetics** (EM)
- **Plasma & Neutrals** — **Relativistic PIC**, Stationary **Fluid** (ρ, $\boldsymbol{p}$, $\mathcal{E}$) with Conductivity
- **Photons** — **macroparticle** transport, photoemission, photoionization
- **Discretizations** — *Fields*: Finite Elements + Time integrators (various)
  Particles: Velocity Verlet (+ Boris Push for EM)
  Fluids: Forward Euler, SDIRK
- **Domains** — **0D, 2D** Cylindrical, **2D/3D** Cartesian
- **Meshes** — hex/quad (ES/EM), tet/tri (ES/EM/PIC)
- **Field BCs** — Voltage (ES), **1D circuits** (EM), Periodic, Dirichlet, Z, PML
- **Particle BCs** — Periodic, Reflecting, Diffuse Scattering, Absorbing,
  Secondary emission, Foil transmission
- **Surface models** — e^{-}/ions (beam, **SCL**, GTF), neutrals (**thermal desorption**)
  e^{-}/photons (**ITS/HDS5 source**), **surface heating**
- **Collisions** — **DSMC**, MCC (cross-section or rate-based)
  two body (in)elastic, excitation, **ionization**, CX, chemical reactions
- **Particle controls** — **merge** schemes with **Gauss-law-preserving** techniques
- **Massively parallel** — CPUs, GPUs
- **Performant** — scaling demonstrated to 2048 nodes, 1.3B elements, 65.6B particles
- **Portable** — Kokkos enables coverage for SNL HPCs, NRL (Nautilus, Narwhal), Tri-lab:
  - ✓ LANL Trinity (ATS-1)
  - ✓ LLNL Sierra (ATS-2)
  - ✓ LANL crossroads (ATS-3)
  - ✓ SNL Astra (Vanguard)
  - ❑ LLNL El Capitan (ATS-4)
- **Controls** — **Restart** (checkpoint) capability available
- **Output** — **high fidelity formats**: `Exodus II` (mesh data), `HDF5` (particle data), csv (histories)



Kokkos MPI+X parallelism enables Empire on platforms *without* platform-specific code



Cornerstone for performance portability across next-generation HPC architectures at multiple DOE laboratories, and other organizations

Slide from Cyr, E. C. et al. The EMPIRE Code Suite: Status (Oral Presentation). Z Fundamental Science Workshop (ZFS) 2018. July 29 - August 1, 2018. Albuquerque, NM USA. SAND2018-8046C

Trilinos Use in EMPIRE: package list

Data Services

- **Teuchos** — Param lists
- **Kokkos, KokkosKernels** — Portability
- **Tpetra** — Linear algebra builder
- **Zoltan2** — Mesh decomposition
- **Pamgen** — inline mesh generation

Discretiz

- **Shards** — Cell topologies
- **Intepid2** — FE basis library
- **Phalanx** — DAG assembly
- **Panzer** — Front end to SEACAS, STK, Percept
- **SEACAS** — I/O Exodus
- **STK** — Sierra Mesh Toolkit
- **Percept** — Mesh refinement

Linear Solvers

- **Belos** — Krylov
- **Ifpack2** — Iterative methods (Jacobi, SOR, …)
- **Amesos2** — Sparse direct solvers
- **Anasazi** — Eigen solvers
- **Stratimikos** — Front end to solvers
- **Teko** — Seg block solvers
- **MueLu** — Algebraic Multigrid

Nonlinear Solvers

- **Thyra** — Alg abstraction
- **NOX** — Newton-based solvers

Empire directly uses 22 packages (enables 38 due to dependencies)

Trilinos use in `Empire`'s numerical approach: FEM-PIC

Empire's Particle-in-Cell (PIC) scheme solves the equations of motion

$$\frac{d\boldsymbol{x}_p(t)}{dt} = \boldsymbol{v}_p(t),$$

$$\frac{d\boldsymbol{v}_p(t)}{dt} \equiv \boldsymbol{a}_p(t) = \frac{q_p}{m_p}\left[\boldsymbol{E}(t,\boldsymbol{x_p}(t)) + \boldsymbol{v}_p(t) \times \boldsymbol{B}(t,\boldsymbol{x_p}(t))\right]$$

encoded by the *plasma kinetic equation* for each particle (p):

$$\frac{df(t,\boldsymbol{x},\boldsymbol{v})}{dt} \equiv \frac{\partial f}{\partial t} + \boldsymbol{v}\cdot\frac{\partial f}{\partial \boldsymbol{x}} + a\cdot\frac{\partial f}{\partial \boldsymbol{v}} = \left(\frac{\partial f}{\partial t}\right)_{coll}$$

with fields evolved according to the Maxwell curl equations:

$$\frac{\partial \boldsymbol{B}}{\partial t} = -\nabla \times \boldsymbol{E}$$

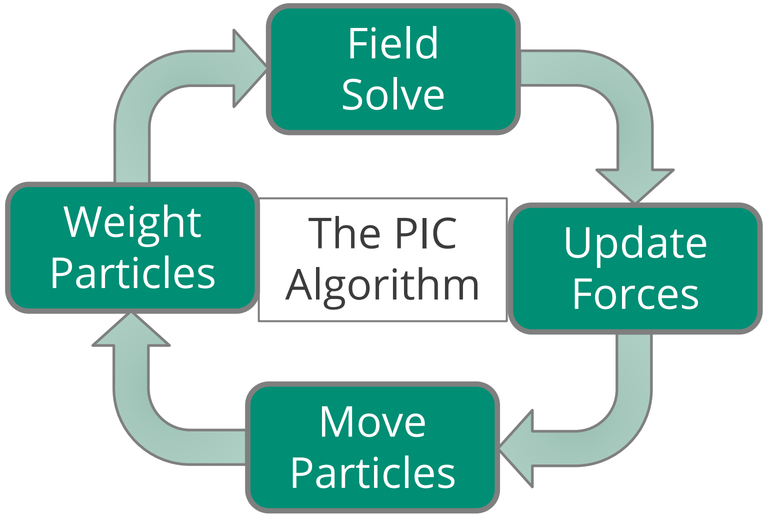
$$\frac{\partial \boldsymbol{E}}{\partial t} = \frac{1}{\epsilon\mu}\nabla \times \boldsymbol{B} - \frac{1}{\epsilon}\boldsymbol{J}$$

$$\xrightarrow[\text{solved in weak form}]{\text{solved in strong form}}$$

$$\begin{pmatrix} \Delta t^{-1}\mathbb{I}_{\mathcal{F}} & \mathbb{K}_h \\ -\mathbb{K}_h^T\mathbb{M}_{\mathcal{F}}(\mu^{-1}) & \Delta t^{-1}\mathbb{M}_{\mathcal{E}}(\epsilon) \end{pmatrix} \begin{pmatrix} \Delta\mathbf{B} \\ \Delta\mathbf{E} \end{pmatrix} = -\begin{pmatrix} \mathbf{r}_{\mathbf{B}} \\ \mathbf{r}_{\mathbf{E}} \end{pmatrix}$$

where $\mathbb{K}$ = discrete curl operator, $\mathbb{M}$ = mass matrix, $\mathbb{I}$ = identity matrix, $\mathcal{F}$ and $\mathcal{E}$ label operators acting on face and edge spaces, h is the characteristic mesh dimension which labels quantities as spatially discretized versions of their continuum counterparts, Δt = timestep width, $\boldsymbol{r}$ = residuals

Using compatible discretization decisions[2,3] ensures the Maxwell divergence constraints are satisfied for all time



Flow diagram showing a pure PIC timestep[1]

[1] Pawlowski, R. et al. *EMPIRE: A Performance Portable Plasma Simulation Code* (Oral presentation). 2021 Trilinos User Group Meeting (TUG21). SAND2021-15038C
[2] Nédélec J-C. *Mixed finite elements in* $\mathbb{R}^3$. Numerische Mathematik, 35(3):315–341, 1980.
[3] Raviart P-A. and Thomas, J. T. *A mixed finite element method for 2nd order elliptic problems*. Mathematical aspects of finite element methods, volume 606, pages 292–315. 1977

Trilinos use in `Empire` *Example*: EM Solver

$$\begin{pmatrix} \Delta t^{-1}\mathbb{I}_{\mathcal{F}} & \mathbb{K}_h \\ -\mathbb{K}_h^T \mathbb{M}_{\mathcal{F}}(\mu^{-1}) & \Delta t^{-1}\mathbb{M}_{\mathcal{E}}(\epsilon) \end{pmatrix} \begin{pmatrix} \Delta\mathbf{B} \\ \Delta\mathbf{E} \end{pmatrix} = -\begin{pmatrix} \mathbf{r}_{\mathbf{B}} \\ \mathbf{r}_{\mathbf{E}} \end{pmatrix}$$

$$\mathbf{B} \in \mathbf{H}_{\nabla\cdot}(\Omega)$$

$$\mathbf{E} \in \mathbf{H}_{\nabla\times}(\Omega)$$

Block LU Decomposition

$$\begin{pmatrix} \Delta t^{-1}\mathbb{I}_{\mathcal{F}} & \mathbb{K}_h \\ -\mathbb{K}_h^T \mathbb{M}_{\mathcal{F}}(\mu^{-1}) & \Delta t^{-1}\mathbb{M}_{\mathcal{E}}(\epsilon) \end{pmatrix} = \begin{pmatrix} \mathbb{I}_{\mathcal{F}} & 0 \\ -\Delta t \mathbb{K}^T \mathbb{M}(\mu^{-1}) & \mathbb{I}_{\mathcal{E}} \end{pmatrix} \begin{pmatrix} \Delta t^{-1}\mathbb{I}_{\mathcal{E}} & \mathbb{K}_h \\ 0 & \mathbb{S}_{\mathcal{E}} \end{pmatrix}$$

Assemble Schur Compliment as monolithic matrix

$$\mathbb{S}_{\mathcal{E}} = \Delta t^{-1}\mathbb{M}_{\mathcal{E}}(\epsilon) + \Delta t \mathbb{K}_h^T \mathbb{M}(\mu^{-1})\mathbb{K}_h$$

Solve for $\Delta\boldsymbol{E}$ with PCG:

$$\mathbb{S}_{\mathcal{E}}\Delta\mathbf{E} = -\mathbf{r}_{\mathbf{E}} + \Delta t \mathbb{K}_h^T \mathbb{M}(\mu^{-1})\mathbf{r}_{\mathbf{B}}$$

Explicit back solve for $\Delta\boldsymbol{B}$:

$$\Delta\mathbf{B} = -\Delta t \mathbb{K}_h \Delta\mathbf{E} - \Delta t \mathbf{r}_{\mathbf{B}}$$

Meshing:
STK, Percept, SEACAS, Panzer

Data Structures:
Kokkos, KokkosKernels, Tpetra

Assembly:
Shards, Intrepid2, Panzer, Thyra

Linear Solve:

- Uses RefMaxwell AMG with Conjugate Gradient
- Chebyshev smoother
- Precond setup once
- Belos, Teko, MueLu, Ifpack2, Amesos2, KokkosKernels, Zoltan2

Bettencourt, et. al., *EMPIRE-PIC: A Performance Portable Unstructured Particle-in-Cell Code*, 2021
Lourenco Beirao de Veiga, Konstantin Lipnikov, and Marco Manzini, *Mimetic Finite Difference Method for Elliptic Problems*.
Bochev et al., *An algebraic multigrid approach based on a compatible gauge reformulation of Maxwell's equations*, 2008.

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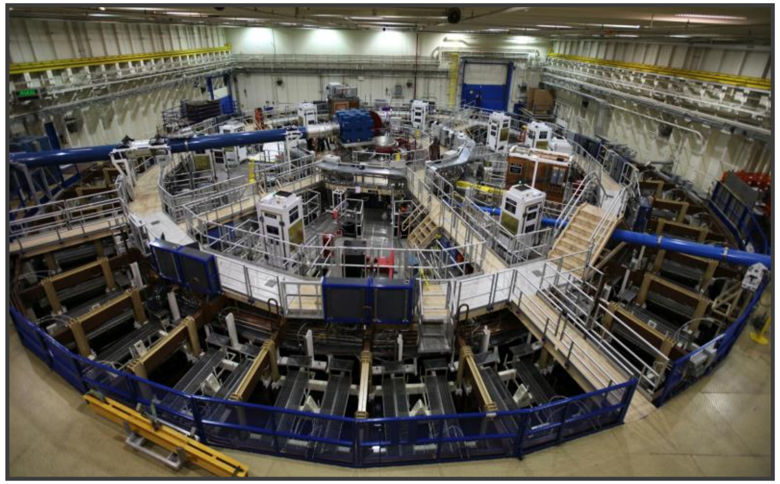
Pulsed Power at Sandia



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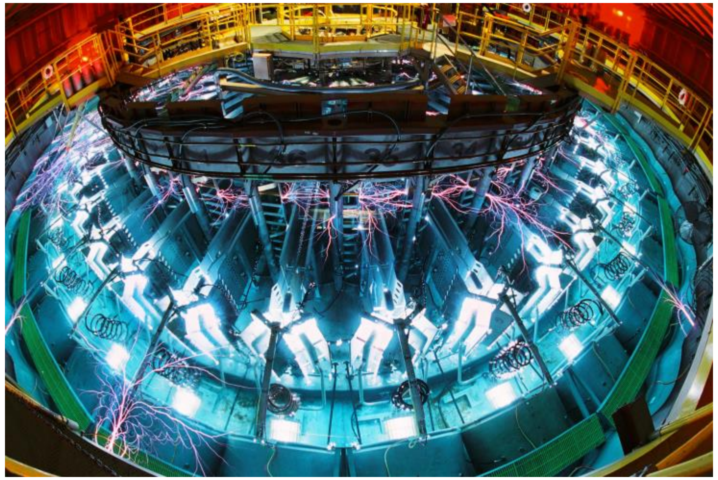
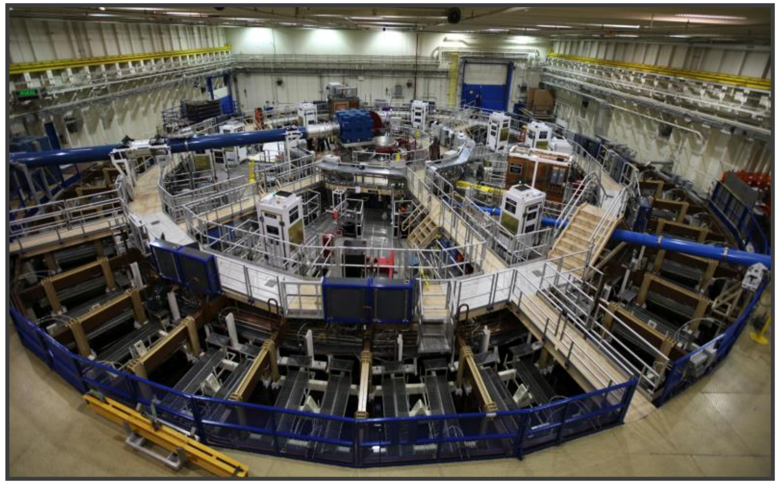


Saturn

HERMES-III

[1]Note: only the "big 3" are shown above, see https://www.sandia.gov/pulsed-power/research-facilities/ for more a more expansive list, including "smaller" machines

Pulsed Power at Sandia



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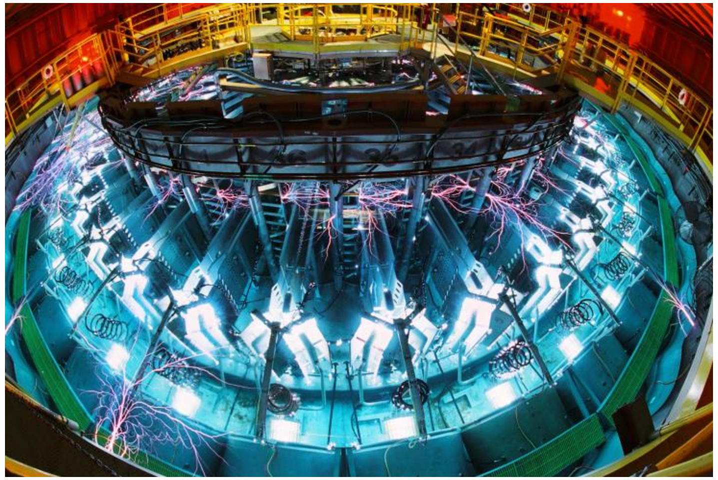

Saturn

HERMES-III

- Delivering on national security: survivability testing

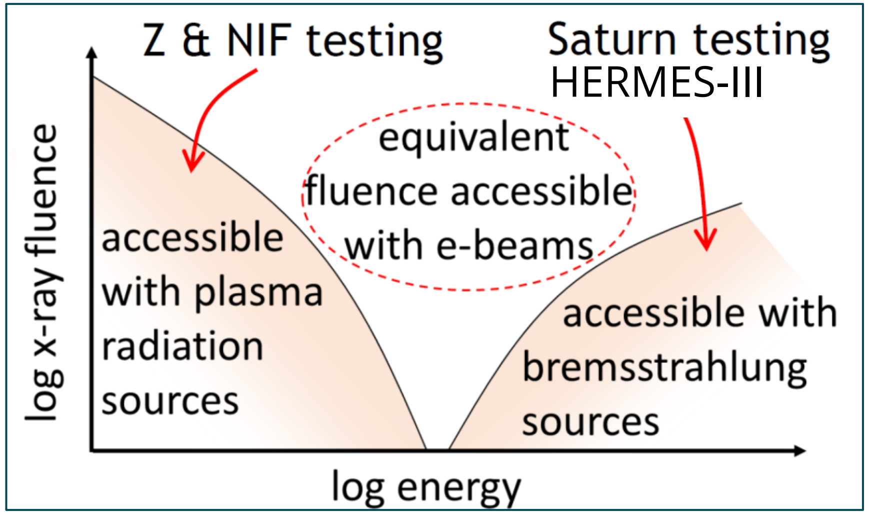

Figure: PPAs create the radiation environments critical for the nation's weapon survivability testing

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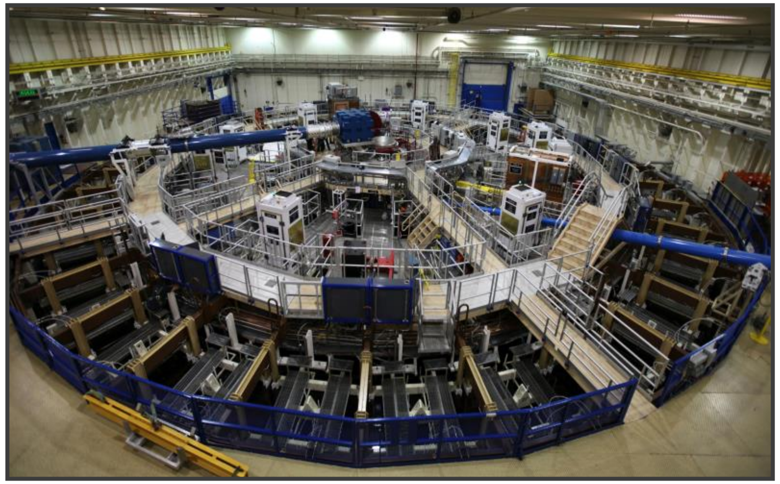

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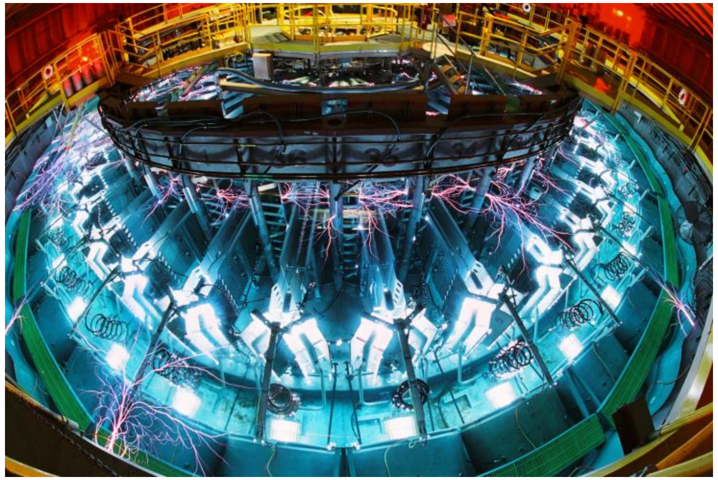
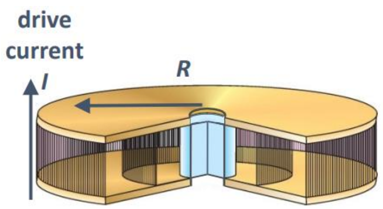


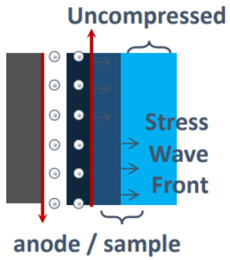
Saturn

HERMES-III

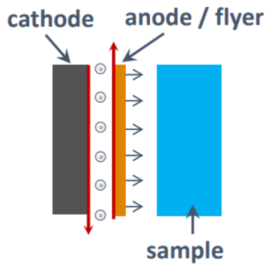
- Delivering on national security: survivability testing
- Enabling "big science" research[2]: material EOS, opacities HED physics, fusion



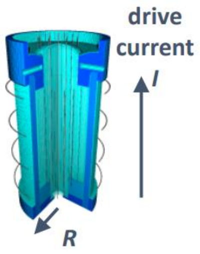
X-ray sources



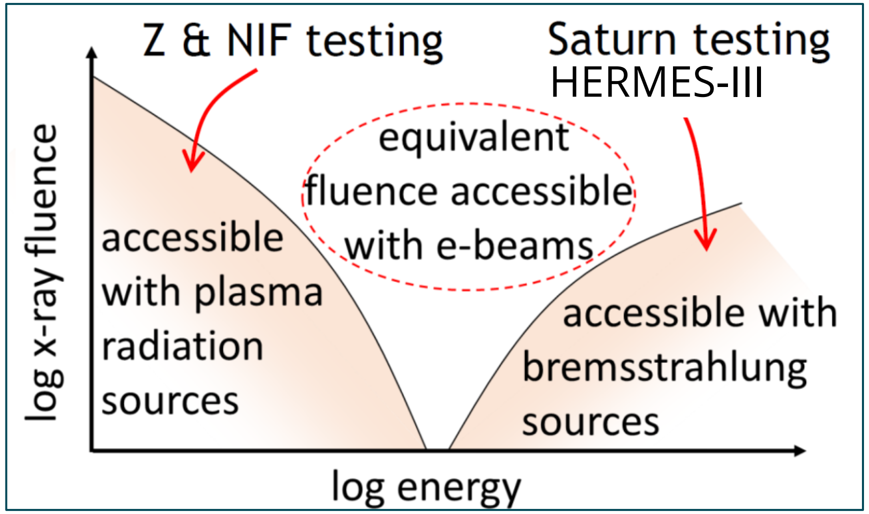
isentropic compression expts



shock expts



fusion



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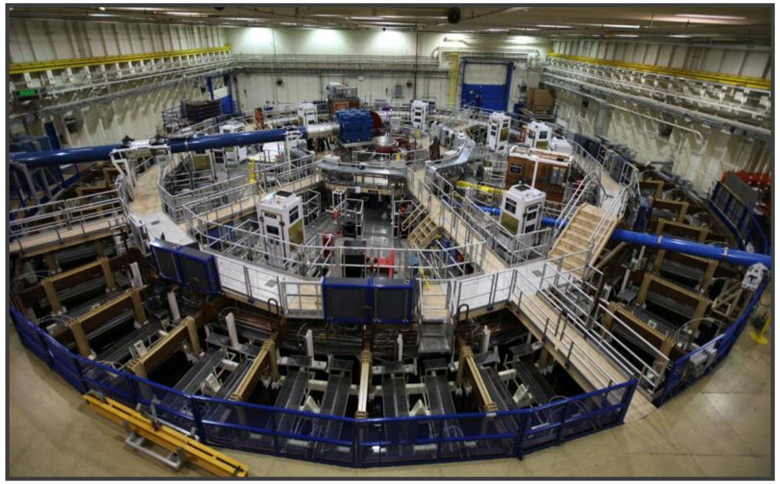
[2]Target figures from D. Sinars et al. *Review of pulsed power-driven high energy density physics research on Z at Sandia.* Phys. Plasmas 27, 070501 (2020)

Pulsed Power at Sandia



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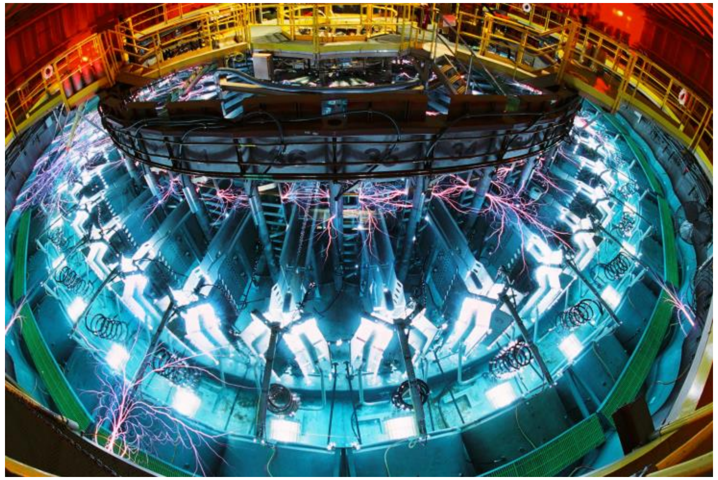


Saturn

HERMES-III

- Delivering on national security: survivability testing
- Enabling "big science" research[2]: material EOS, opacities HED physics, fusion
- **There is significant programmatic interest to progress modeling capabilities such as RAMSES** to enable simulation-based decisions in pulsed power: to support refurbishments, to vet new ideas for meeting design targets, and to extrapolate into new operating spaces

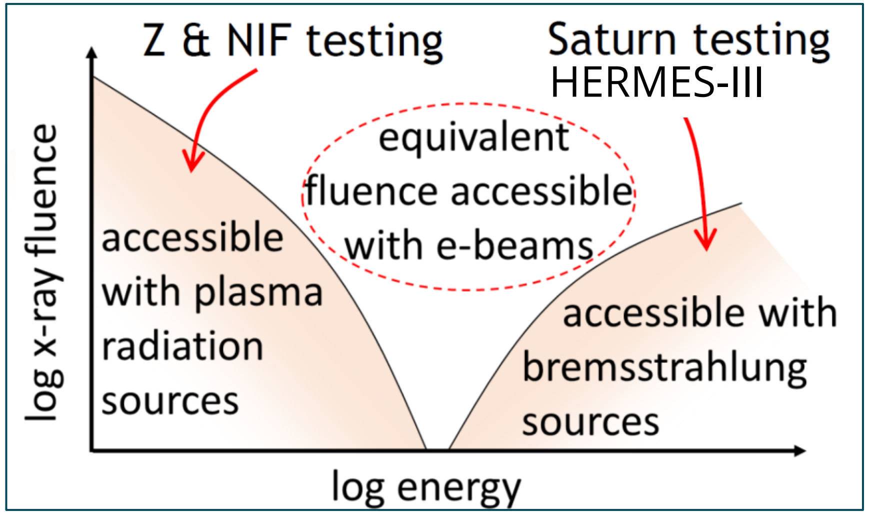


Figure: PPAs create the radiation environments critical for the nation's weapon survivability testing

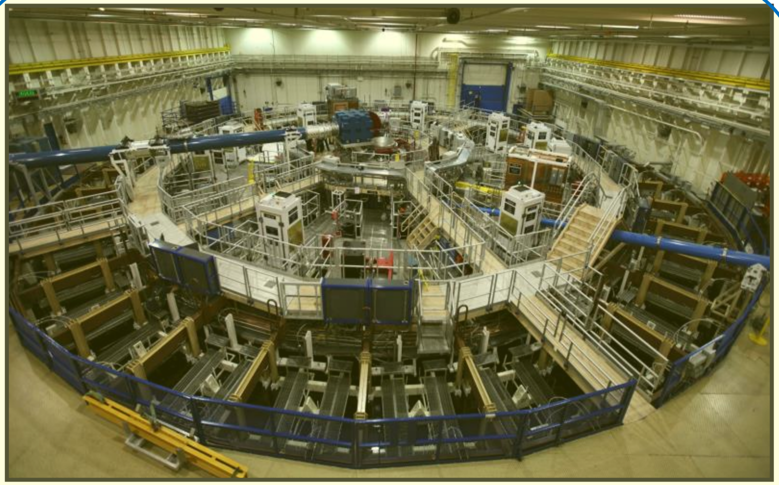
[1]Note: only the "big 3" are shown above, see https://www.sandia.gov/pulsed-power/research-facilities/ for more a more expansive list, including "smaller" machines

[2]Target figures from D. Sinars et al. *Review of pulsed power-driven high energy density physics research on Z at Sandia.* Phys. Plasmas 27, 070501 (2020)

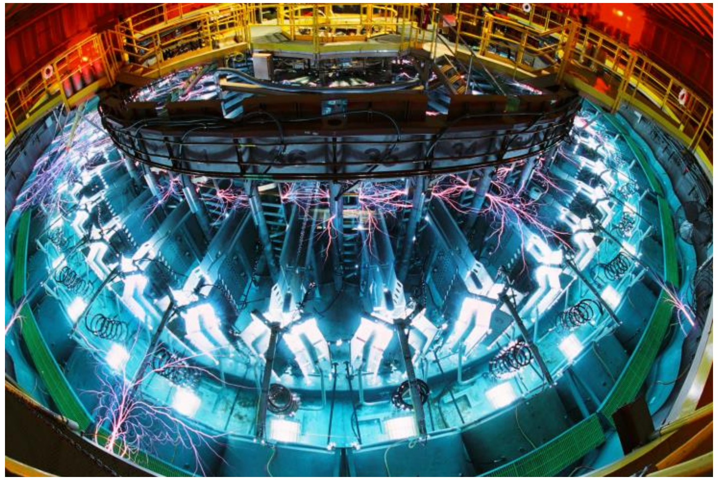
Outline

- RAMSES' role in SNL's mission space
- Code overviews: ITS, Empire
- Pulsed power at Sandia
- RAMSES Simulation Results and Impact to Pulsed Power
- Outlook and Future Impacts

RAMSES Simulation Results and Impact to Pulsed Power



Z



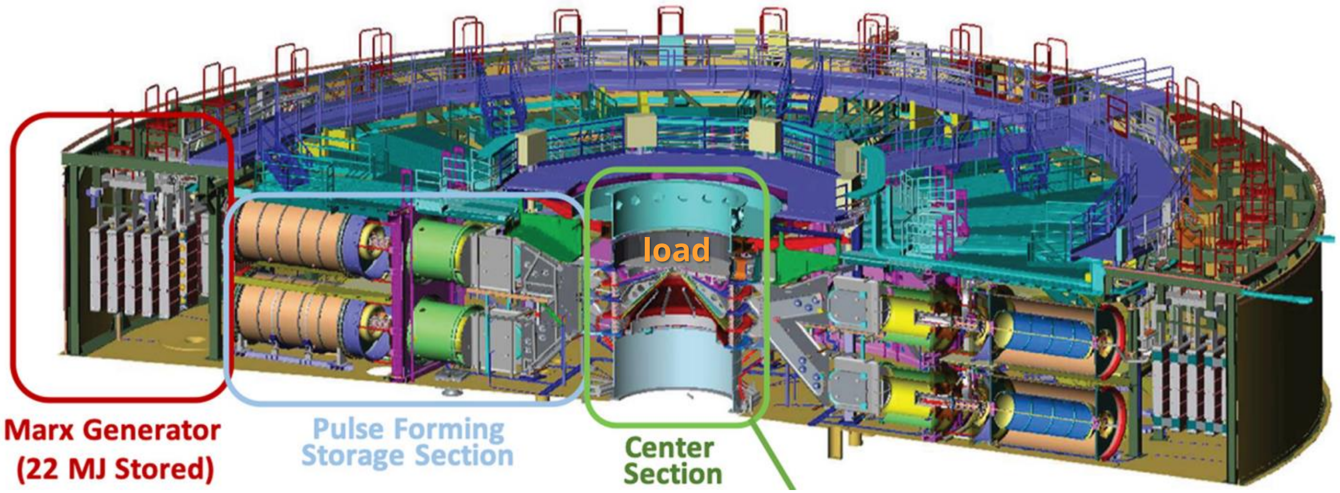
Saturn

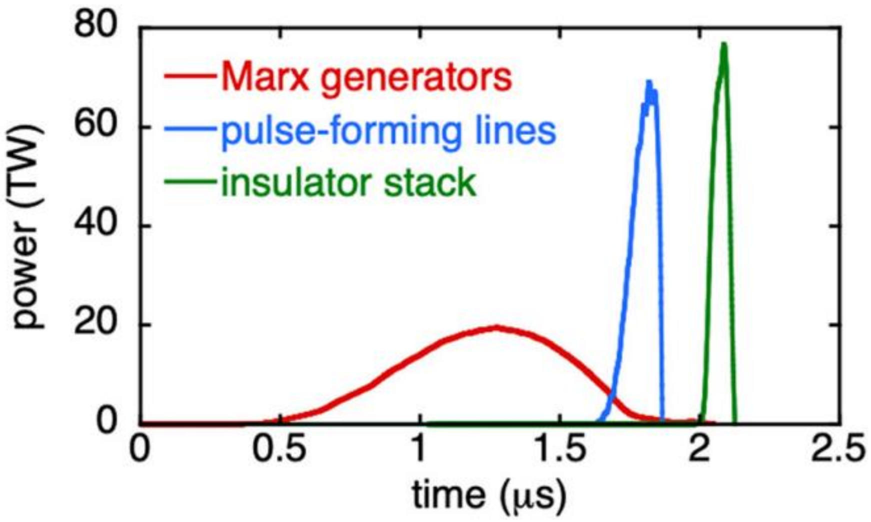
HERMES-III

- *Work covered in this talk*: Z upgrade
- *Work impacting behind-the-scenes*: next-generation pulsed-power (NGPP)

System Overview: Z accelerator

*An 80 TW pulsed-power accelerator used to drive various **loads** spanning cold X-ray sources (e.g., Tungsten wire arrays), flyer plates (dynamic materials research), implosion targets (EOS and opacities research), and fusion targets (MagLIF)*





Pulsed-power driver:

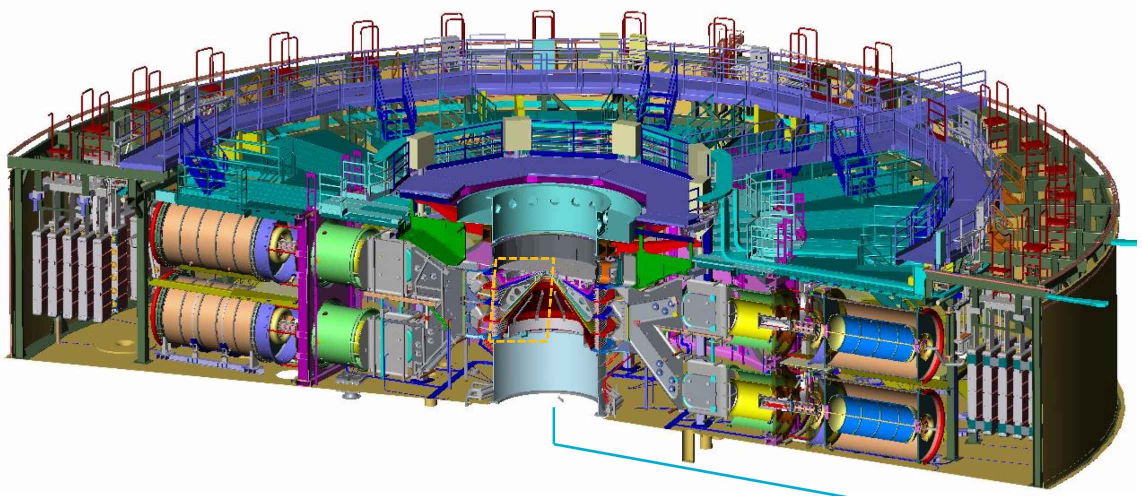
- Marx generators → pulse-forming lines → convolute → load
  ≤ 26 MA (80 TW) peak; load dependent

- Energy storage: 36 Marx banks, 20 MJ total
- Pulse Compression: 1.5 μs → 600 ns → 100 ns

Figures from D. Sinars et al. *Review of pulsed power-driven high energy density physics research on Z at Sandia.* Phys. Plasmas 27, 070501 (2020)

Computational challenges on Z: vastness of scales

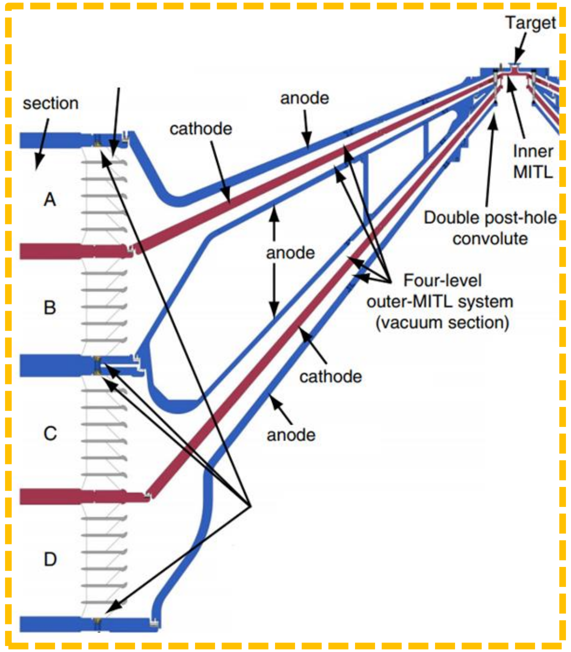
Power flow over system size



system size	(m)
pulse duration	(100 ns)
EM wave speeds in media	$(v/c \leq 1)$
near-vacuum	$(10^{-5}$ Torr)

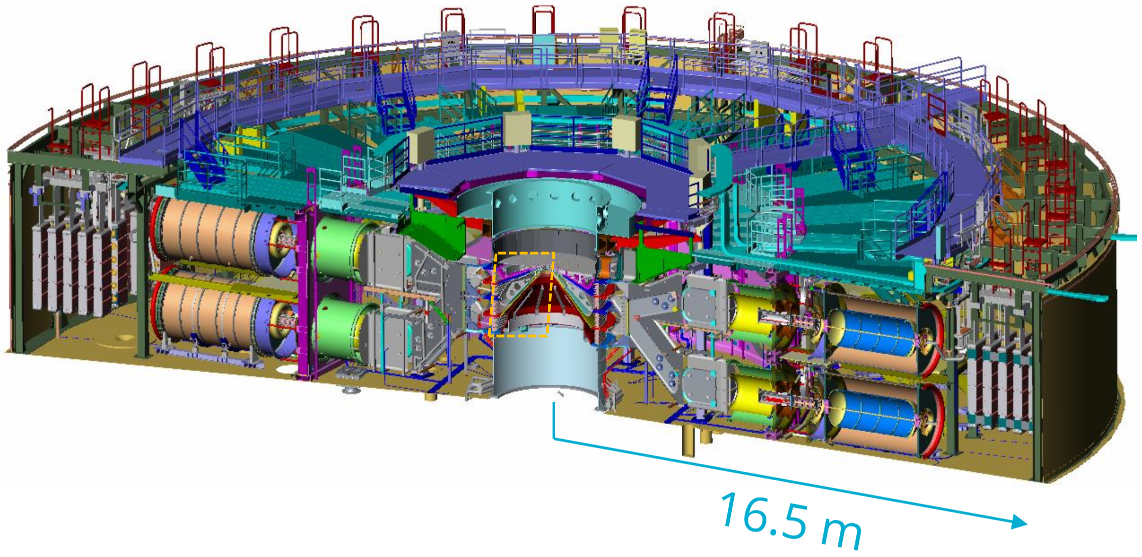
Computational challenges on Z: vastness of scales

Detailed MITL physics



vs.

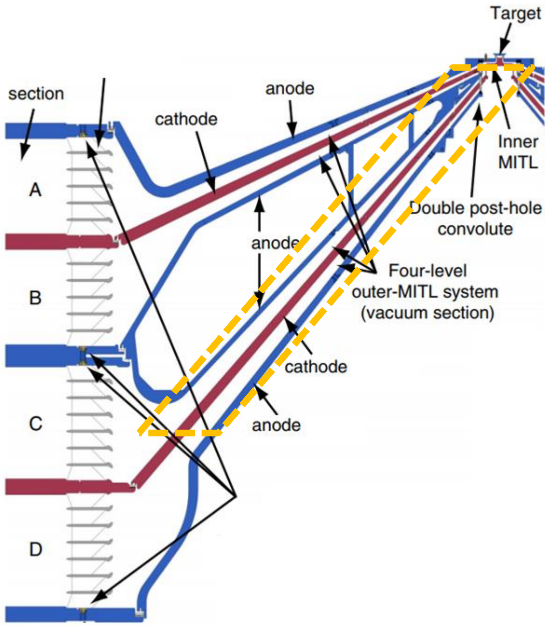
Power flow over system size



space:	Debye lengths	(μm)	vs.	system size	(m)
time:	electron freqs	(THz)	vs.	pulse duration	(100 ns)
velocities:	desorbed neutrals	($v/c \sim 10^{-6}$)	vs.	EM wave speeds in media	($v/c \leq 1$)
densities:	plasma densities	($\leq 10^{18}\ \mathrm{cm}^{-3}$)	vs.	near-vacuum	(10^{-5} Torr)

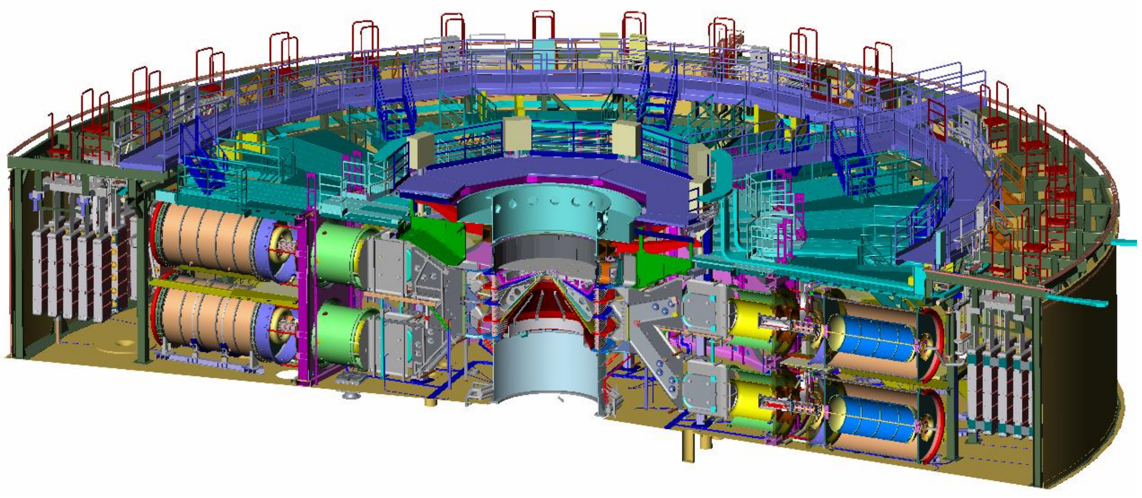
Computational challenges on Z: multitude of processes

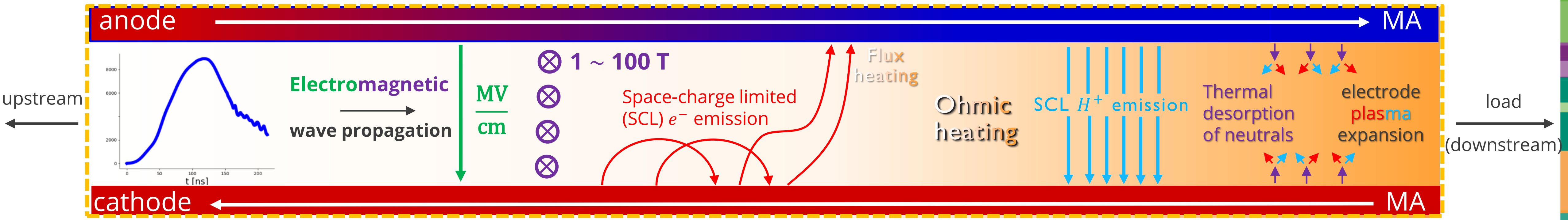
Detailed MITL physics



vs.

Power flow over system size



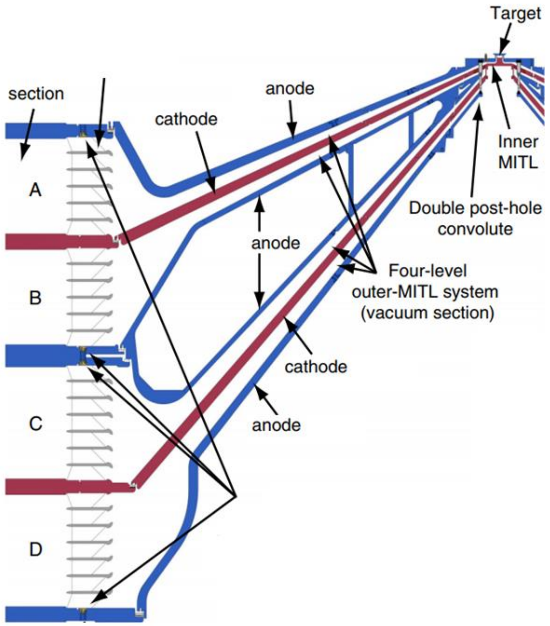


Most germane processes to correctly simulating pulsed power operation, i.e. a non-exhaustive list!

How can we simulate a meters-long system requiring micron resolution over 100 ns at 10^{-14}s timesteps?

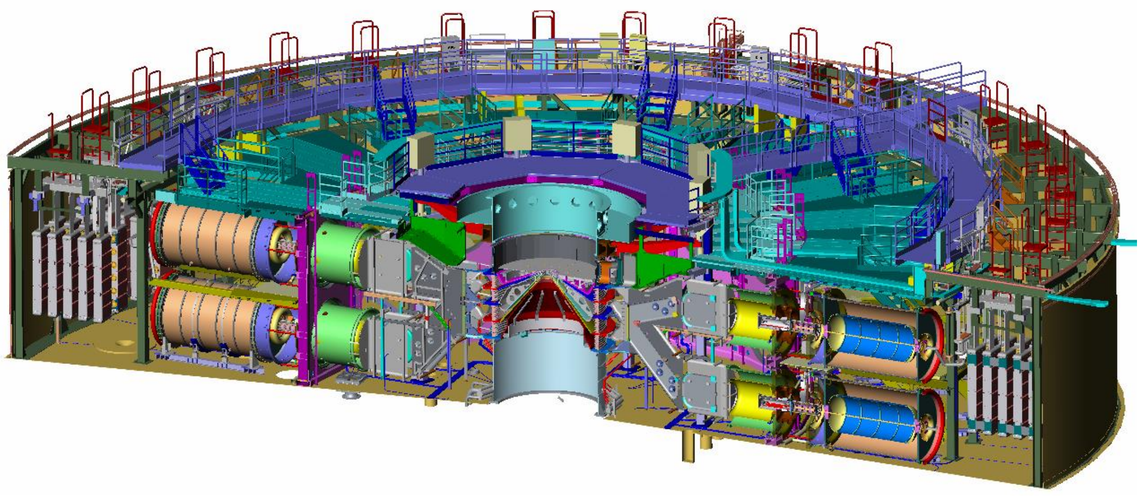
Computational challenges on Z

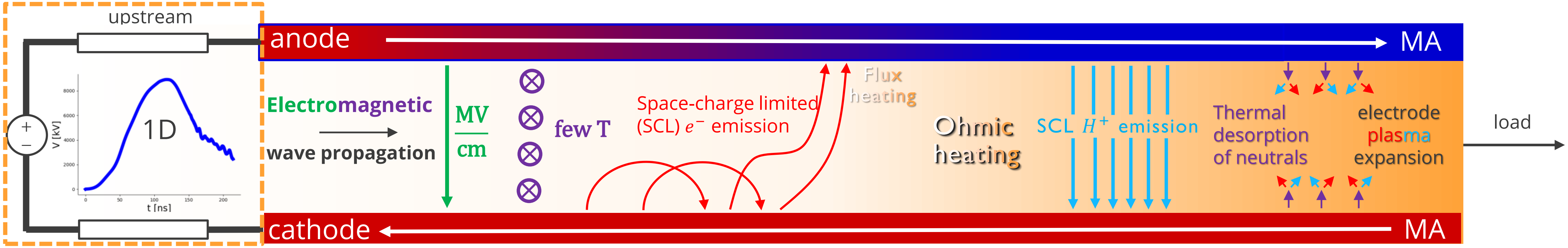
Detailed MITL physics



vs.

Power flow over system size

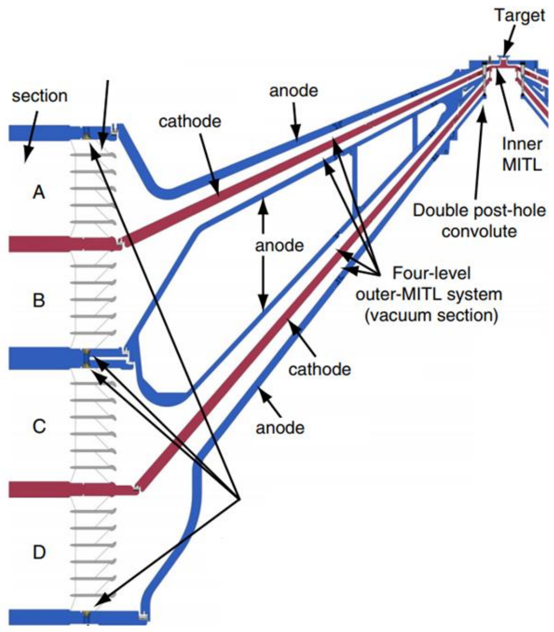




Solution: 1D-3D computational model – TEM wave propagation in 1D transmission line domains (meters) are coupled to a single 3D EM-PIC domain downstream (centimeters) simulating the details MITL physics

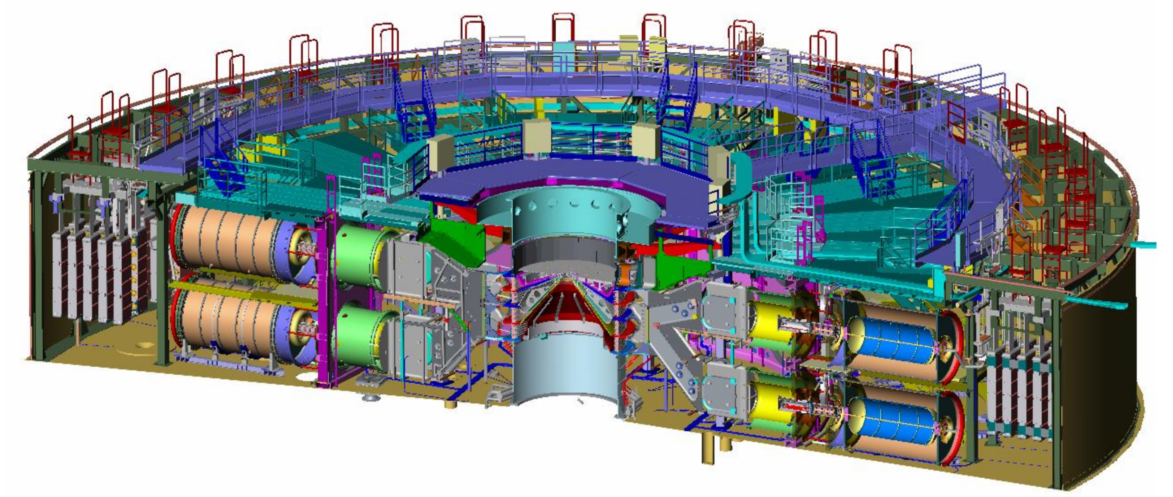
Computational challenges on Z

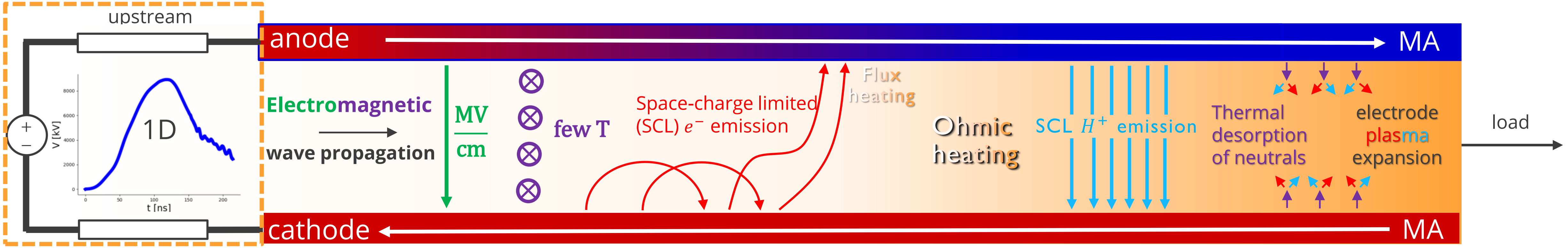
Detailed MITL physics



vs.

Power flow over system size



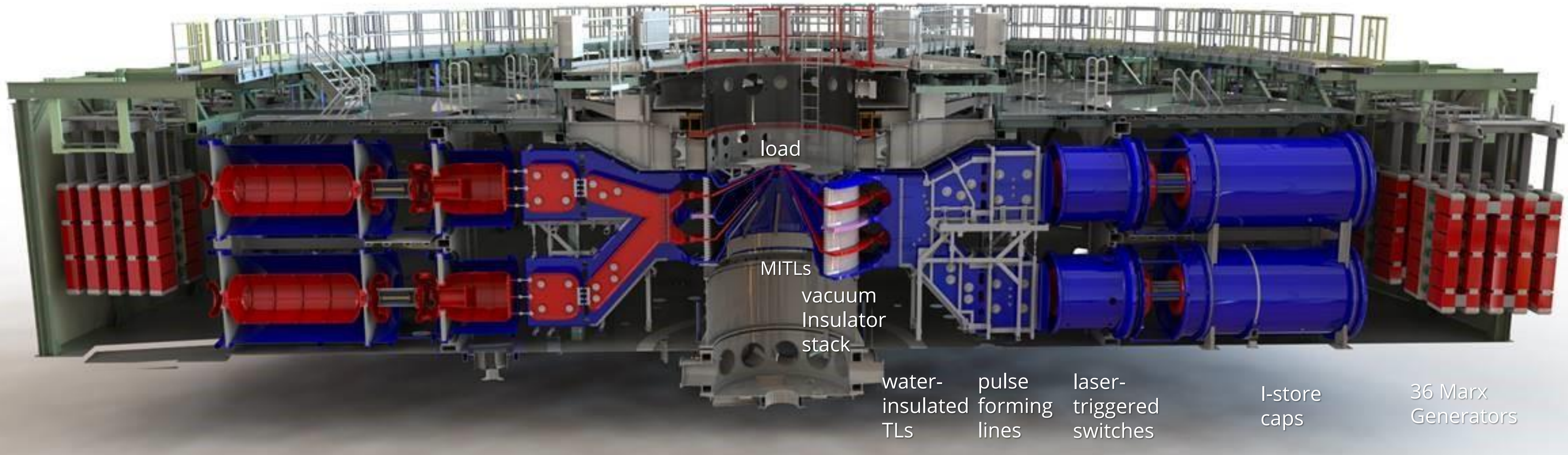


Solution: 1D-3D computational model – TEM wave propagation in 1D transmission line domains (meters) are coupled to a single 3D EM-PIC domain downstream (centimeters) simulating the details MITL physics

Similar, if not worse, "vastness" of scales and "multitude of processes" occupy the parameter spaces in all pulsed power devices!

Self-consistent machine-scale simulations enabled through 1D transmission line – 3D EM PIC domain coupling

1. A 1D/2D full circuit model for Z was developed in BERTHA



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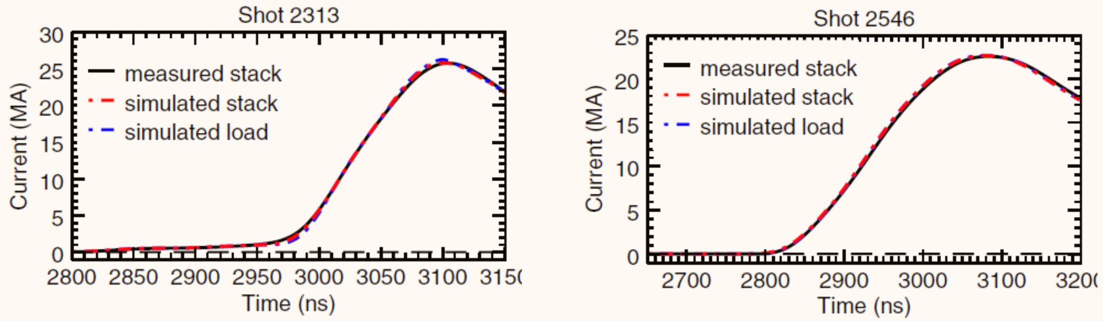
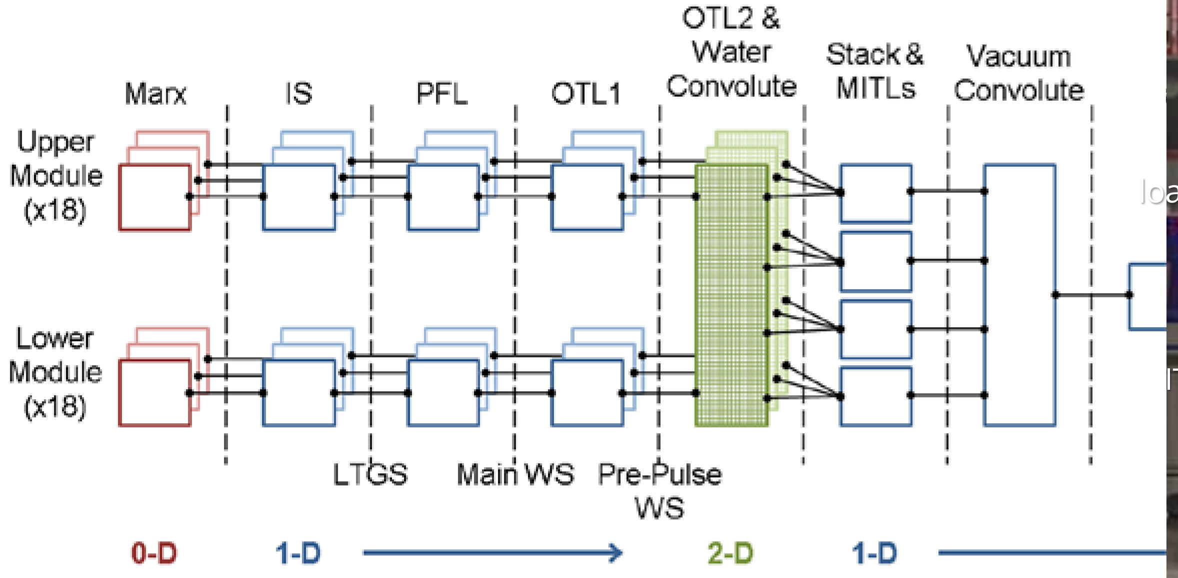
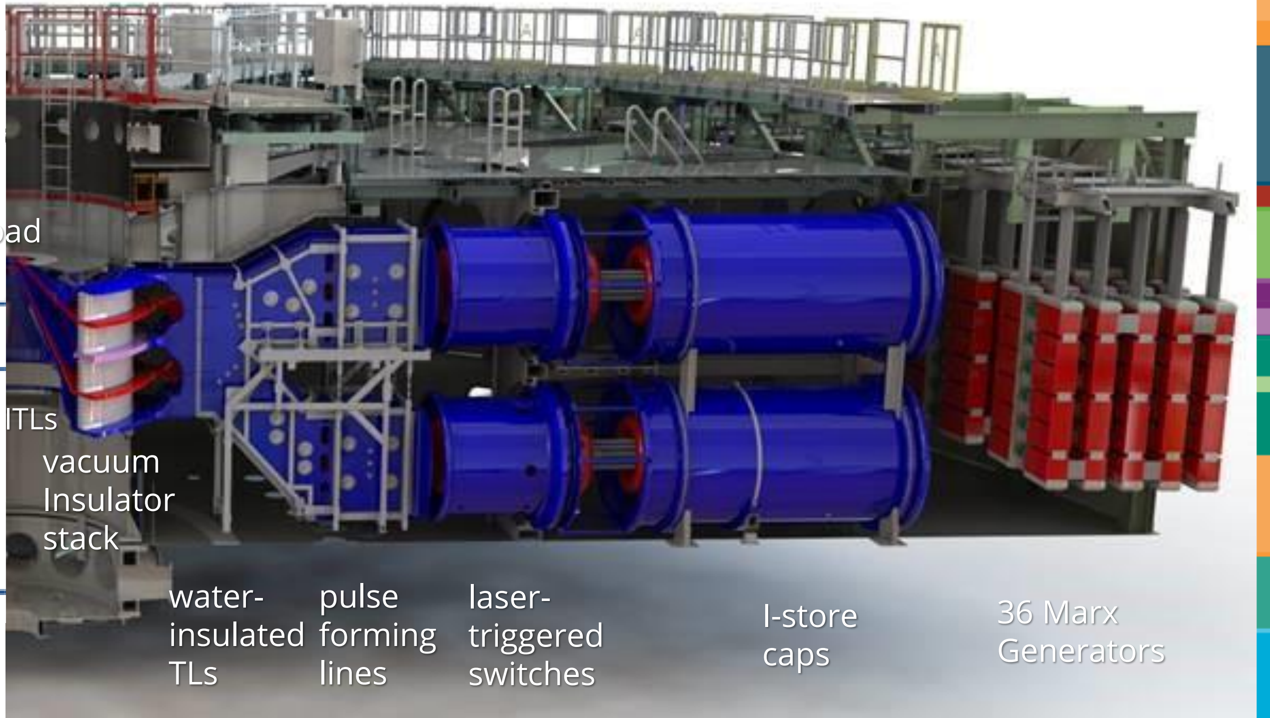


circuit model predictions agree with measurements for various shots

Full BERTHA circuit model



(Hutsel, B. T. Phys. Rev. Accel. Beams **21**, 030401)



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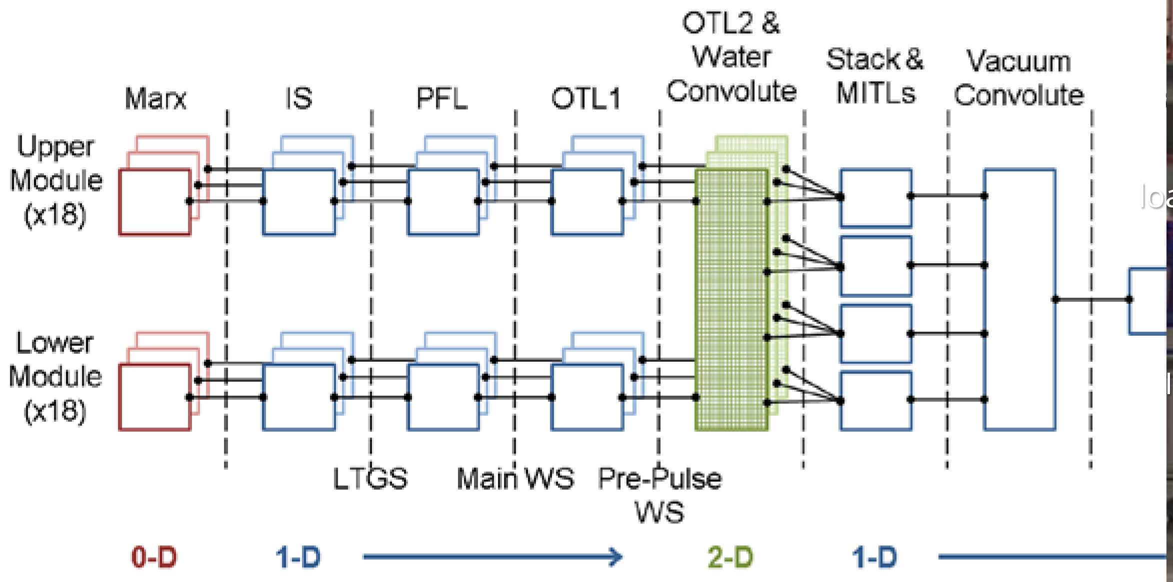
Full BERTHA circuit model

1D
Empire transmission lines



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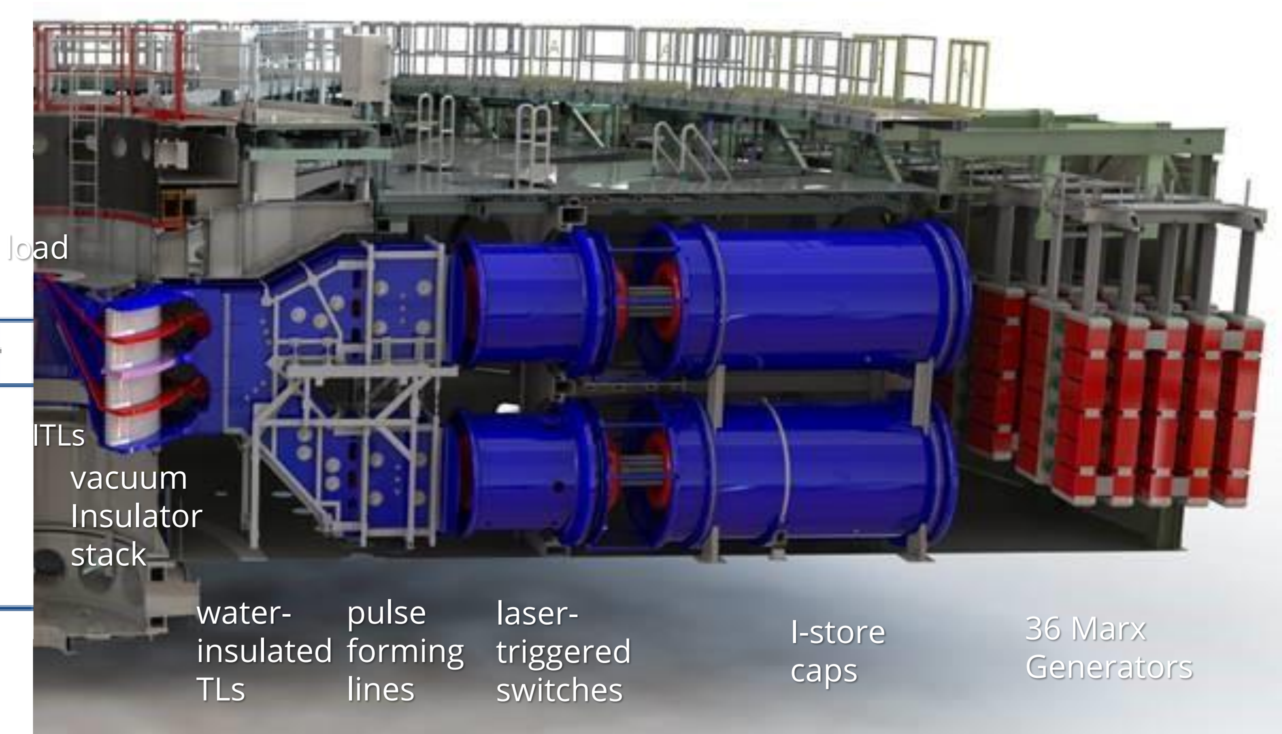

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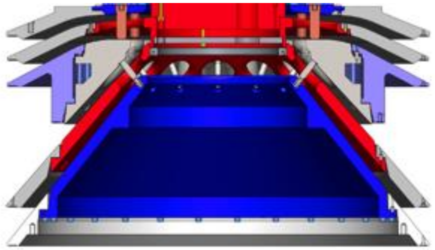
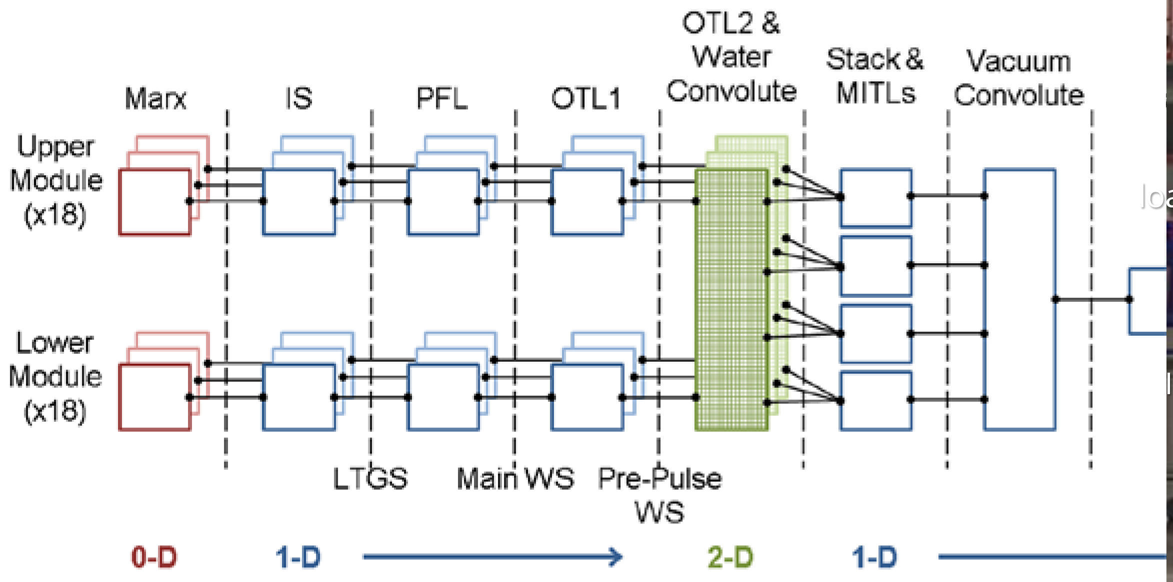


Fig: convolute hardware

Full BERTHA circuit model

3D Empire EM-PIC

1D Empire transmission lines



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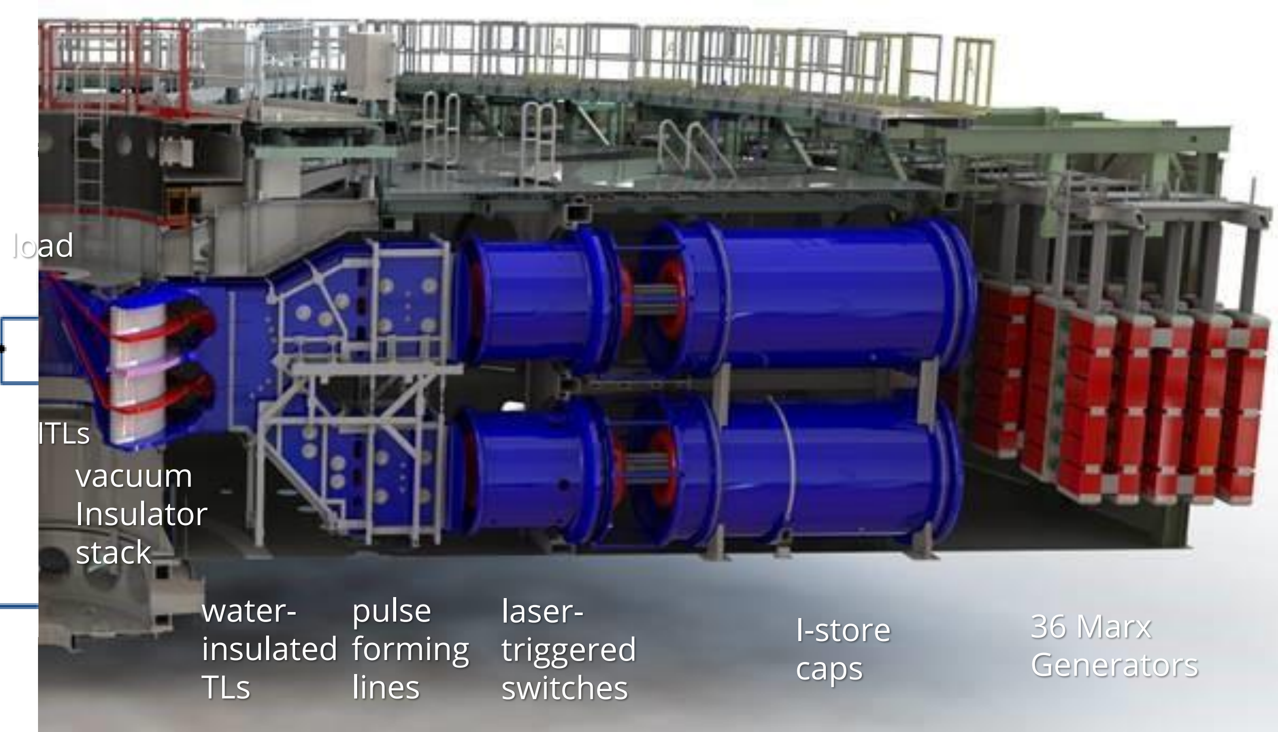

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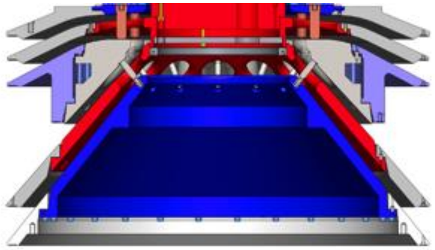
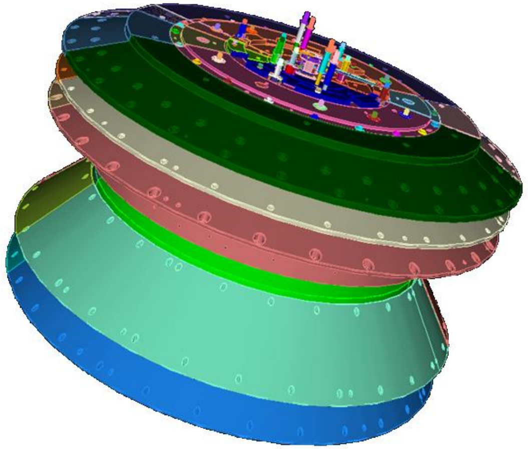


Fig: convolute hardware



CAD
(Z convolute hardware)

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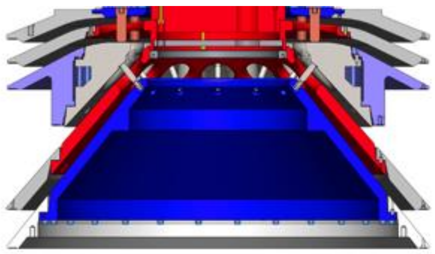

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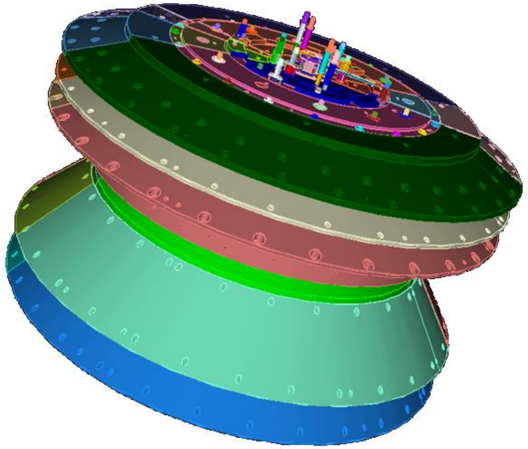

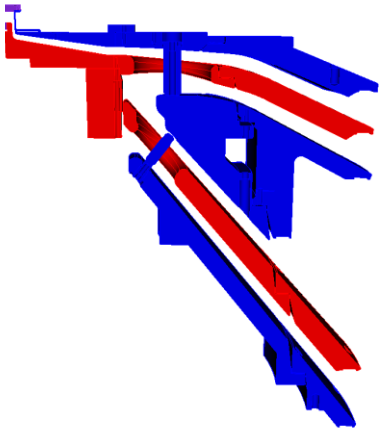

CAD
(Z convolute hardware)

CAD
(minimum periodic unit)

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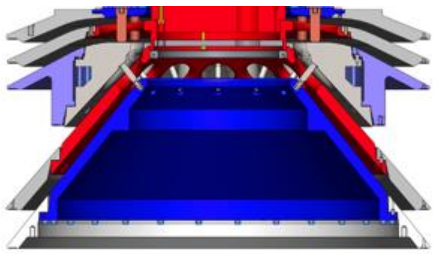

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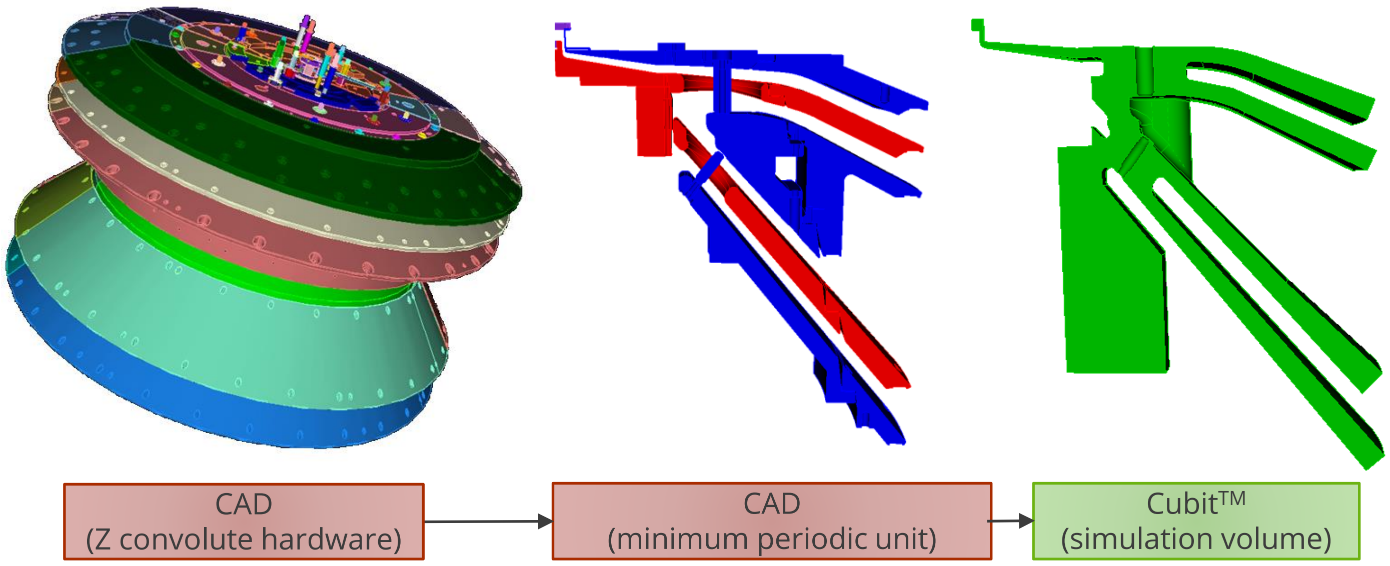

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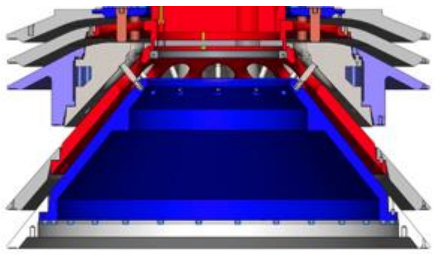
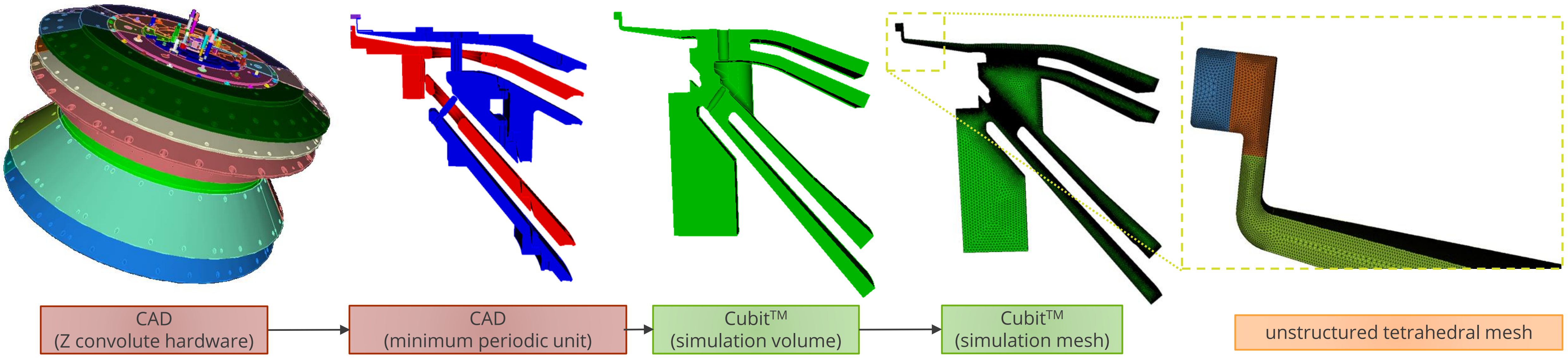


Fig: convolute hardware



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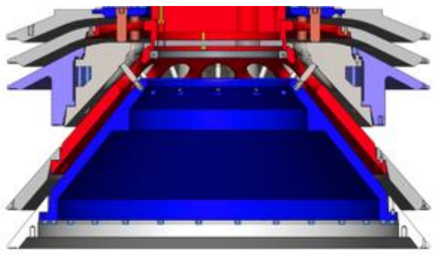

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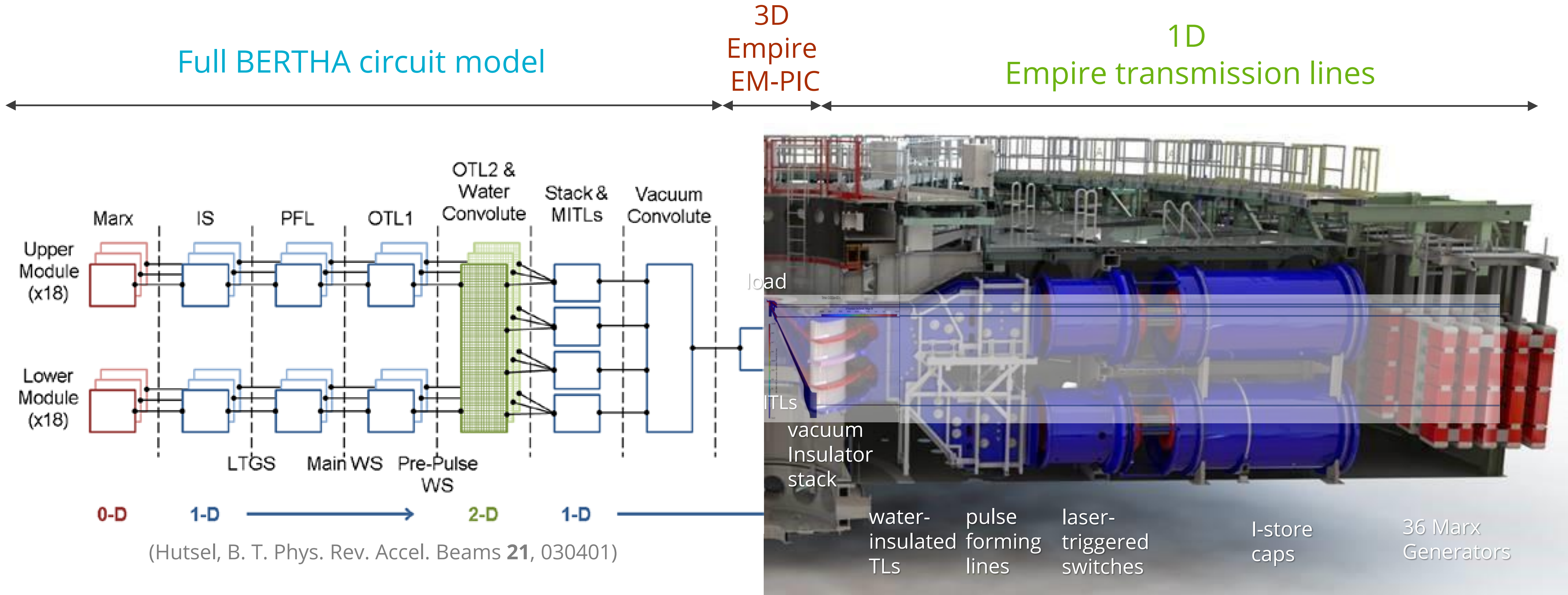
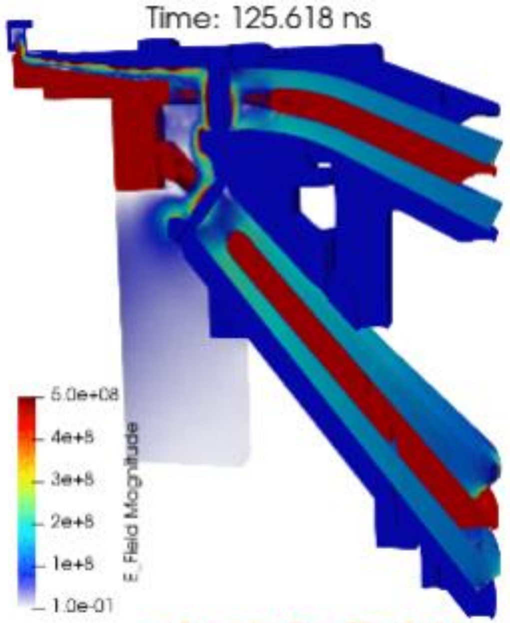


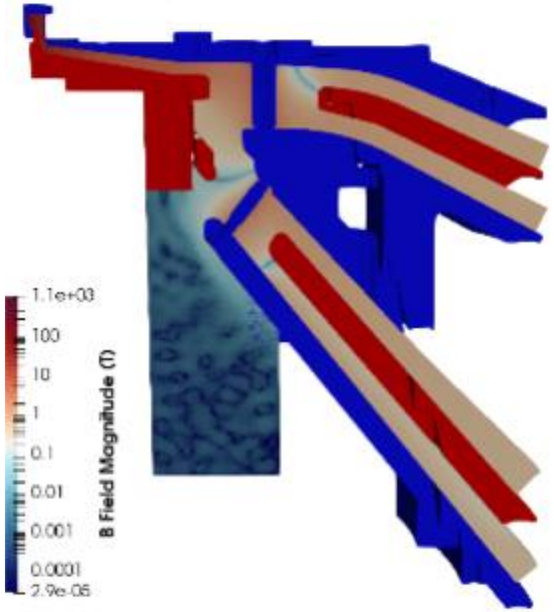
(Hutsel, B. T. Phys. Rev. Accel. Beams **21**, 030401)

We can simulate *all* major processes germane to power flow Z

animation



electric fields



magnetic fields

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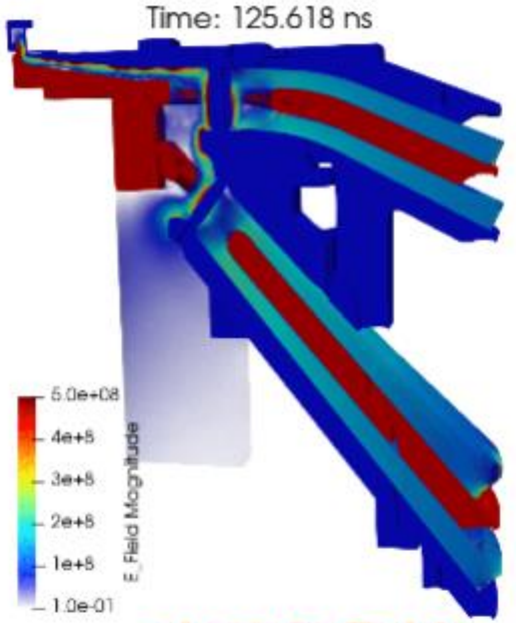
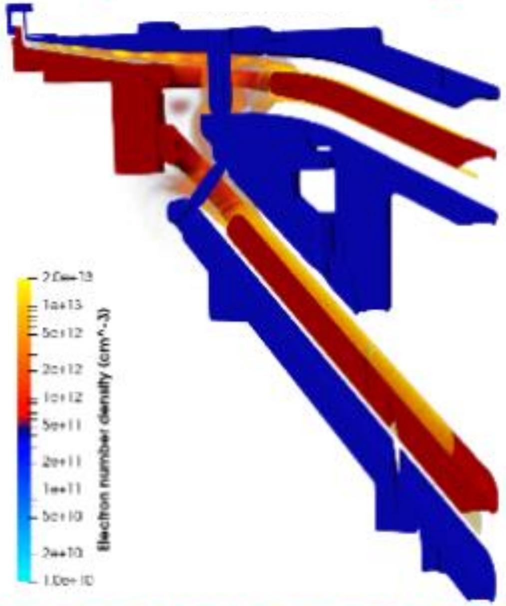
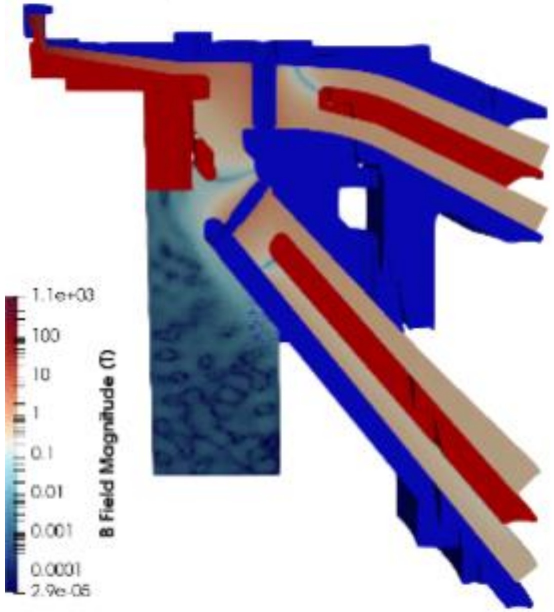


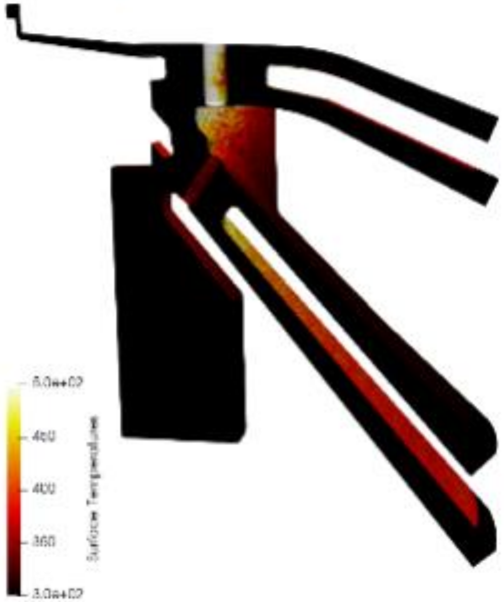
electric fields



cathode plasma emission (e^-)



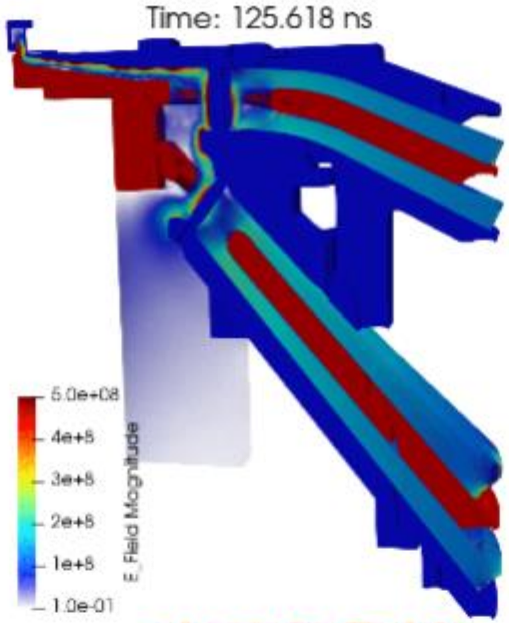
magnetic fields



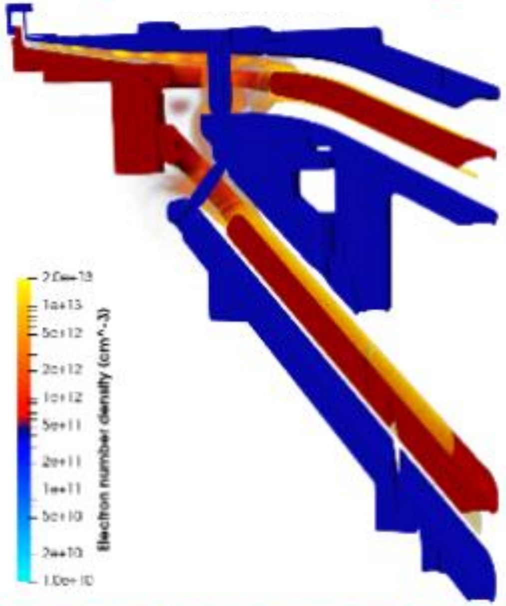
electrode heating from B fields

We can simulate *all* major processes germane to power flow Z

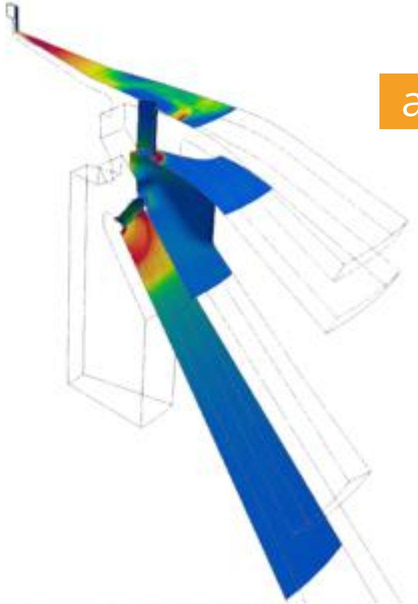
animation



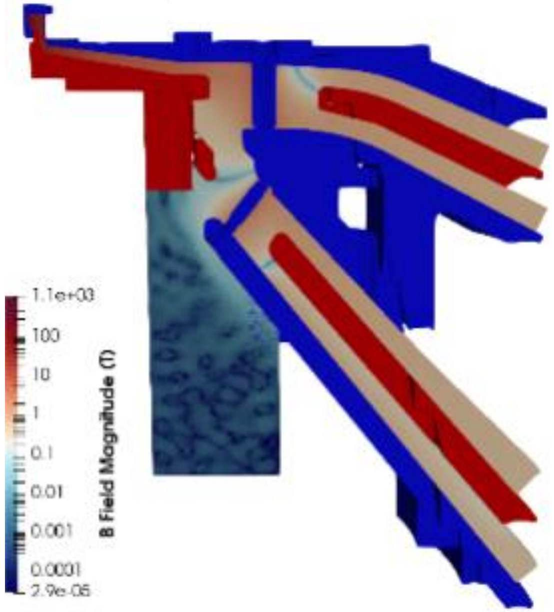
electric fields



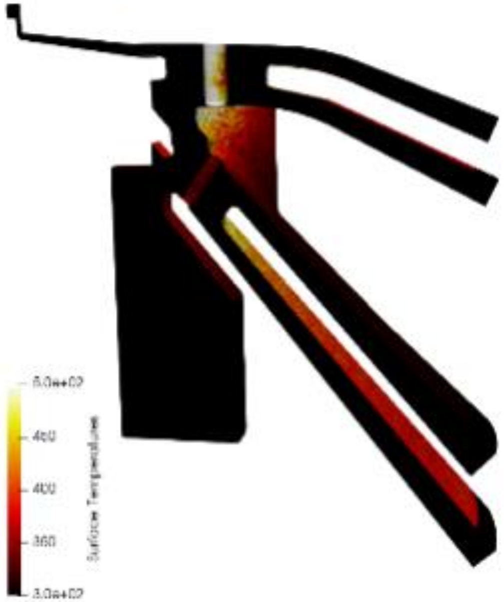
cathode plasma emission (e^-)



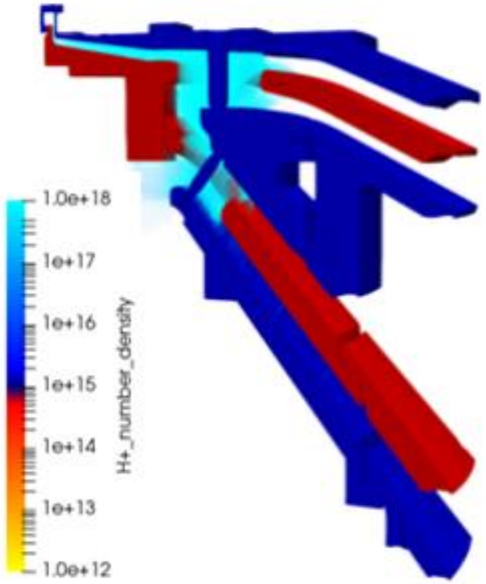
anode heating from e^- fluxes



magnetic fields



electrode heating from B fields



anode plasma emission (H^+)

Reaching for higher targets in pulsed power: variable-impedance MITLs

- Programmatic interest in higher-current accelerators: “Z upgrade”, “next-generation pulsed power” (NGPP)
- Existing pulsed power has been engineered using constant-impedance vacuum transmission lines
- Recent studies* suggest MITLs having a variable geometric impedance give significant advantages

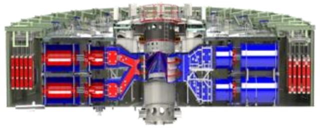
⇒ potential means to reduce inductance and deliver more current to the load

Help Wanted

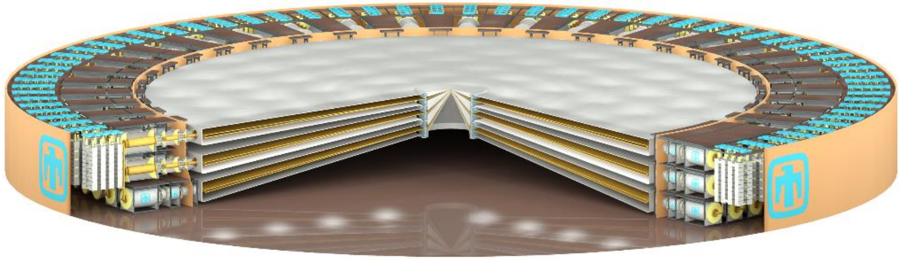
essential qualifications:
- a pulse of $\tau < 120$ ns
- faster dI/dt
- deliver I_{load}: $\gg 26$ MA

desired qualifications:
- Minimizing inductance L_{driver} $\left(I \approx \tau \frac{dI}{dt} = \tau \frac{V}{L}\right)$ highly desired!

Apply inside!



Z

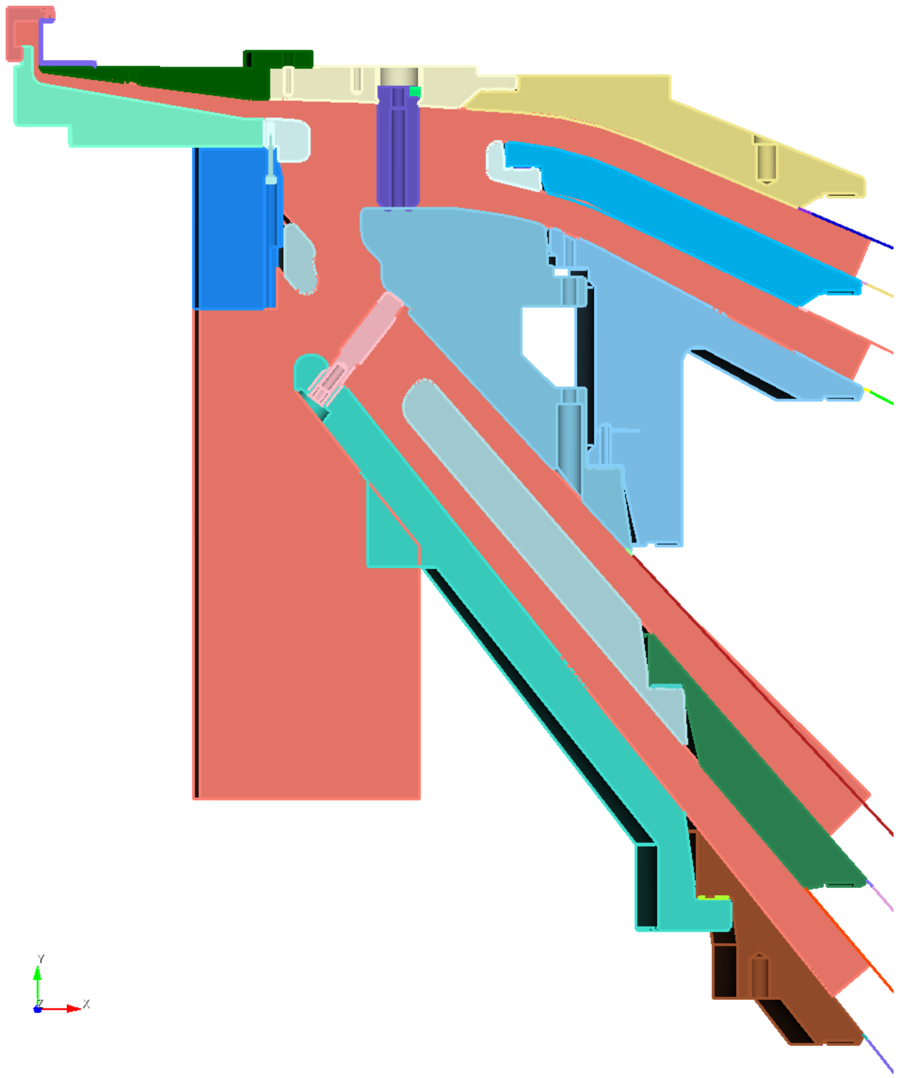


NGPP (potential concept)

We are **using Empire to vet this concept as a potential enabling technology** to reach design targets **for Z upgrade and NGPP**

*R. B. Spielman, "Pulsed-Power Innovations for Next-Generation, High-Current Drivers," in IEEE Transactions on Plasma Science, vol. 50, no. 9, pp. 2621-2627, Sept. 2022, doi: 10.1109/TPS.2022.3196188.

Towards Z upgrade: our ModSim work looks to optimize impedance profiles for *all* levels of Z



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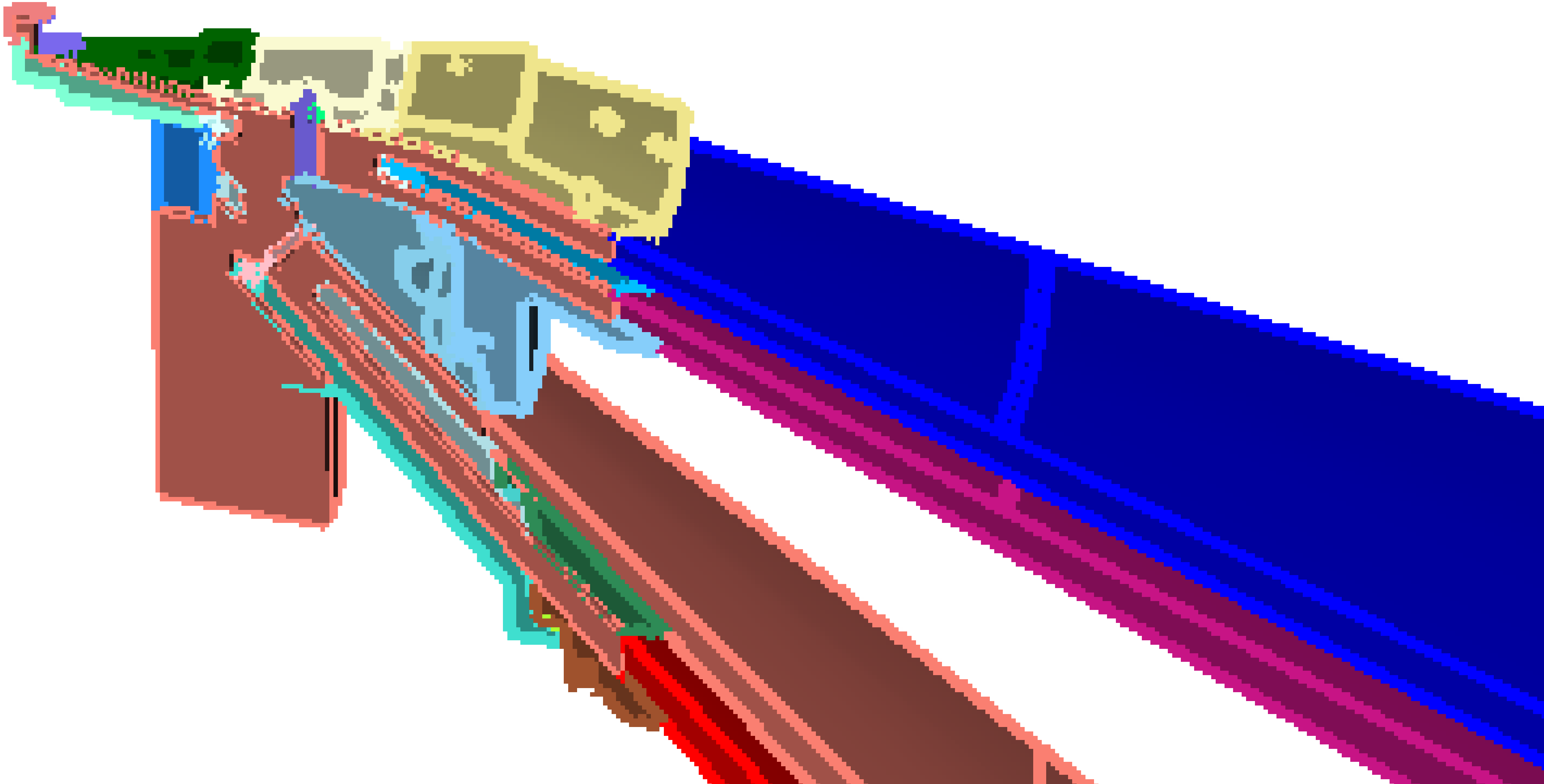

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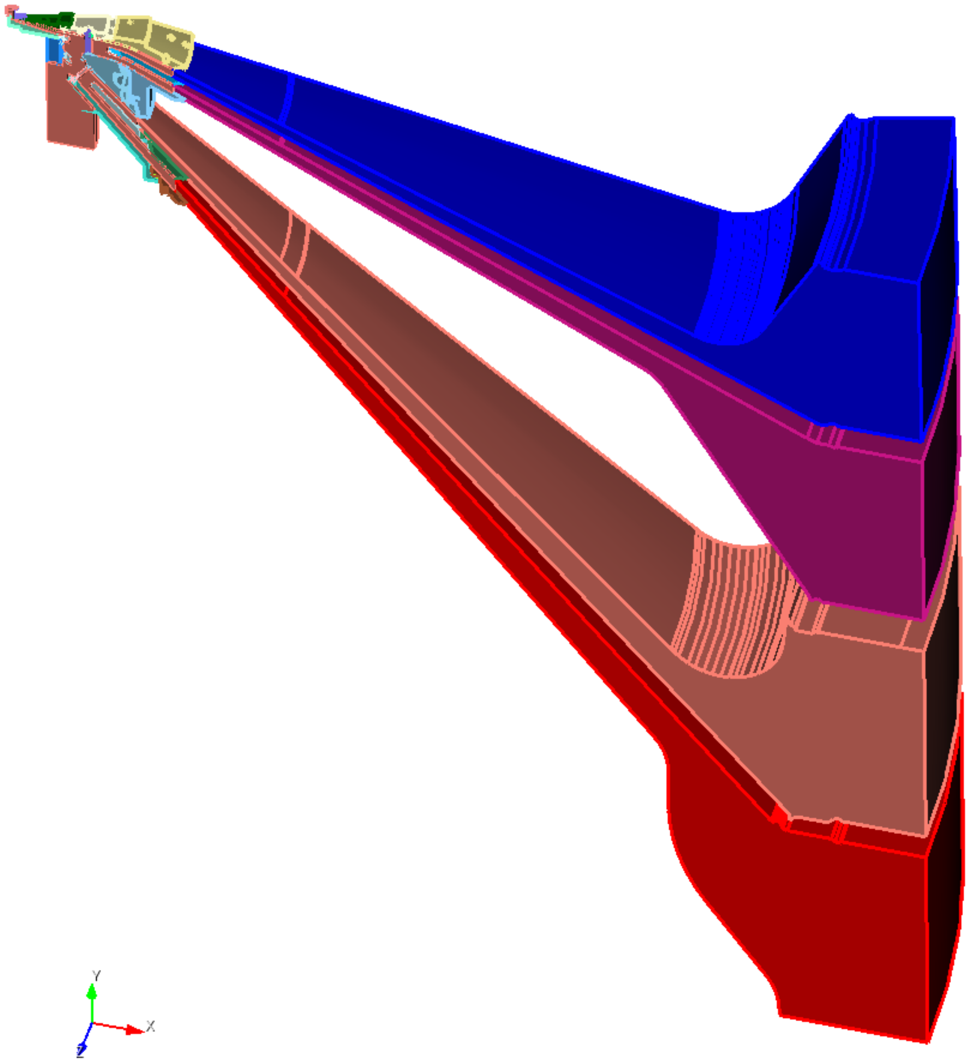


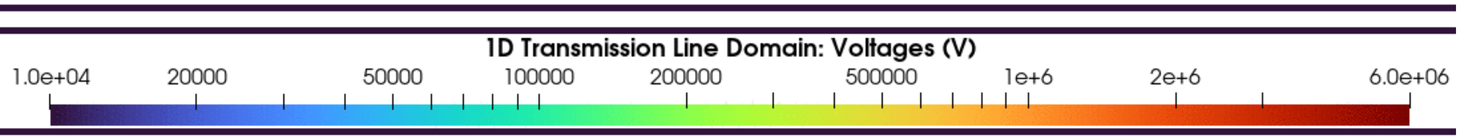
- Proposing **non**-constant impedance transmission lines asks us as a program to reconsider a decades-old foundational idea which lead to successful pulsed-power accelerators ⇒ **viability must be demonstrated**

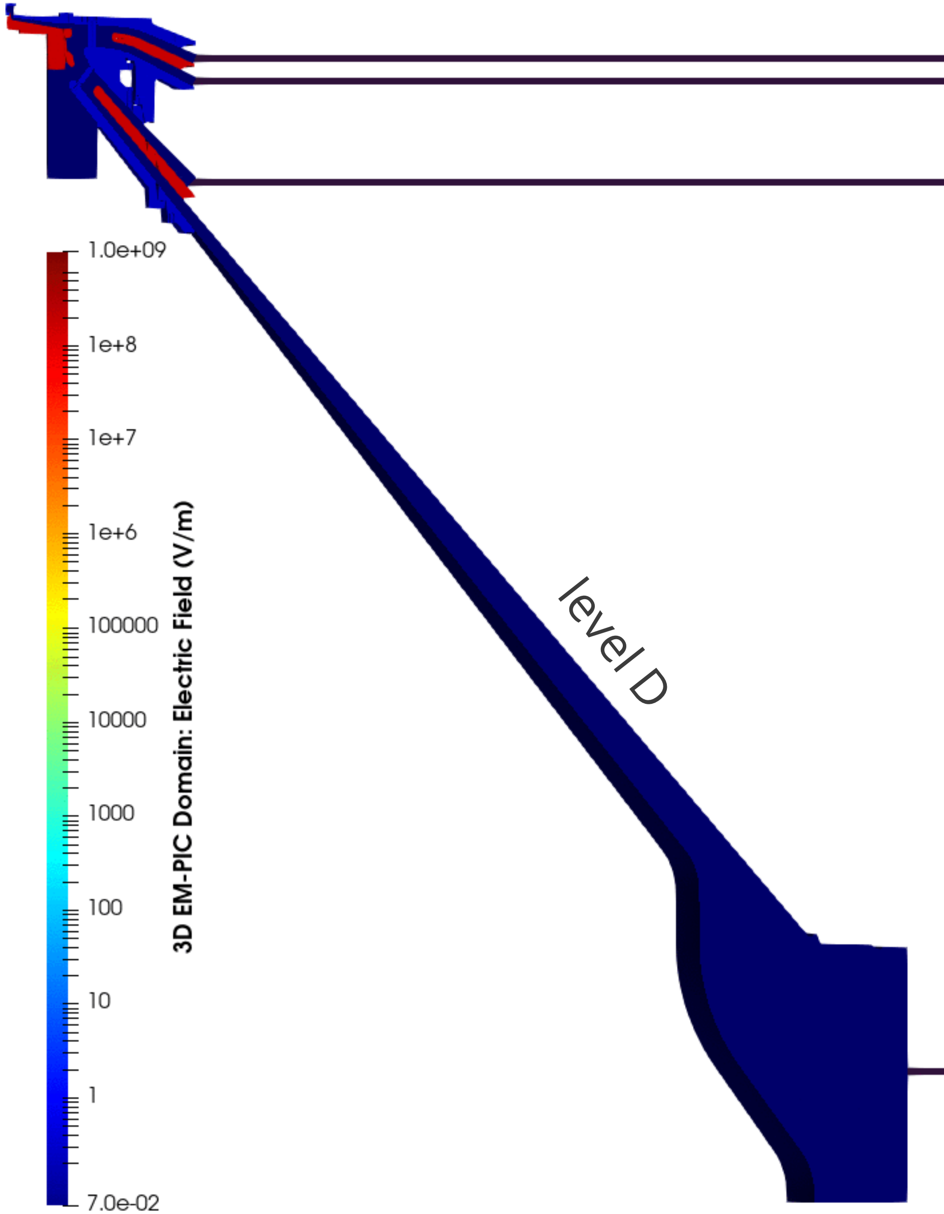
- **Currently**, **we are characterizing** baseline (Z today) vs. variable-impedance **redesigns for the highest inductance line ("level D")** *to demonstrate the working design principle*

Fully 3D EM-PIC Empire simulations including the entire level D show encouraging agreement with measurements

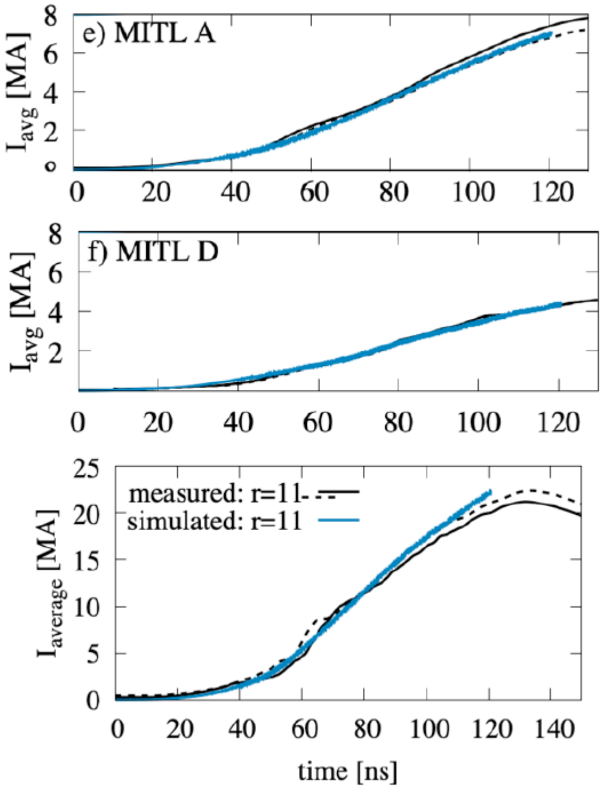
animation

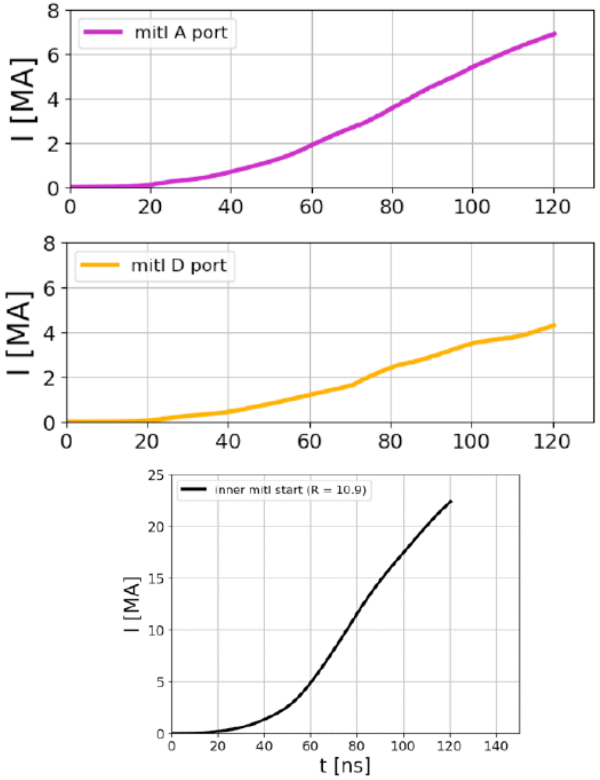
Time: 0.000e+00 s





CHICAGO[1] vs. measurements vs. Empire

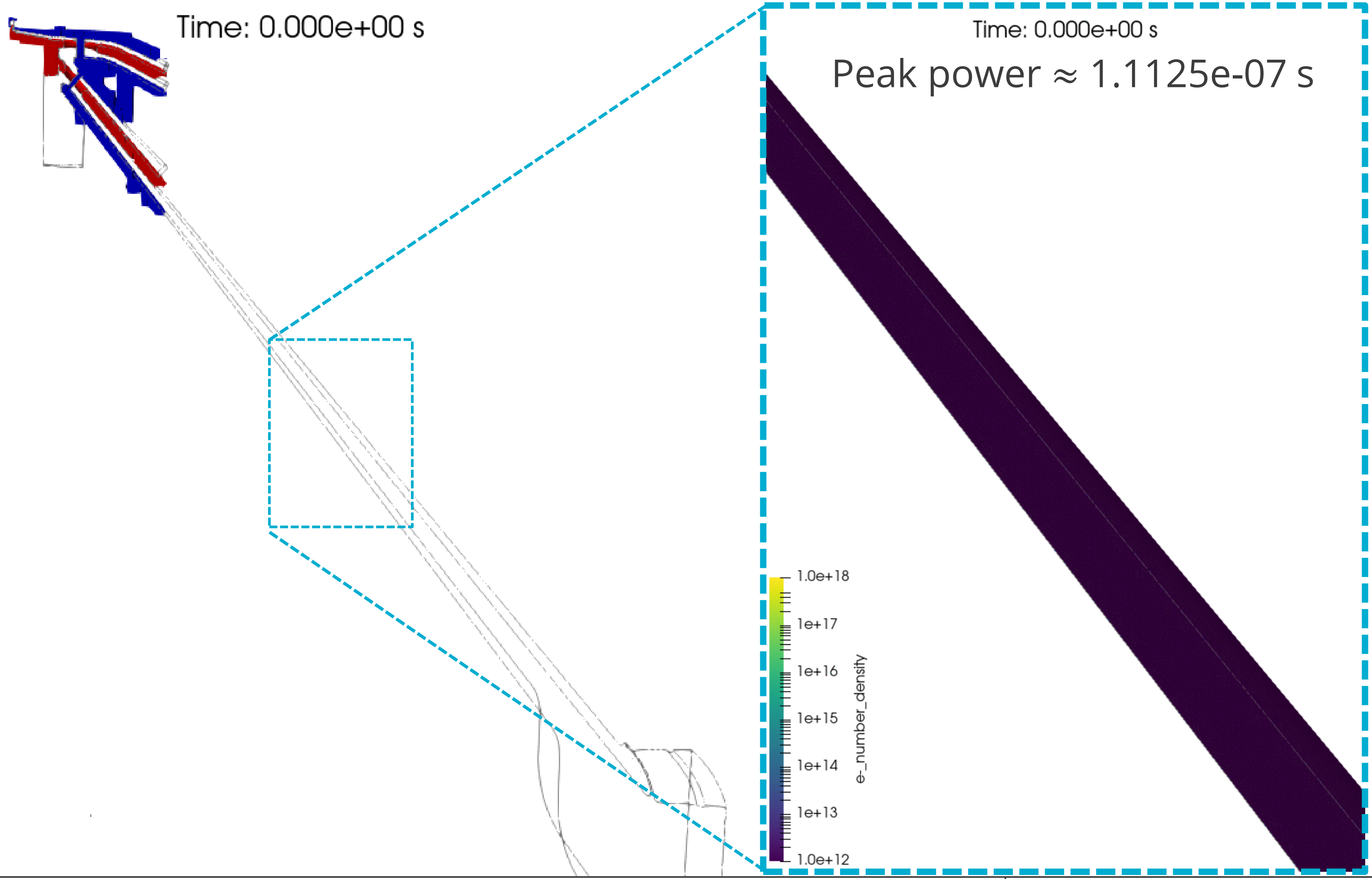




[1]CHICAGO simulation done by N. Bennett, published in Laity, George R. et al. Plasma Grand Challenge LDRD final report. SAND2021-0718. doi:10.2172/1813907.

Fully 3D EM-PIC Empire simulations including the entire level D show encouraging operational characteristics ⇒ *well* below safety limits

animation

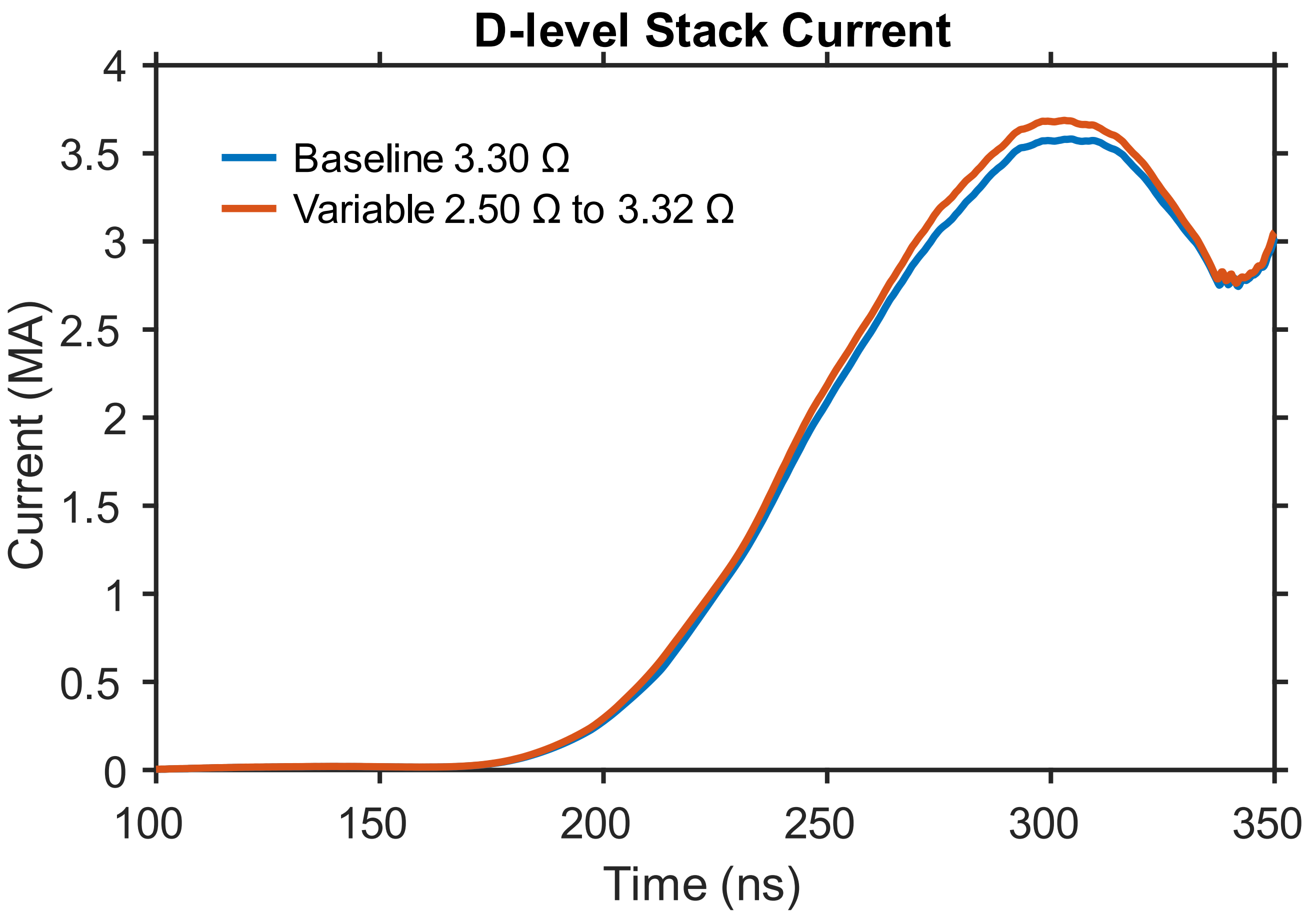


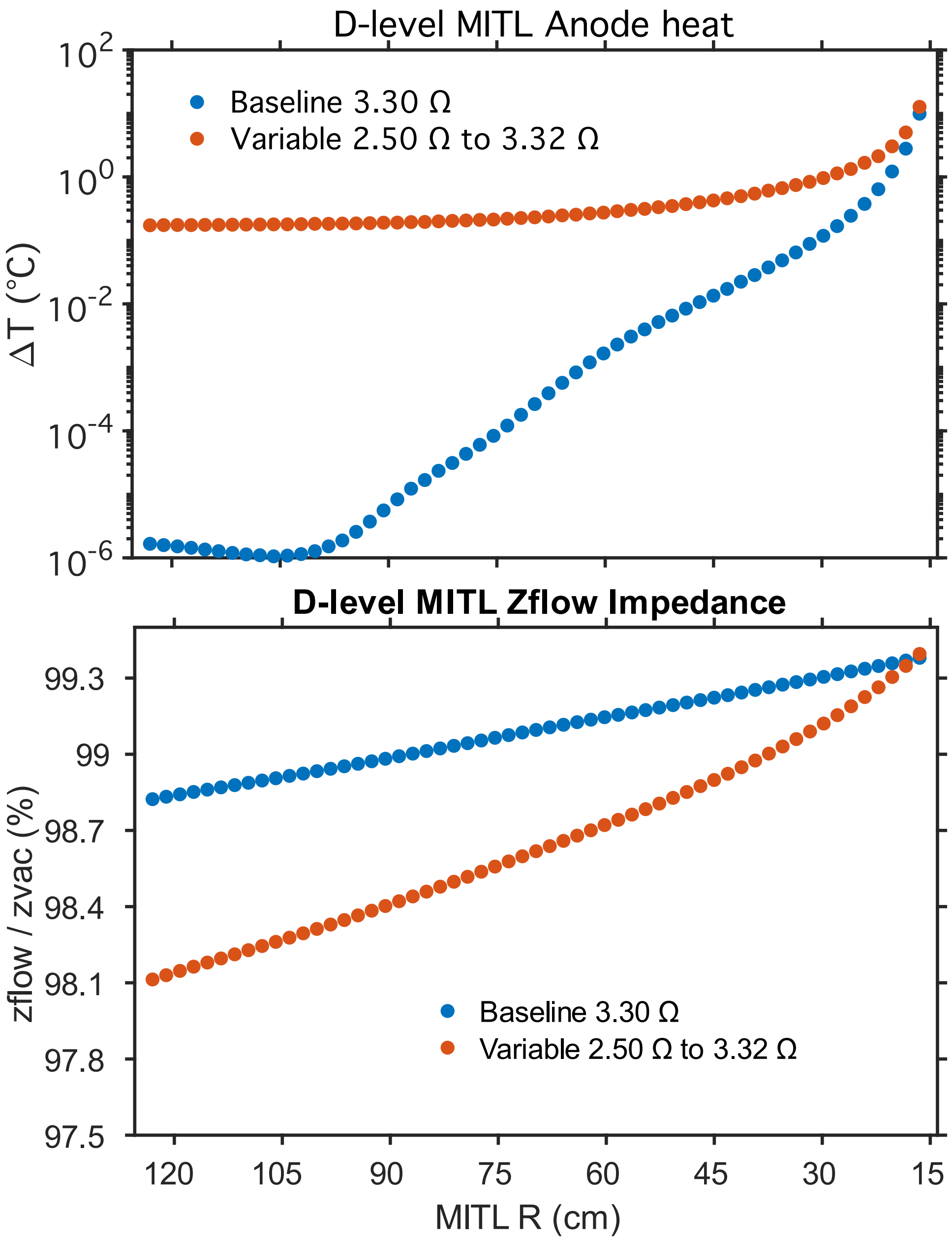
- Can be used to vet *many* candidate designs, providing detailed reports of machine performance
- Any re-design must maintain operational and *safety* limits ⇒ electron flows, surface heating must be safely under design limits
- Testbed results show variable-impedance transmission lines insulate *extremely well*
- ***Next***: Empire simulations of variable impedance versions: can up to 0.5 MA more current be delivered while satisfying safety limits?

Simulation details

- *Meshes*: 153,061,360 elements + thermal grids inside materials
- *Particles*: 1.40e+08 electrons, 1.58e+07 protons; maximum
- *Resources*: 7680 cores / 160 CTS-1 nodes
- *Duration*: 160 ns over 190623 steps, 30 wall-hours
- *Output*: 3.8 TB (mesh data), 555 MB (history data)

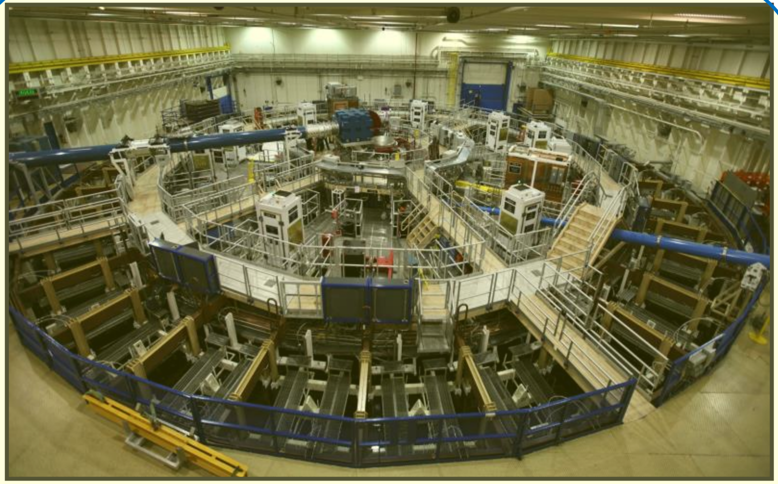
SCREAMER circuit simulations demonstrate a variable impedance MITL results in *higher* current while staying *well* below safety limits





- *Proof-of-concept*: modestly tailoring just **one** line results in ~ 3% **more current** (above)
  - ➢ greater gains possible with further (careful) reduction of inductance
- Tailoring ***all*** levels will translate to ***significant* gains**

RAMSES Simulation Results and Impact to Pulsed Power



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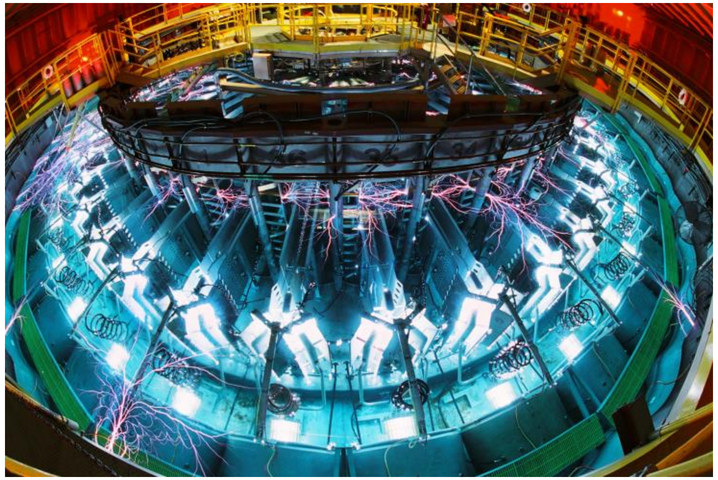
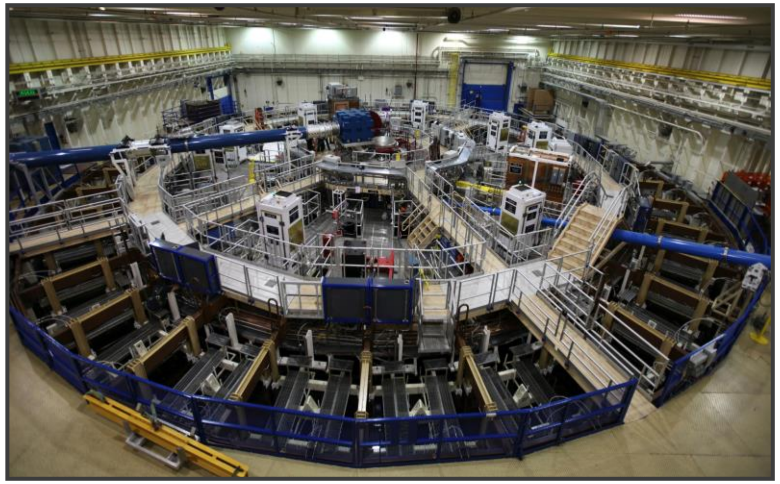


Saturn

HERMES-III

- *Work covered in this talk*: Z upgrade
- *Work impacting behind-the-scenes*: next-generation pulsed-power (NGPP)

RAMSES Simulation Results and Impact to Pulsed Power



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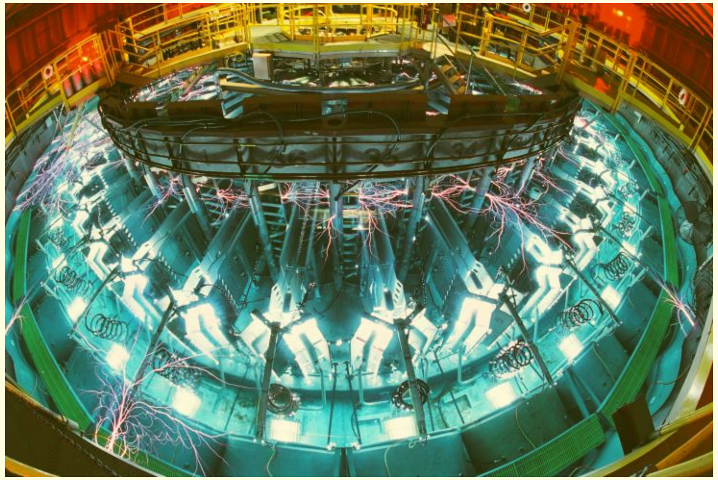


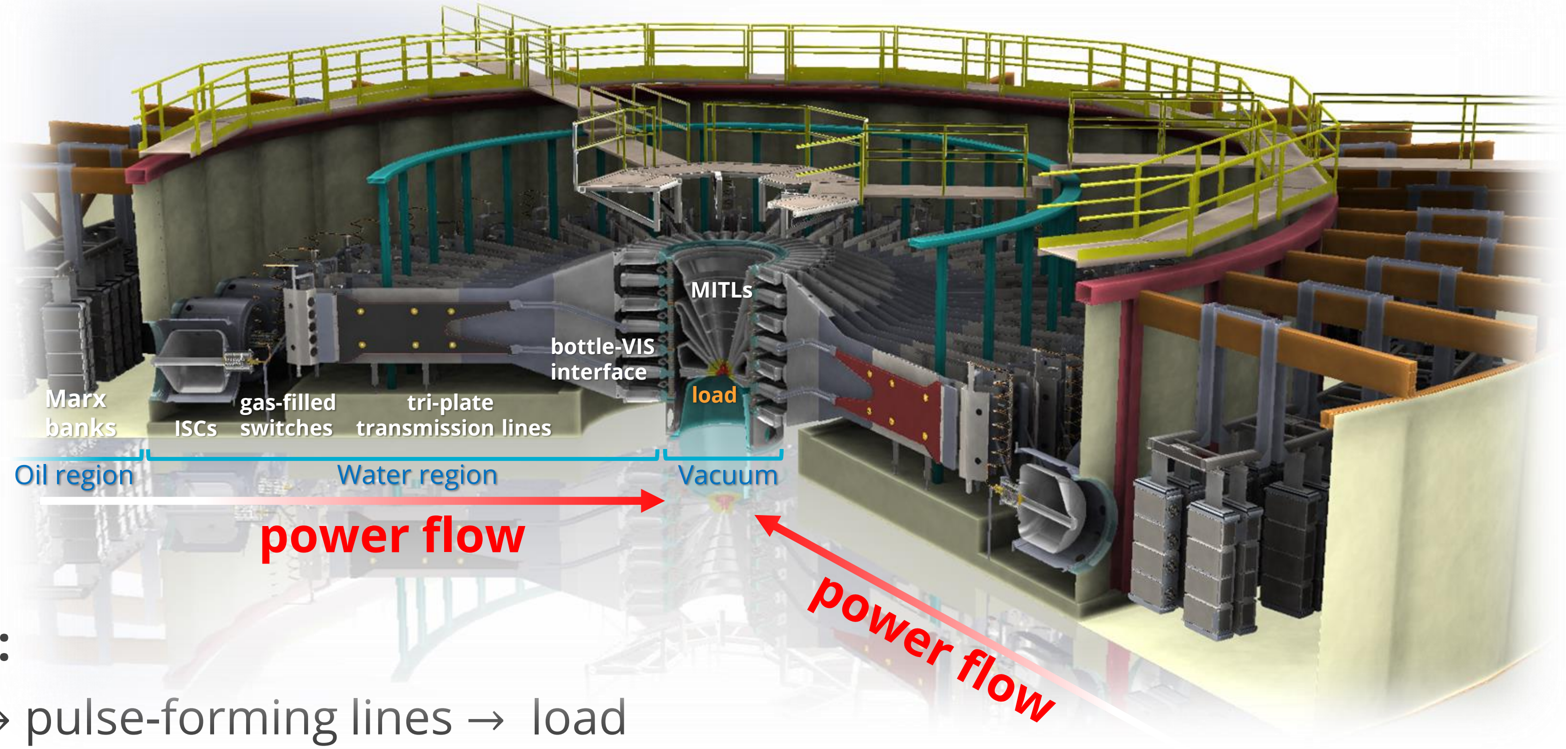
Saturn

HERMES-III

- Saturn Refurbishment Project:
  - Machine-scale power flow simulations
  - Bremsstrahlung diode physics
- Saturn Redesign of the e-beam source

System overview: Saturn accelerator

*A 26 TW pulsed-power accelerator used to drive various **loads** covering both X-ray sources (Bremsstrahlung diode, rod pinch, reflex triode array), and charged beams sources for surrogate testing (e.g., e-beam, ion diode)*



Pulsed-power driver:

- Marx generators → pulse-forming lines → load
- 36 Marx banks, 5.6 MJ total
- 100 ns power pulse delivered to diode

Impacts to Saturn Refurbishment Project

1. A large-domain 3D electromagnetic (EM) model in `EMPIRE` was developed to characterize the power flow from the Saturn water line to the load;

2. A high resolution 3D EM particle-in-cell (EM-PIC) domain for regions approaching the Bremsstrahlung source (completed upstream via 1D circuit coupling) was developed in Empire, enabling self-consistent determination of diode beam characteristics at feasible cost;

3. The beam fluxes calculated by Empire provided inputs to an `ITS` domain modeling the region under the anode convertor which *has lead to the most accurate predictions of the Saturn radiation field to date*

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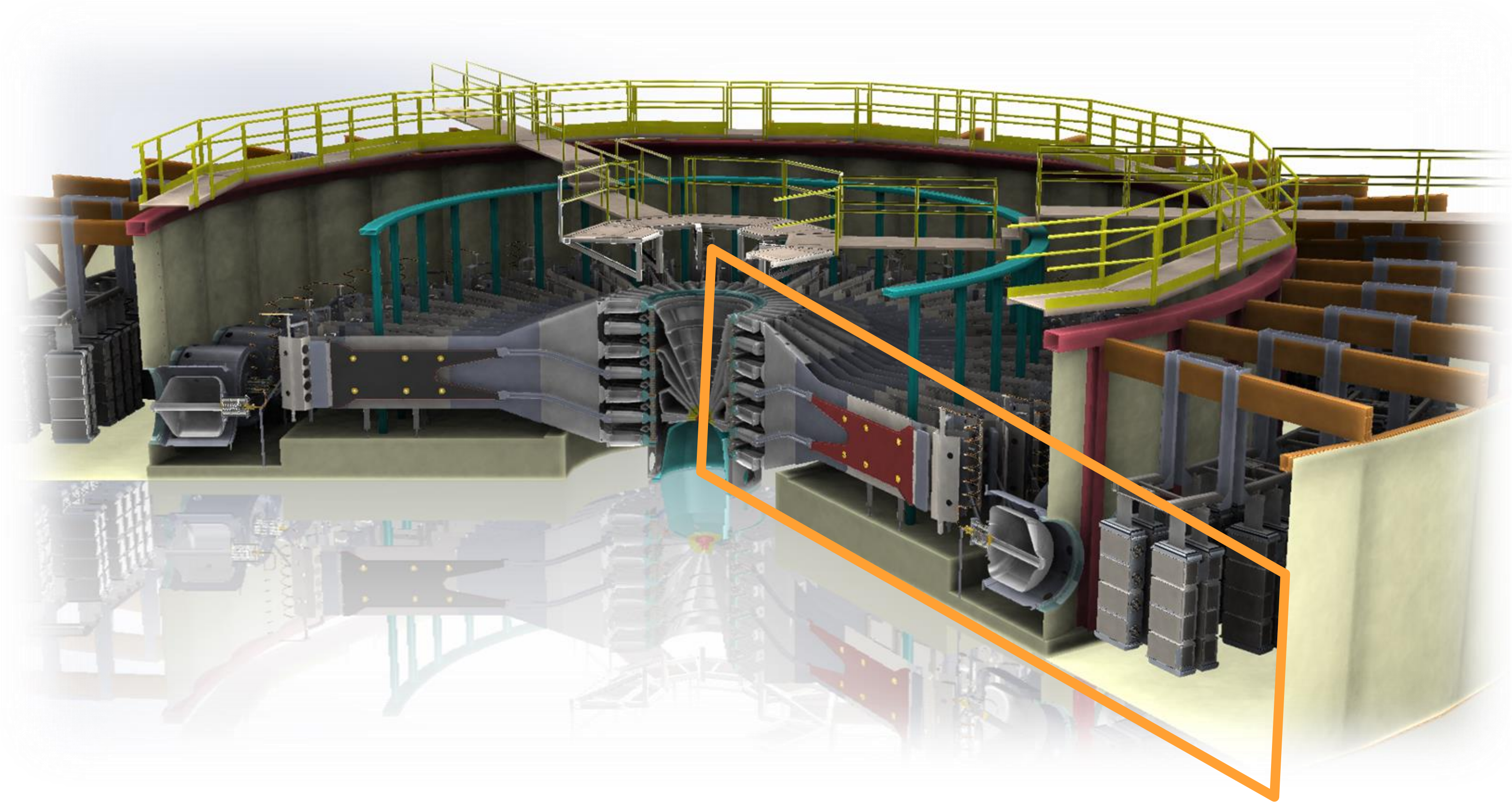
A large-domain 3D electromagnetic model was developed to characterize power flow from the Saturn water line to the load



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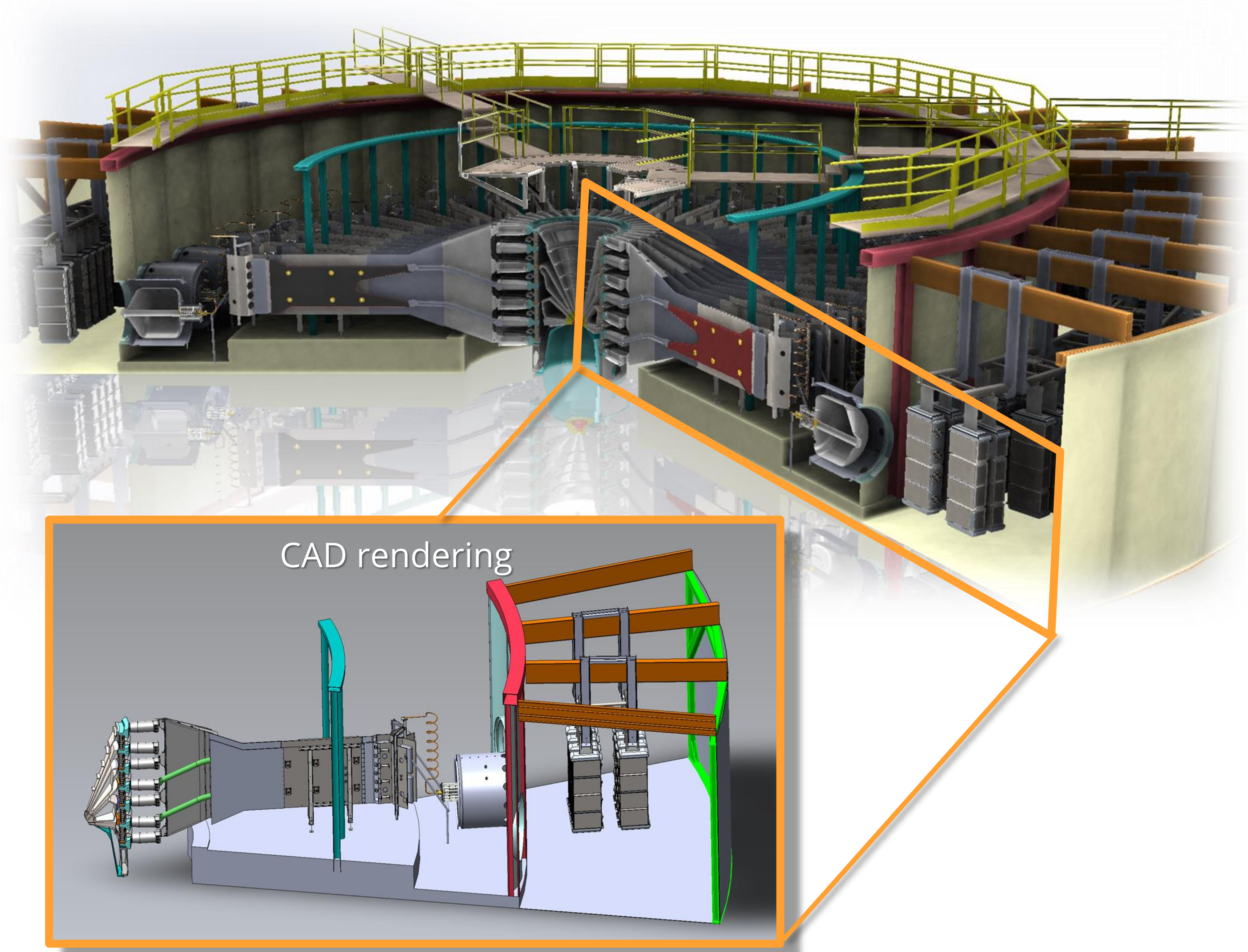

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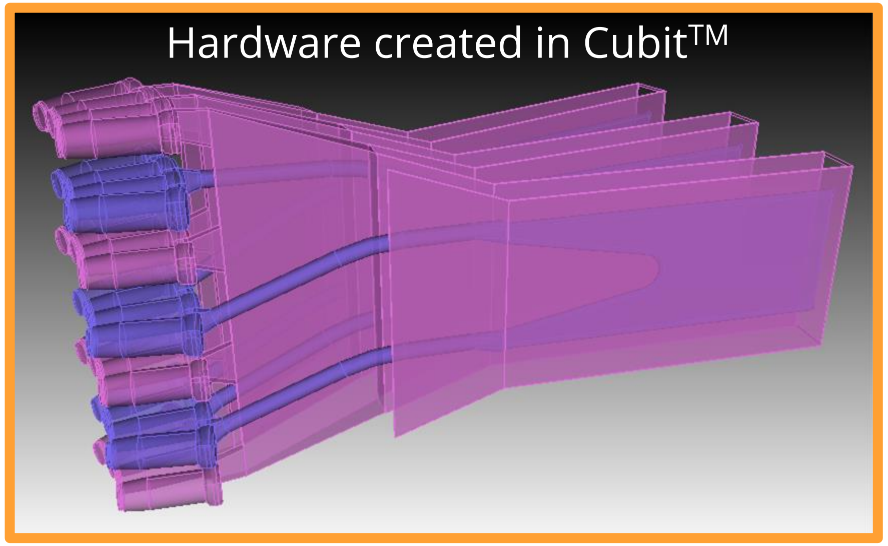

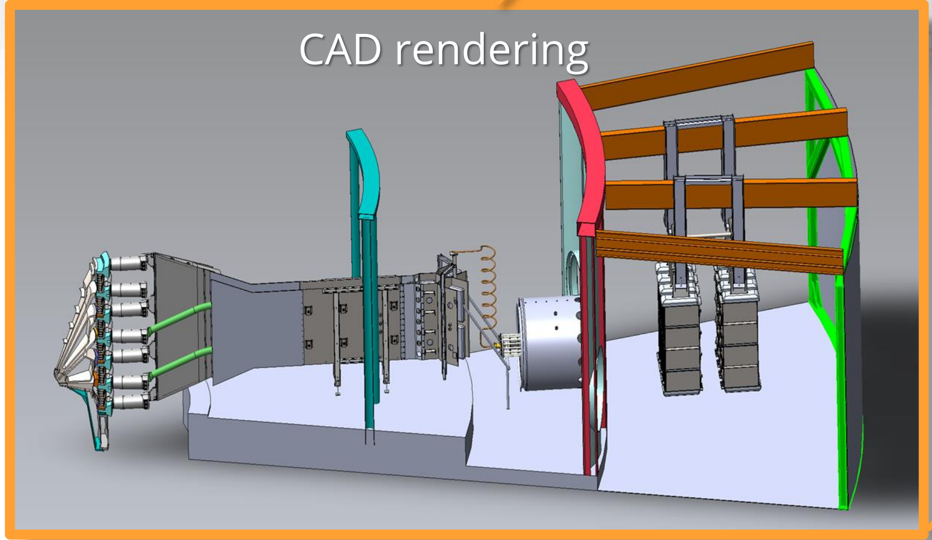

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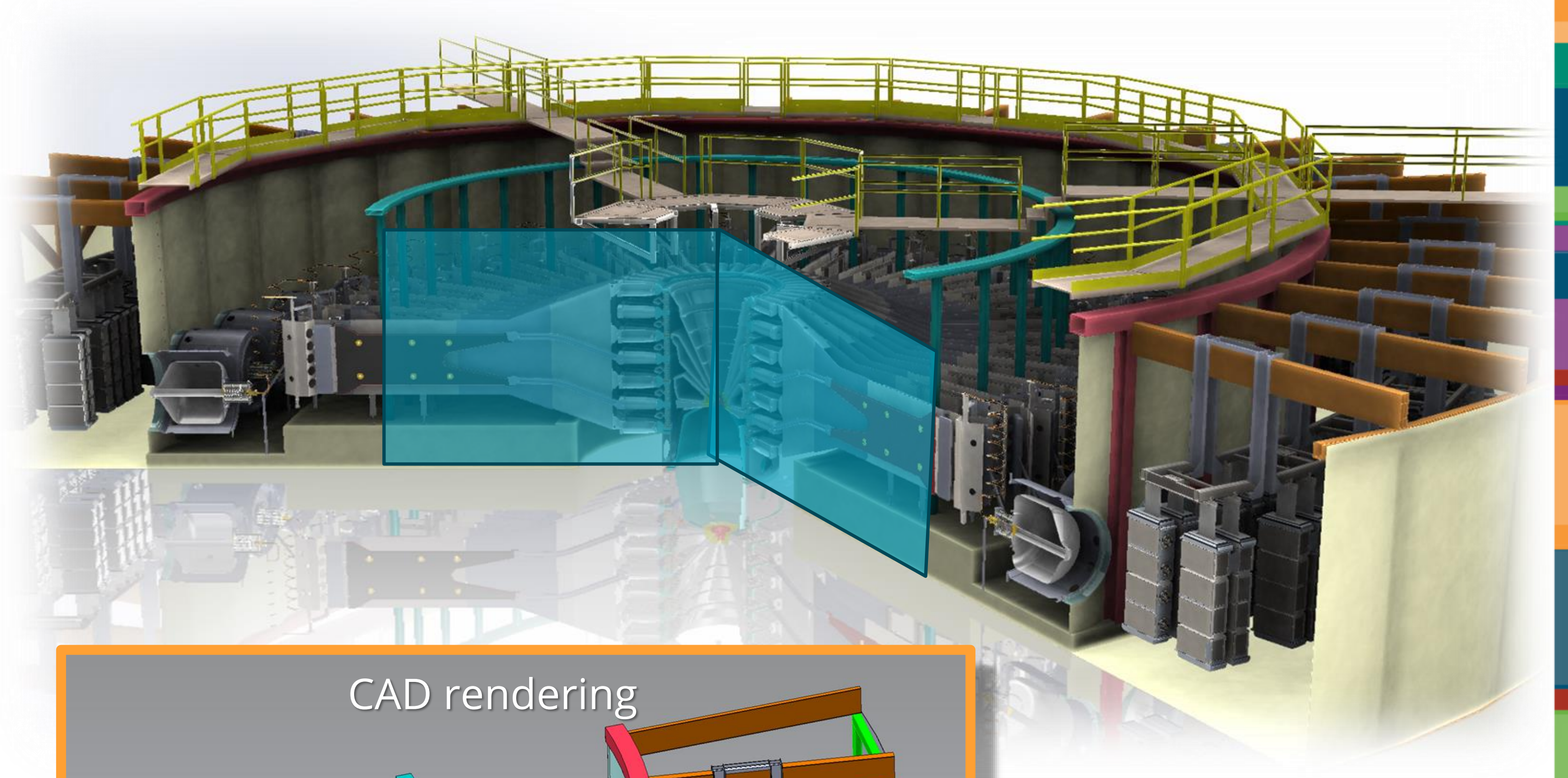
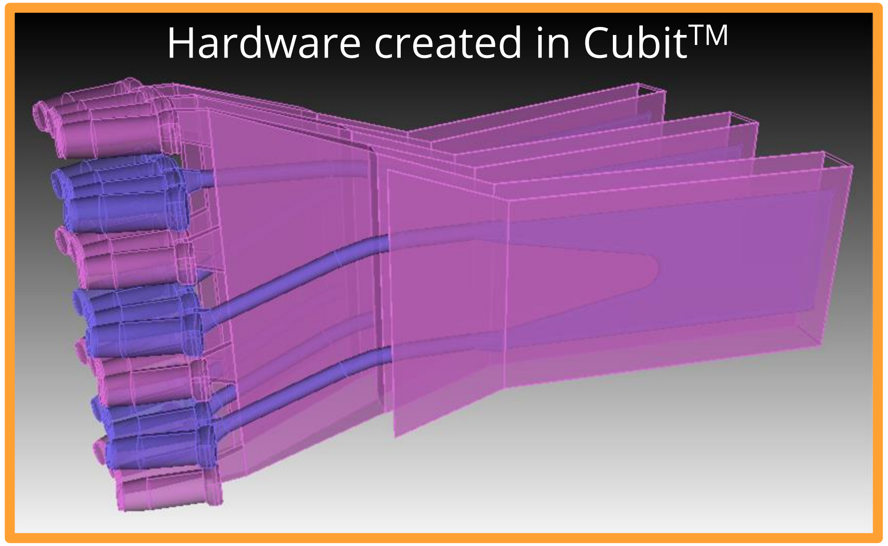
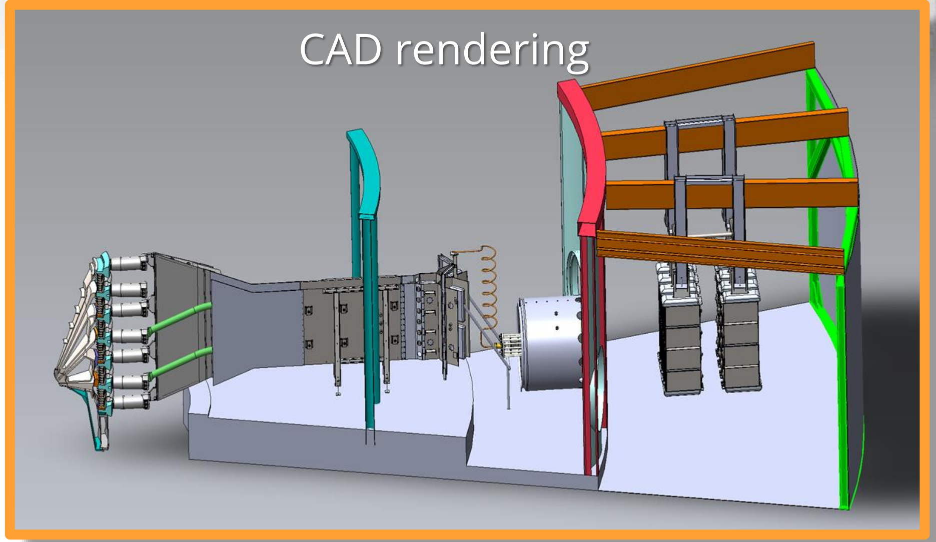


baseline simulation were obtained to better understand power flow





A large-domain 3D electromagnetic model was developed to characterize power flow from the Saturn water line to the load

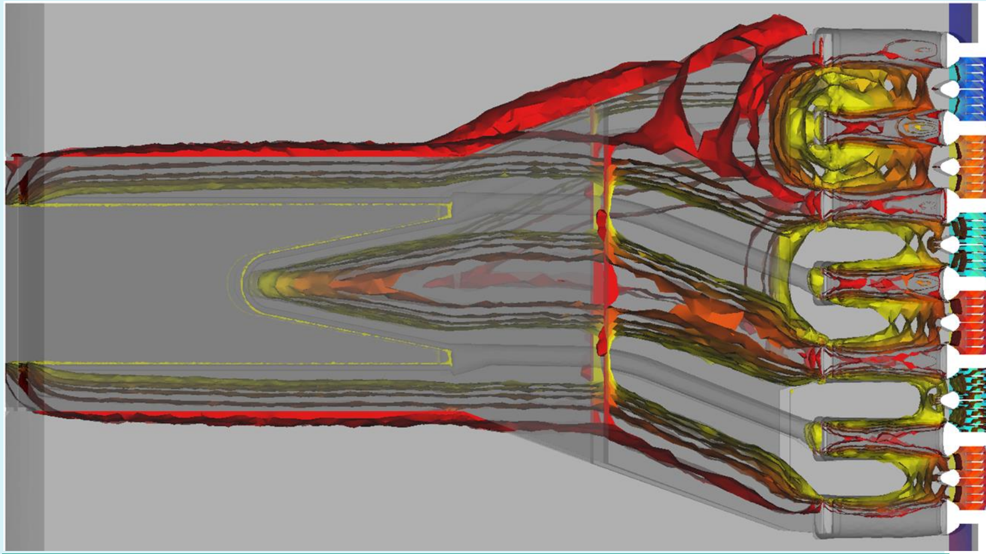
animation

Simulation model enabled
- comparison to 1D circuit model
- investigation of transmission line losses
- identification of impedance mismatches
- " " locations of field enhancements
- decisions for azimuthal field diagnostic locations

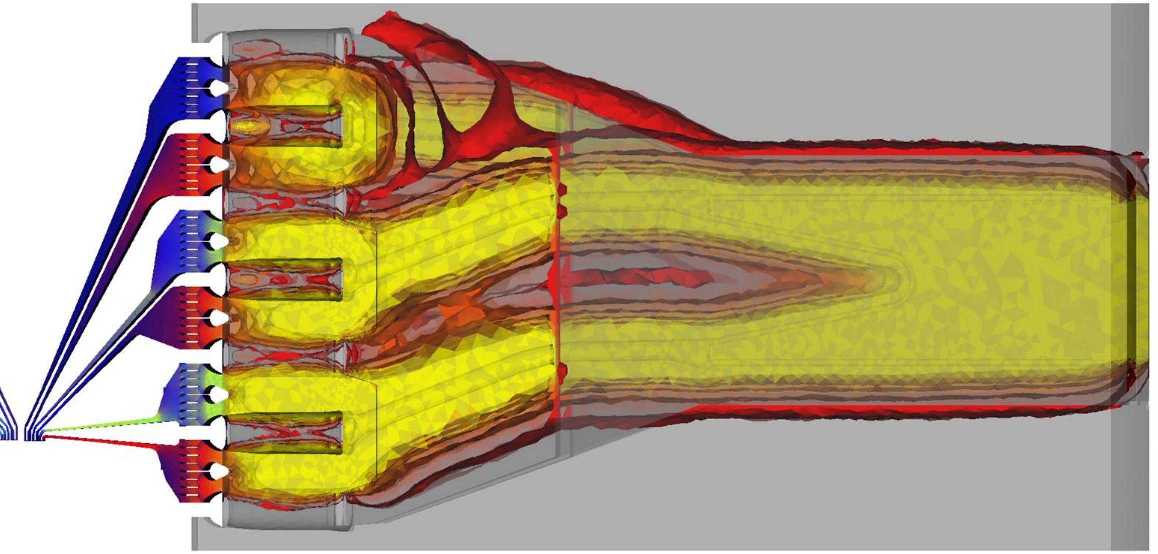
Outlook: the geometric fidelity of this model allows investigation of some impacts of
- switch timing and azimuthal drive asymmetries by driving each line with separate waveforms
- reconfiguring the water convolute region
- " " MITL and diode geometry

Simulation: Peggy Christenson, Visualization: Keith Cartwright

30° angular periodic domain (meters long): 21,973,729 elements ~20 nodes, ~10 wall-hours



Open contours of electric field magnitude show areas of high field gradient while tri-plate structure is recognizable



Filled contours of electric field magnitude indicate regions of maximum electric field

Impacts to Saturn Refurbishment Project

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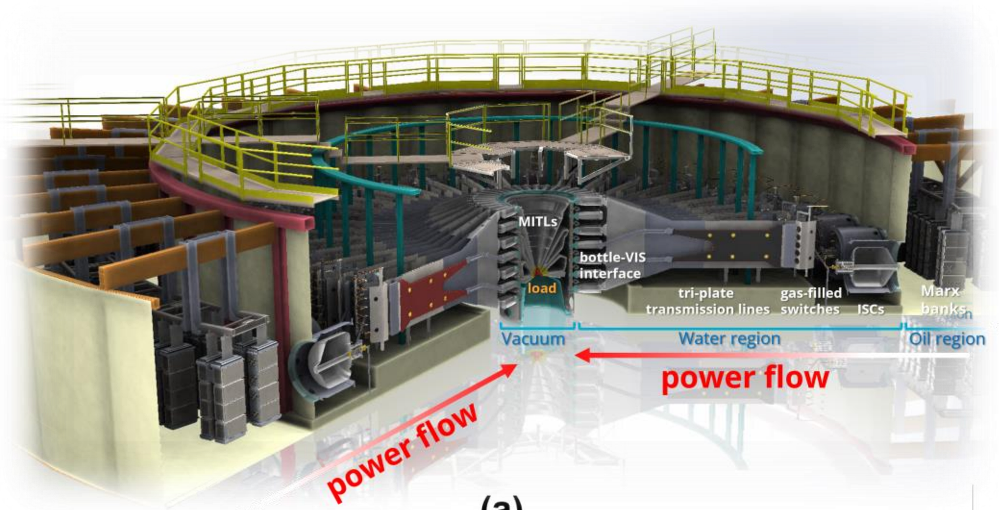
System overview: Saturn Bremsstrahlung Source

Energy driven through the accelerator **(a)** is compressed in space and time so that the power flow entering the vacuum section **(b)** liberates electrons. These electrons are directed towards the high Z anode target in the **3-ring diode load** **(c)** which convert to intense Bremsstrahlung photon output

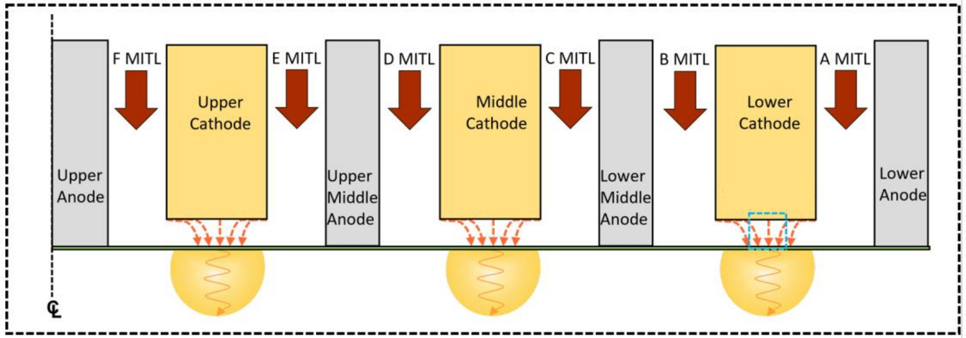
Pulsed-power driver:
- 36 Marx banks, 5.6 MJ total
- 100 ns power pulse delivered to diode

Electron beam generation:
- 10 MA current (total of 3 diodes)
- 1.5 MeV

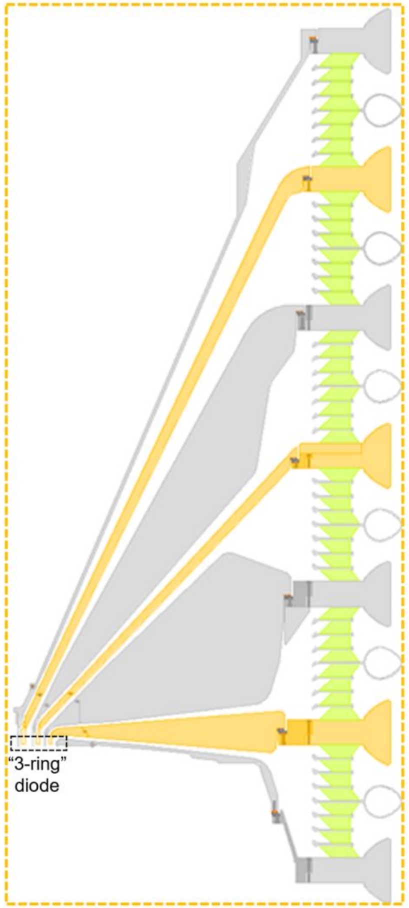
X-ray generation:
- variable spectrum
- 100 keV to 1.5 MeV endpoint energies



(a)



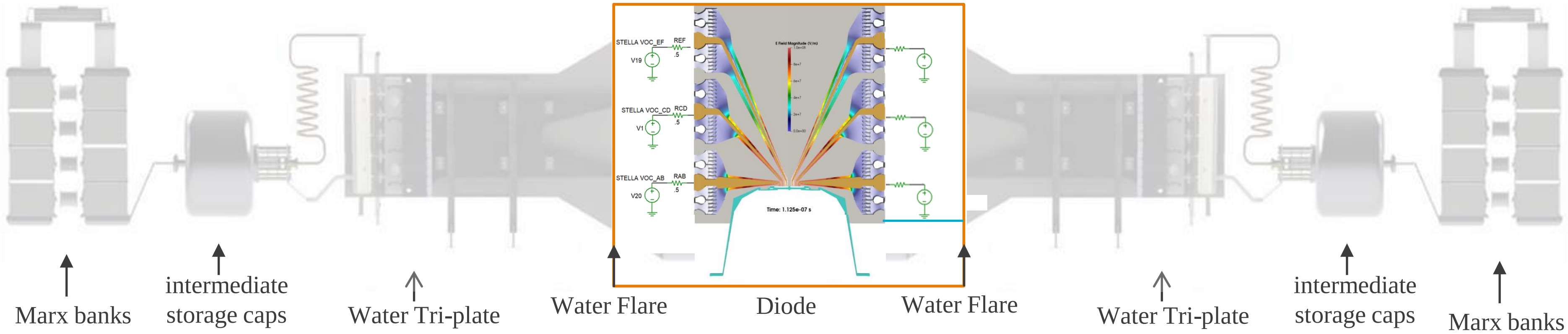
(c)



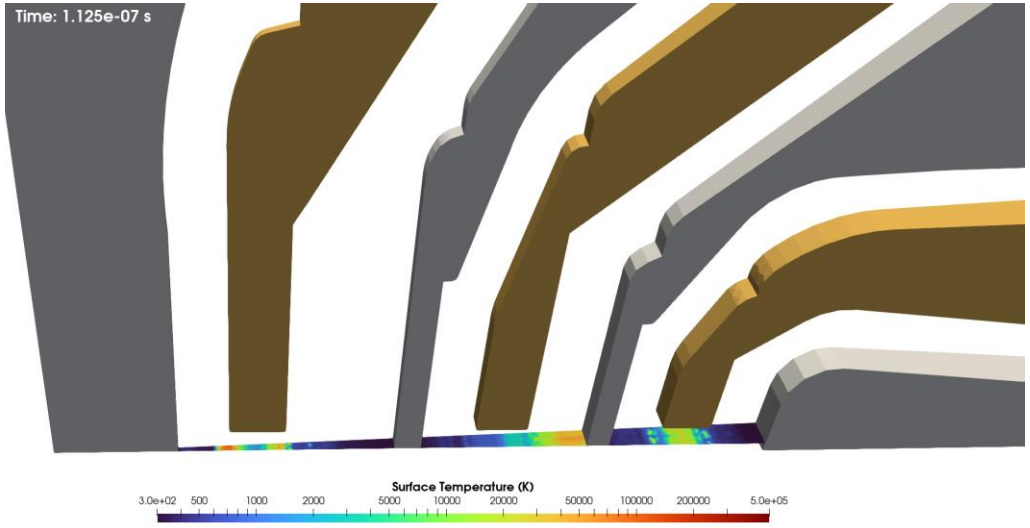
(b)

High resolution EM-PIC diode simulations: we self-consistently follow the power flow conversion from EM waves to the emission of electrons, leading to bipolar flow, reproducing the correct diode beam pinching and steering

animation

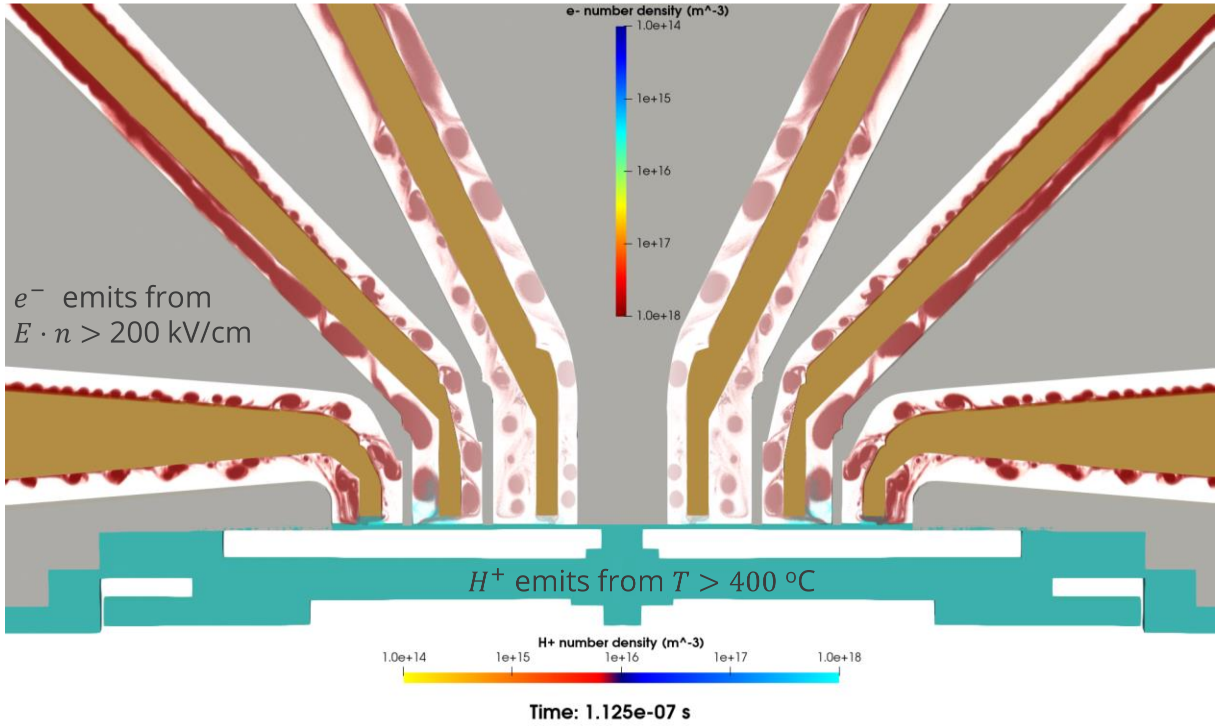


Heterogeneous modeling strategies and HPC resources have enabled machine-scale simulations of detailed processes



We simulate 2.5° azimuthally-periodic domains using 28-87M element meshes on 90-350 HPC nodes. Each simulation takes ≈ 20-30 wall-hours

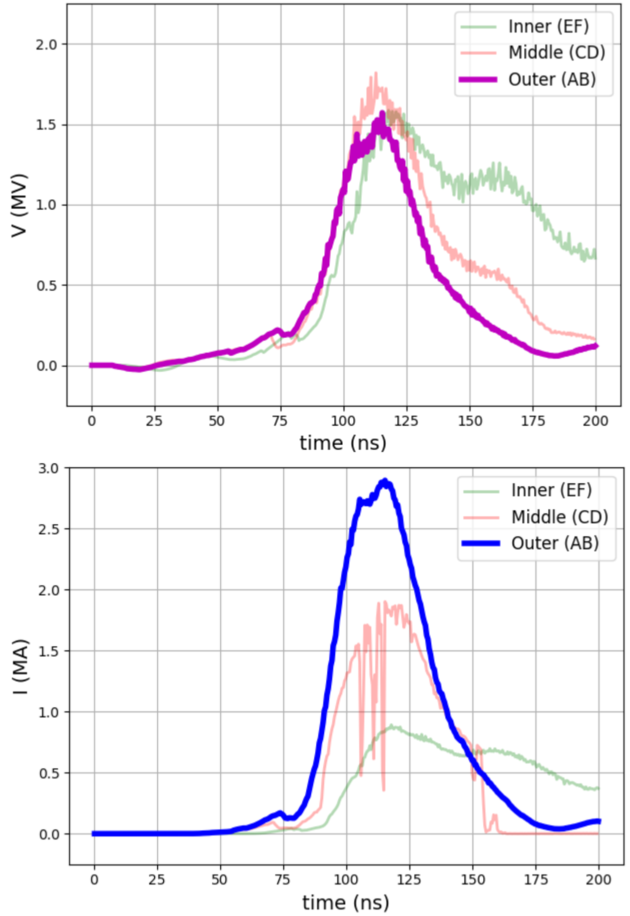
self-consistent surface heating



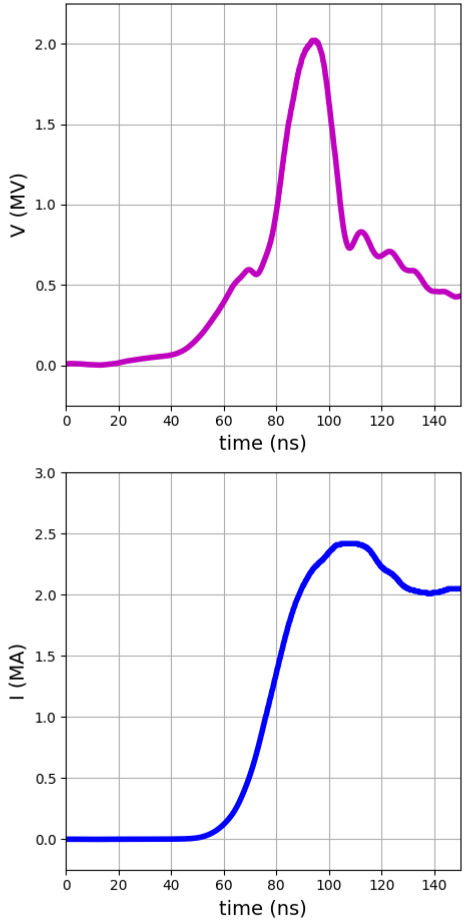
spatially- and time-resolved simulation of bipolar flow

Simulations predict diode currents and voltages in line with extrapolated measurements

1D-3D EMPIRE EM-PIC predictions at load



Extrapolated measurement at the load[1]



AB diode voltage comparisons

- EMPIRE predicts ~ 1.5 MV peak
- Extrapolated measurement ~ 2 MV peak

AB diode current comparisons

- EMPIRE predicts < 3 MA peak
- Extrapolated measurement < 2.5 MA peak

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[1]Savage, Mark et al. *Technical goals of the Saturn recapitalization project*. Presented at the IEEE International Pulsed Power Conference (Virtual). https://doi.org/10.2172/1899658

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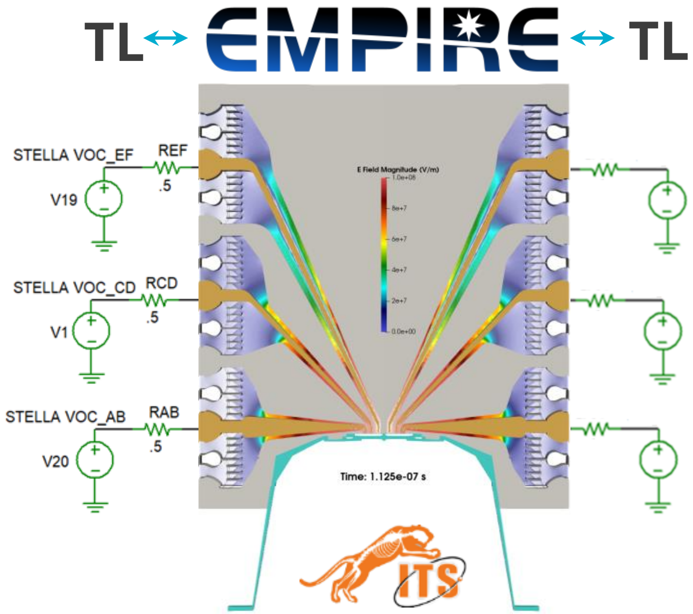
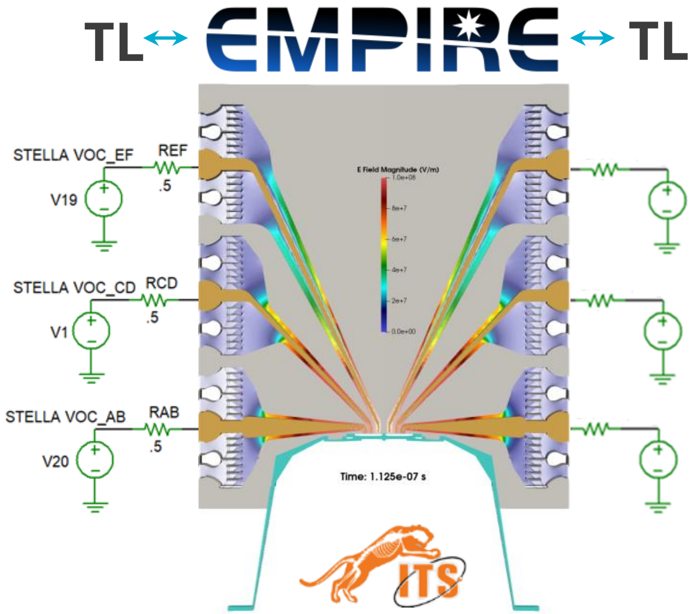
Self-consistent bipolar flow simulations provide high confidence “inputs” for ITS radiation calculations



Coupled simulation model

Self-consistent bipolar flow simulations provide high confidence “inputs” for ITS radiation calculations



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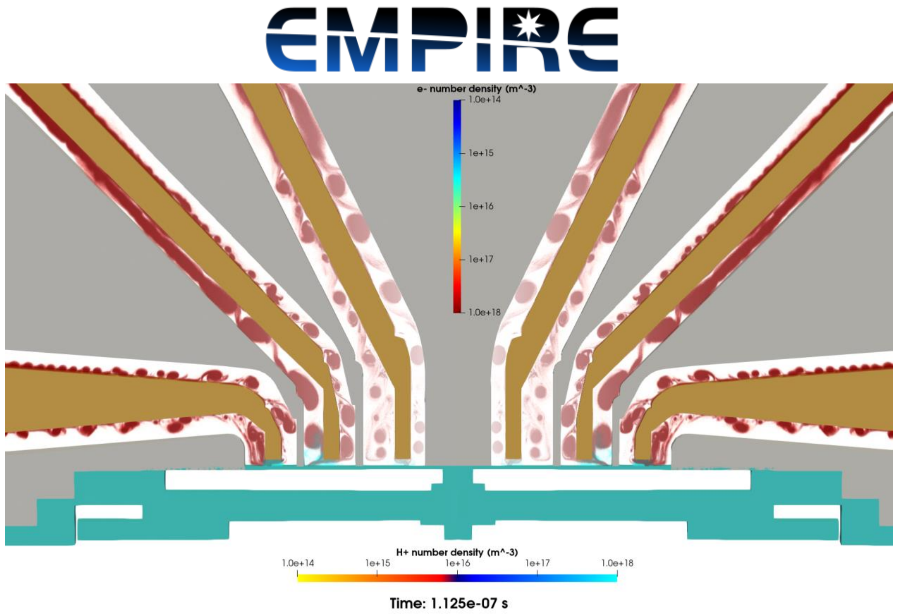
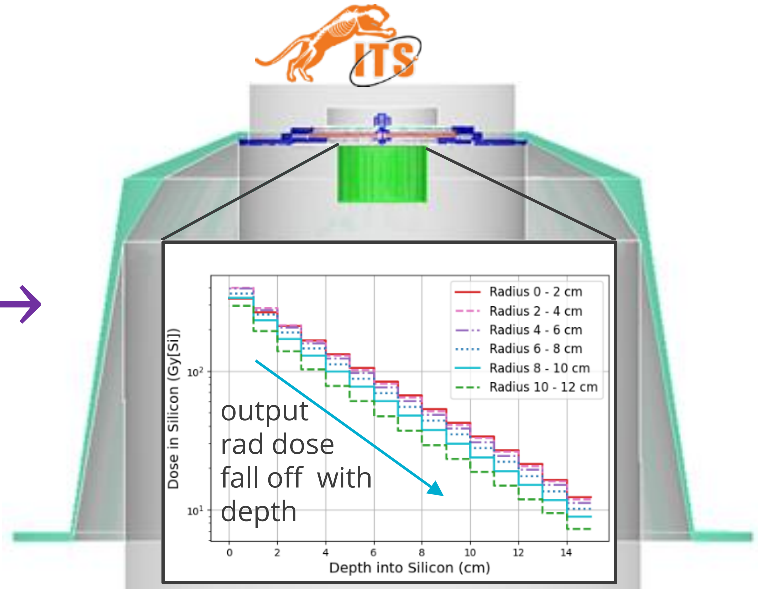


EMPIRE power flow simulation

→



ITS radiation transport calculation

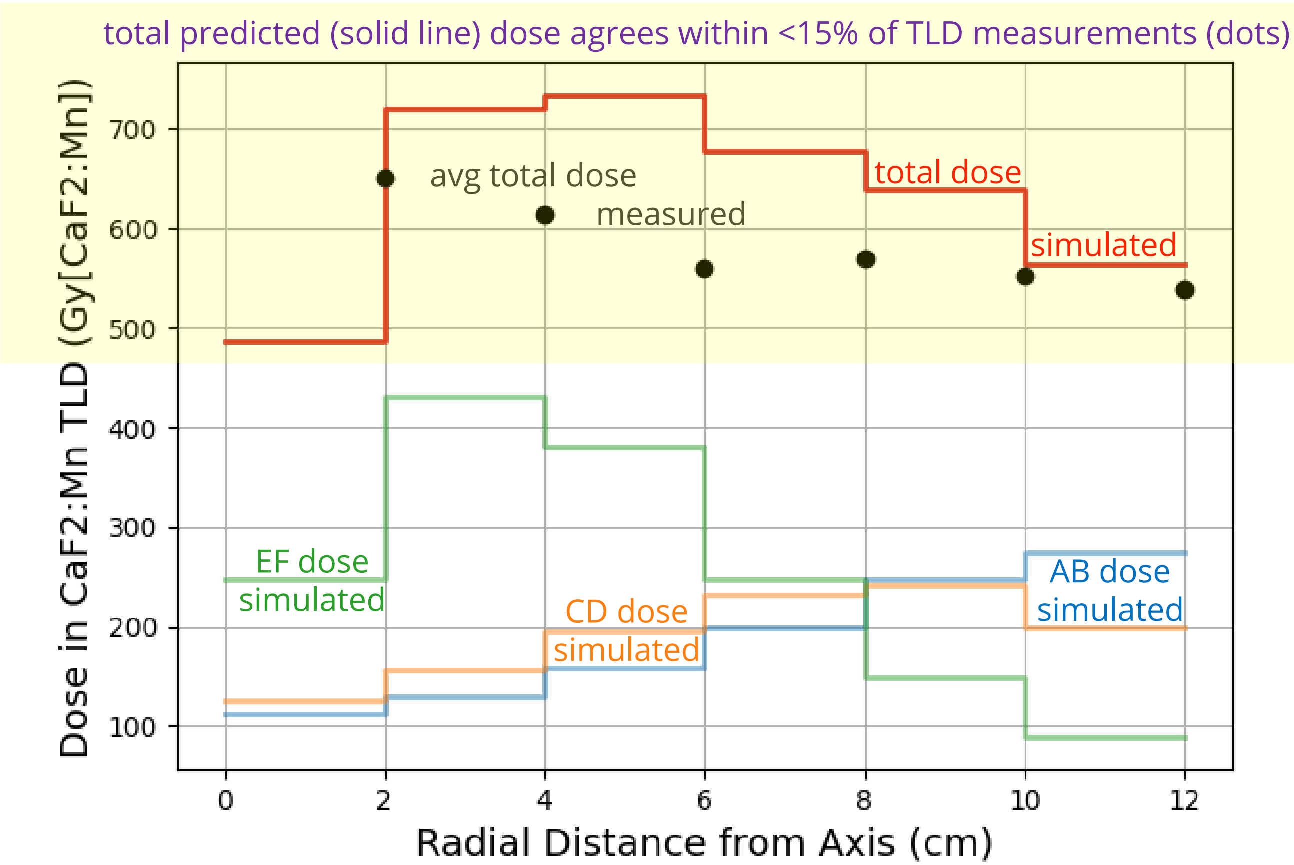
- **Powerflow simulation:** 1D-3D EMPIRE model for $R \leq 115$ cm (water flare to diode), driven by Bruce Weber’s (NRL) empirical CASTLE circuit model.
- **Radiation transport**: radiation field is calculated in ITS (POC: K. R. Depriest[1]) by sampling ≈ 800M trajectories per diode beam “PIC-FLUX-SOURCE” defined from the output of EMPIRE power flow simulations

Contributions: J. D. Douglas (CAD), P. J. Christenson (Cubit geometry creation), D. Sirajuddin (EMPIRE simulations), B. Weber (circuit modeling), T. D. Pointon (ITS/EMPIRE code coupling), R. DePriest (ITS model)

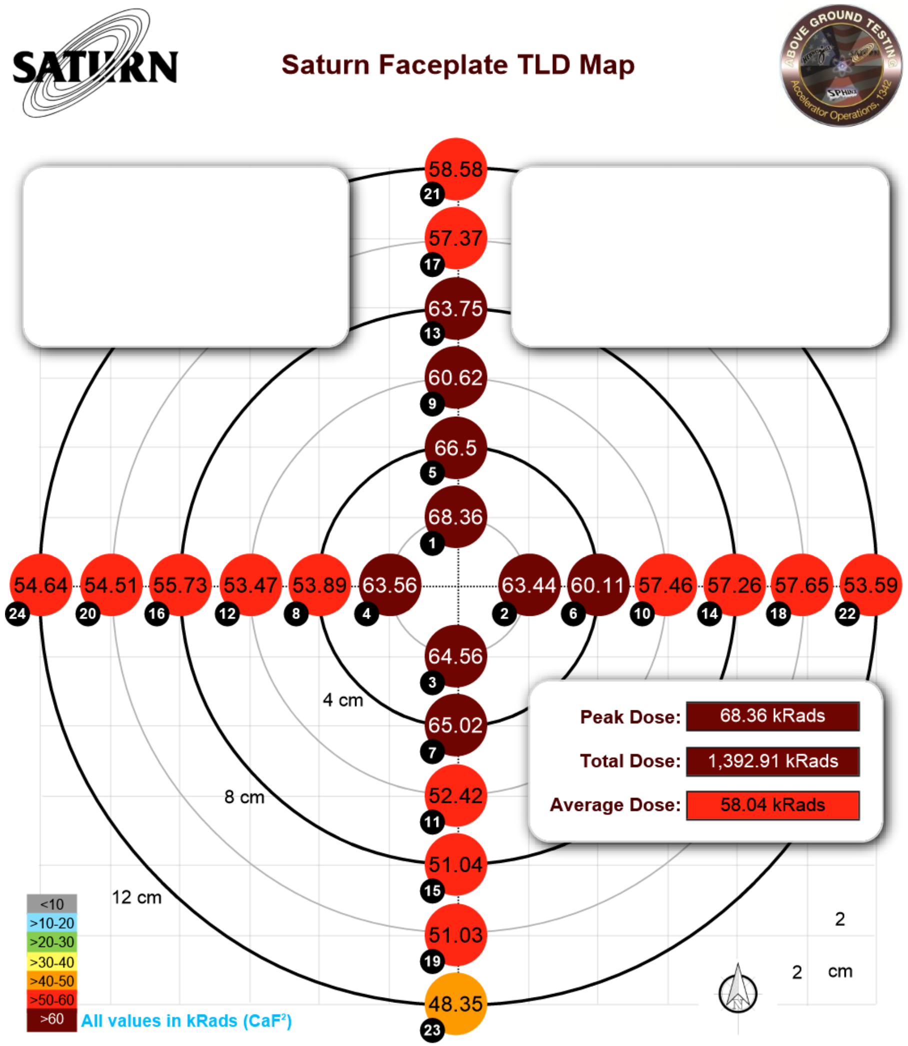
[1]K. R. DePriest, T. D. Pointon, D. Sirajuddin, B. A. Ulmen. *Time- and Energy-Resolved Coupled Saturn Radiation Environments Simulations Using the Integrated Tiger Series (ITS) Code*. September 2022. Technical report (SAND2022-11853). doi:10.2172/1885646

Empire-ITS coupling has lead to the most accurate predictions of the Saturn radiation field to date

Empire-ITS predictions vs. TLD measurements



TLD measurements



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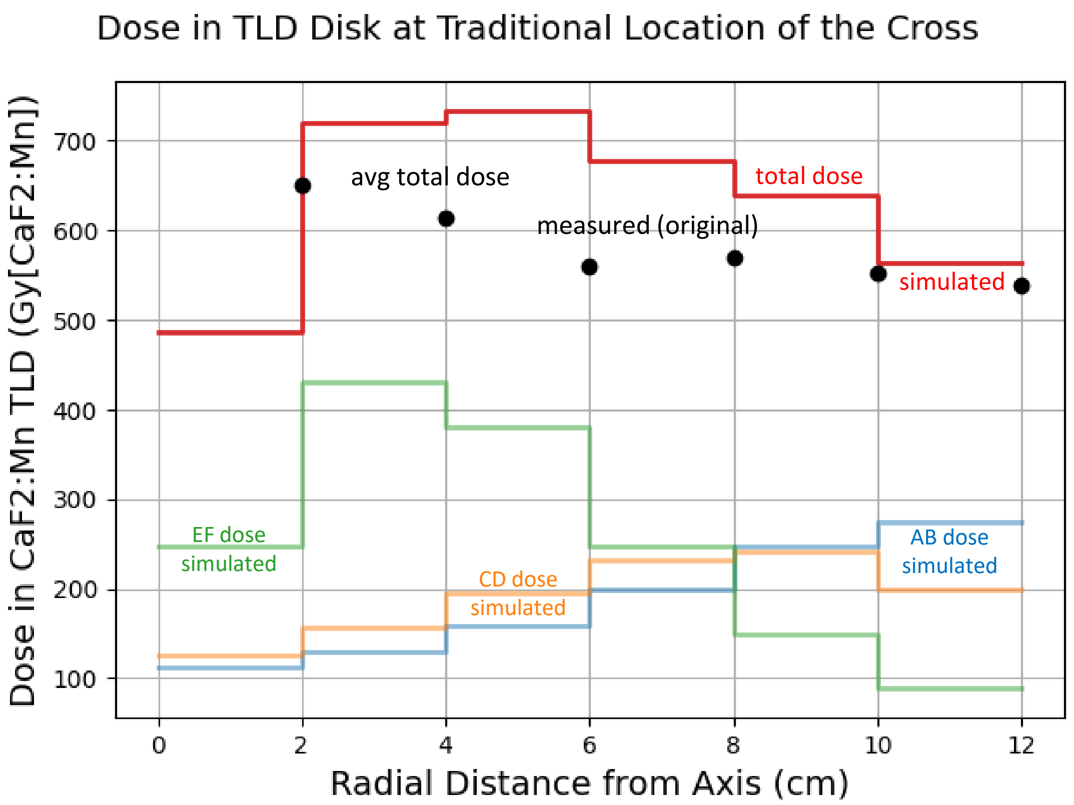
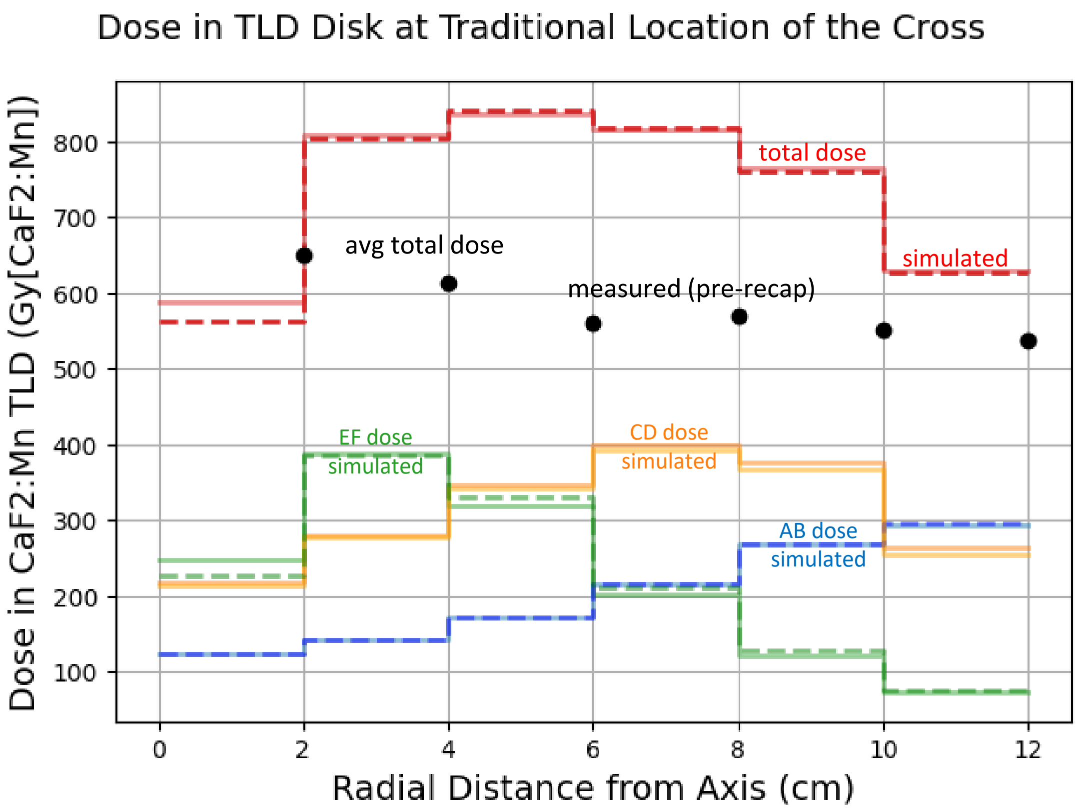
Empire-ITS leveraged to predict radiation field for refurbished geometry design



Original geometry

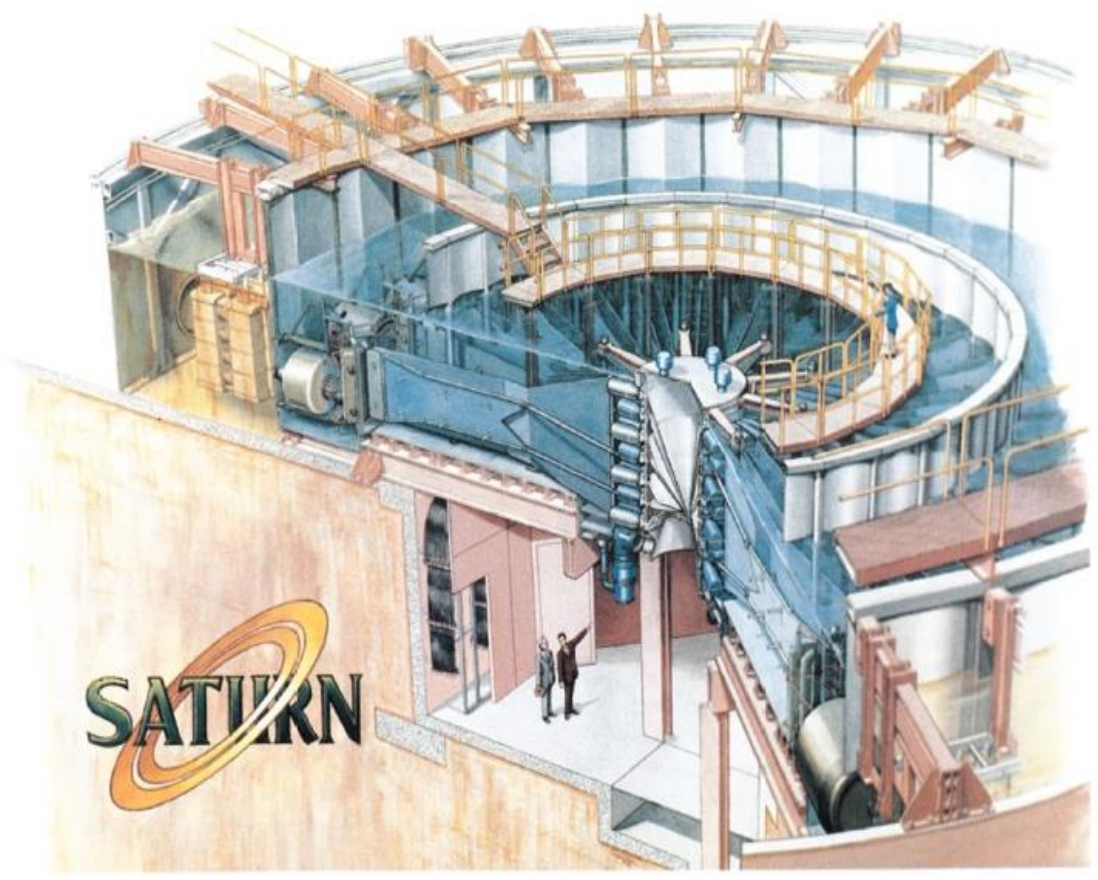


Refurbished geometry

- ✓ Simulated dose from the refurbished hardware proposal (Figure, right) lie within acceptable limits of the original hardware (Figure, left), confirming “do no harm” design principles are upheld
- ✓ Results from different diode gap spacings suggest a weaker dependence on the output radiation dose

System overview: Saturn E-beam Source

Energy driven through the **accelerator (a)** is compressed in space and time, *mixed* in a **convolute region (b)**, and delivered to a 3-ring diode load to generate **electron beam** output into an air drift cell **(c)** underneath



(a)

Pulsed-power driver:

- 24 Marx banks, 3.7 MJ total
- 100 ns power pulse delivered to diode

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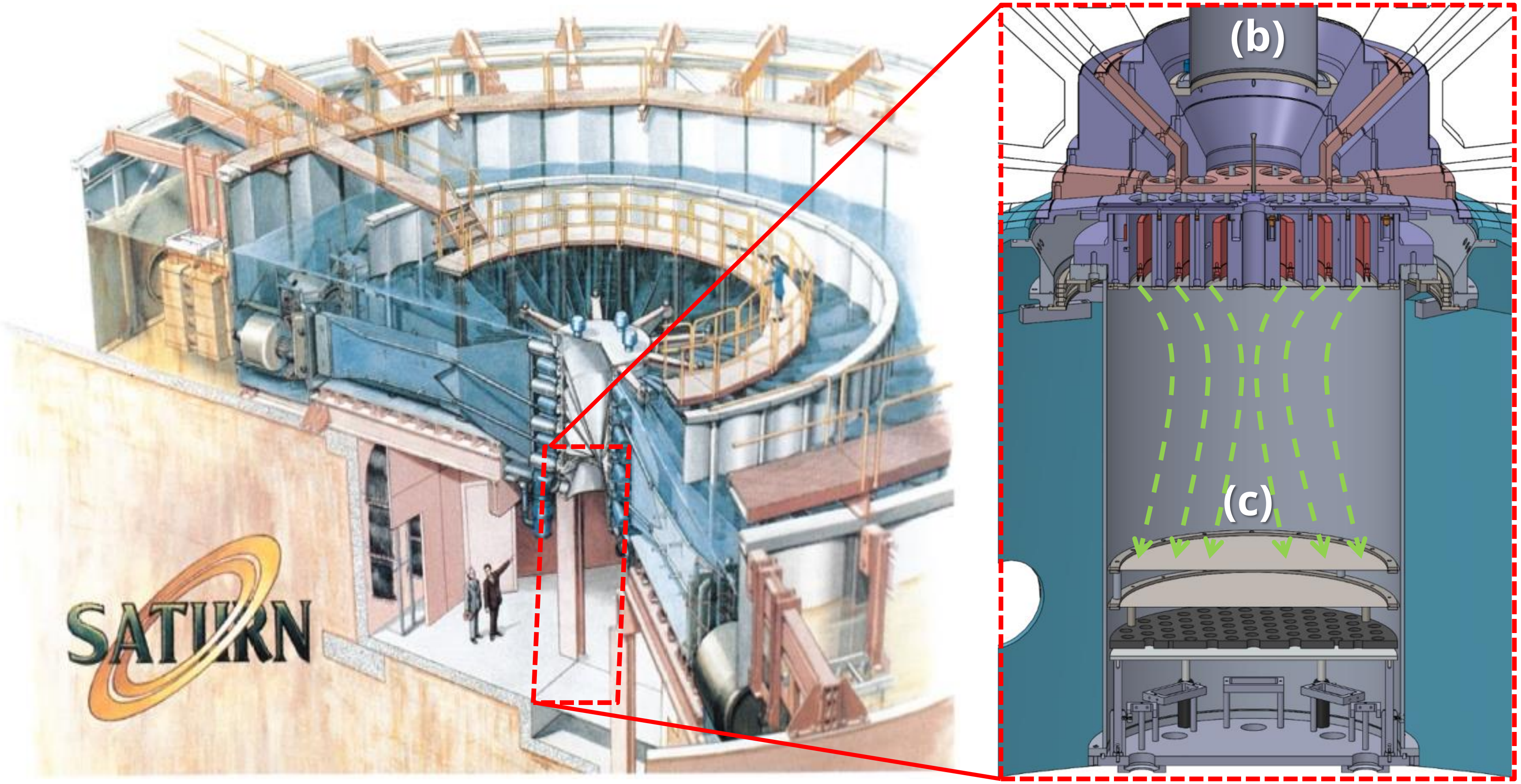

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Pulsed-power driver:

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Electron beam generation:

- 6 MA current (total of 3 diodes)
- 1.3 MeV

[(a)]Artist rendering sourced from: Savage, M. et al. Status of the pulsed power refurbishment of Saturn at Sandia National Laboratories. Proceedings of the IEEE International Pulsed Power Conference held in San Antonio, TX. June 25-29, 2023

Impacts to Saturn Re-design of the e-beam source

1. A high resolution 1D-3D EM-PIC model in `EMPIRE` was developed for the original e-beam source geometry in order to:
   a) characterize the power flow
   b) clarify magnetic field configuration and power mixing in the convolute region, and
   c) reveal vulnerabilities to accelerator hardware from operation (e.g., electron impact damage)

2. Simulations of a re-design have been completed and detailed comparisons to the original geometry analysis have been performed to inform the next design iteration. The results already confirm the design decisions protect vulnerabilities (e.g., diffusing electron beam fluxes and decreasing the energy deposition to surfaces.) without affecting power flow to the load

3. Ongoing work:
   a) Following the beam transit into the air drift cell (underneath) using ITS and/or Empire
   b) Simulations of at least one more design iteration (anticipated: December 2024)

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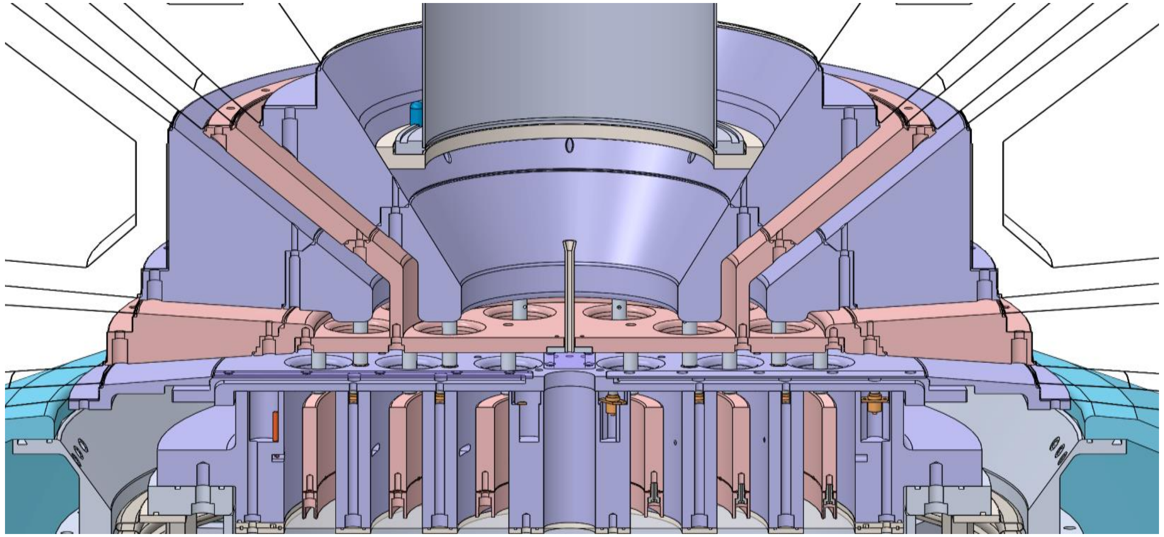
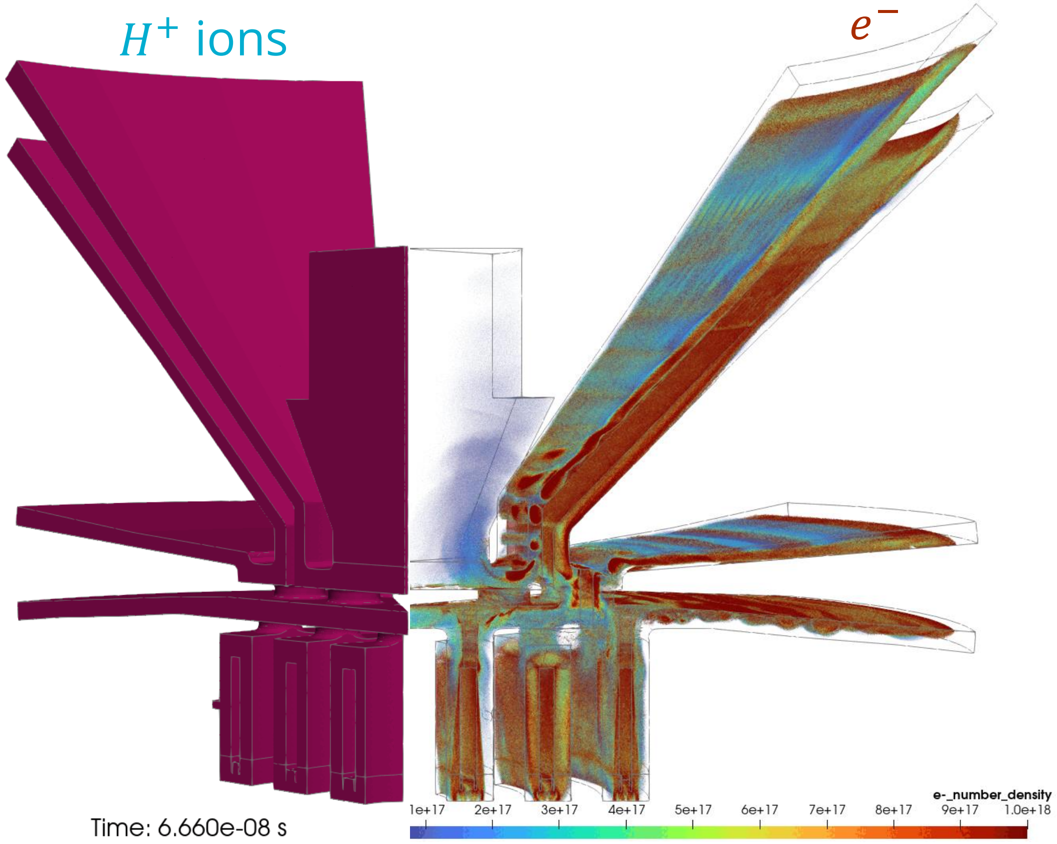
Characterizing power flow in the Saturn E-Beam

animation



CAD rendering



Simulation

Simulation details

- *Meshes*: 286,462,880 elements + thermal grids inside materials
- *Particles*: 4.83e+08 electrons, 2.71e+07 protons; maximum
- *Resources*: 14400 cores / 300 CTS-1 nodes
- *Duration*: 115 ns over 227,844 steps, 30 wall-hours
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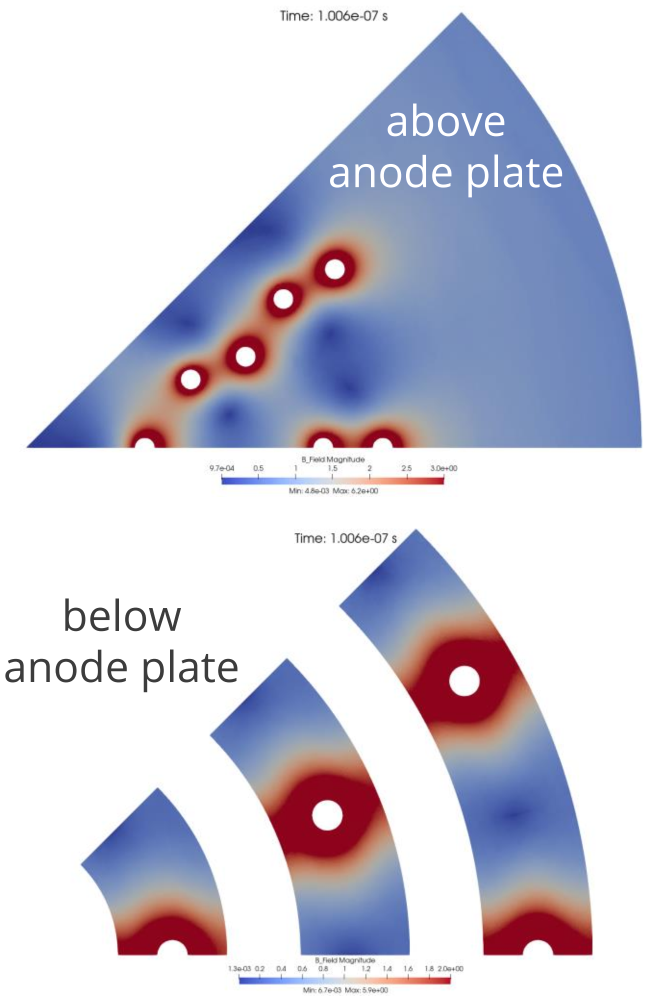
2. Simulations of a re-design have been completed and detailed comparisons to the original geometry analysis have been performed to inform the next design iteration. The results already confirm the design decisions protect vulnerabilities (e.g., diffusing electron beam fluxes and decreasing the energy deposition to surfaces.) without affecting power flow to the load

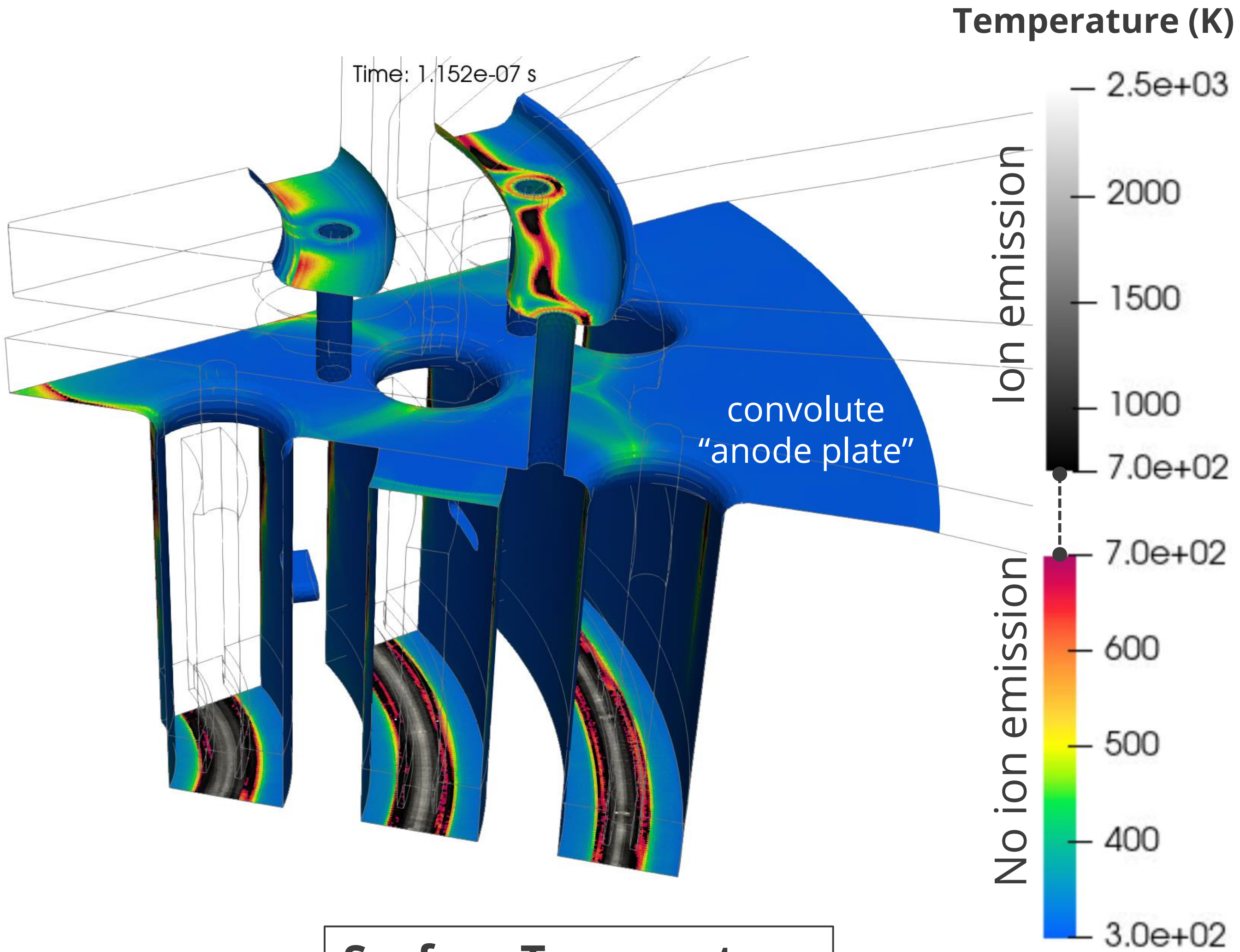
3. Ongoing work:
   a) Following the beam transit into the air drift cell (underneath) using ITS and/or Empire
   b) Simulations of at least one more design iteration (anticipated: December 2024)

Magnetic field configuration and identifying vulnerabilities in the Saturn E-Beam

animation



Magnetic field magnitude



Surface Temperature

- Field nulls break insulation, allowing electron trajectories to impact surfaces
- Anode surfaces locally break down into plasma (grey-black) and damage components

Impacts to Saturn Re-design of the e-beam source

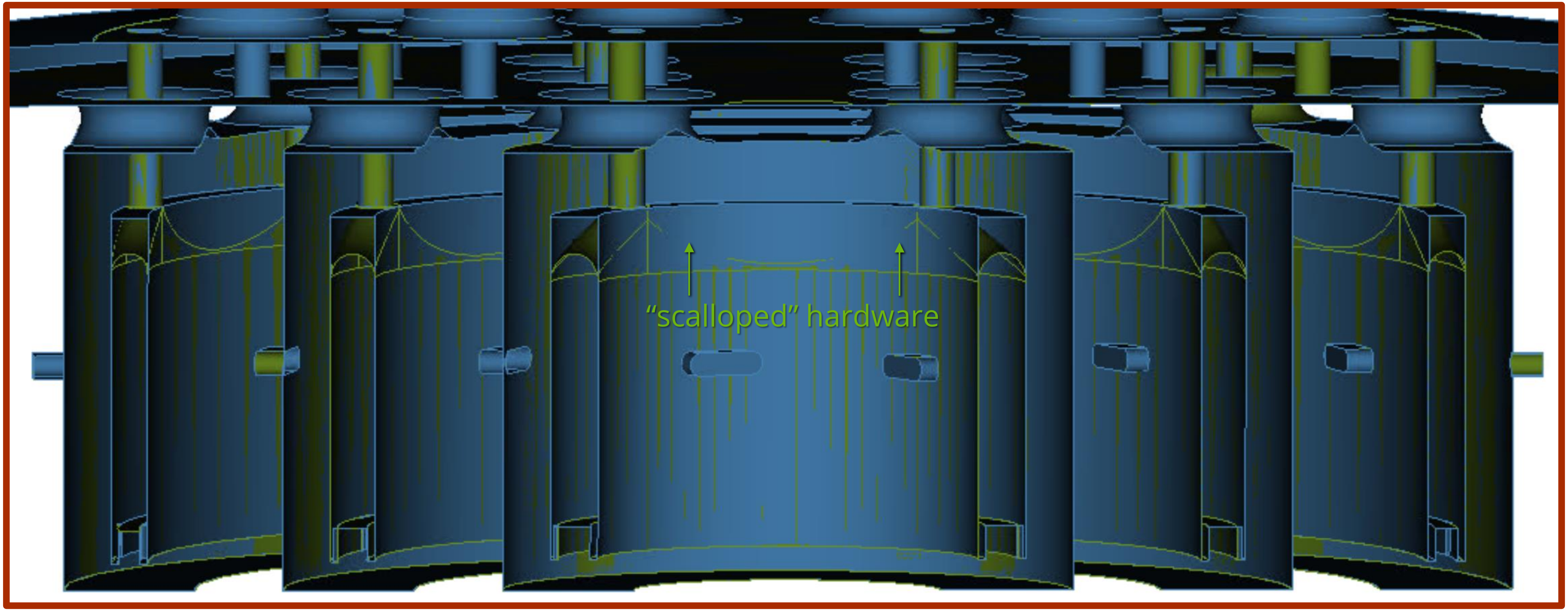
1. A high resolution 1D-3D EM-PIC model in `EMPIRE` was developed for the original e-beam source geometry in order to:
   a) characterize the power flow
   b) clarify magnetic field configuration and power mixing in the convolute region, and
   c) reveal vulnerabilities to accelerator hardware from operation (e.g., electron impact damage)

2. Simulations of a re-design have been completed and detailed comparisons to the original geometry analysis have been performed to inform the next design iteration. The results already confirm the design decisions protect vulnerabilities (e.g., diffusing electron beam fluxes and decreasing the energy deposition to surfaces.) without affecting power flow to the load

3. Ongoing work:
   a) Following the beam transit into the air drift cell (underneath) using ITS and/or Empire
   b) Simulations of at least one more design iteration (anticipated: December 2024)

Saturn e-beam re-design

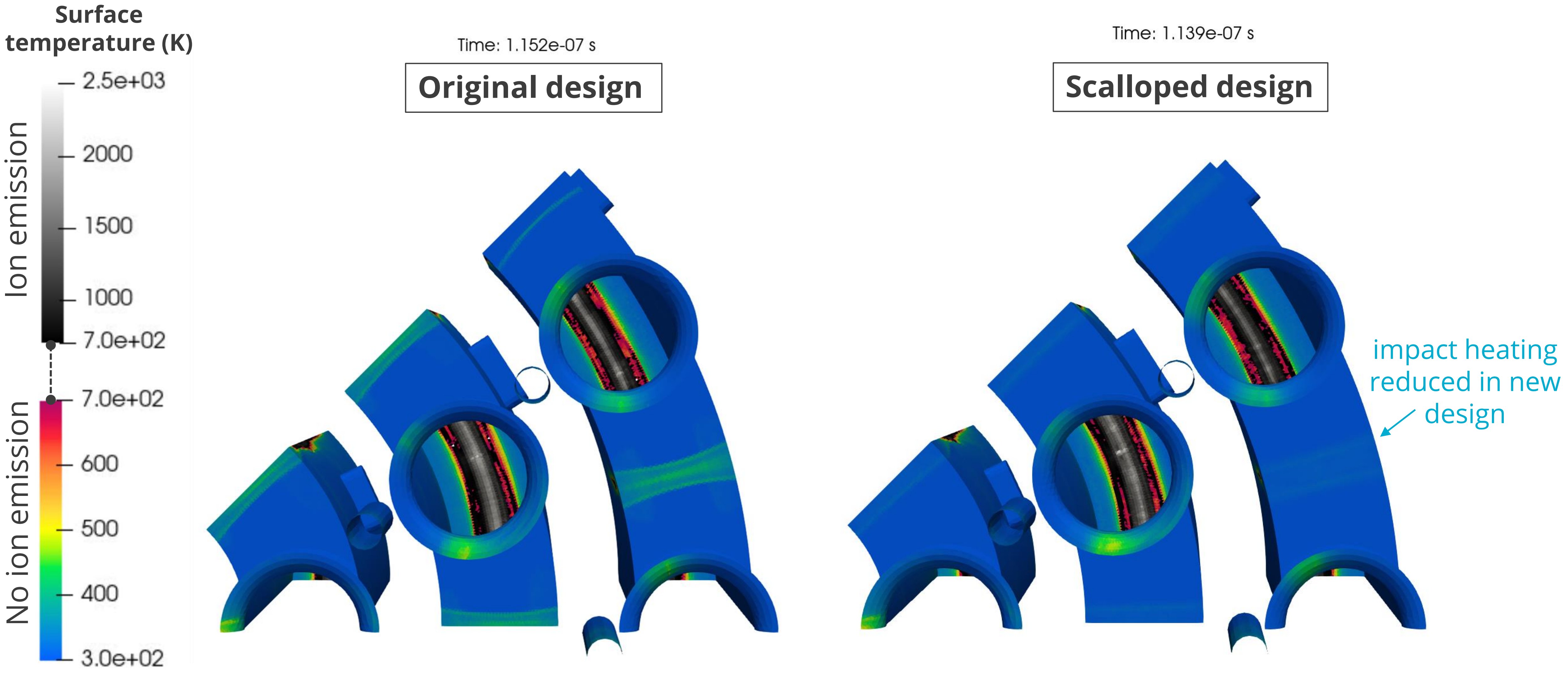
The post hole plates have been redesigned (green) with scalloping to mitigate hardware damage from electron impacts compared to the original design (teal)



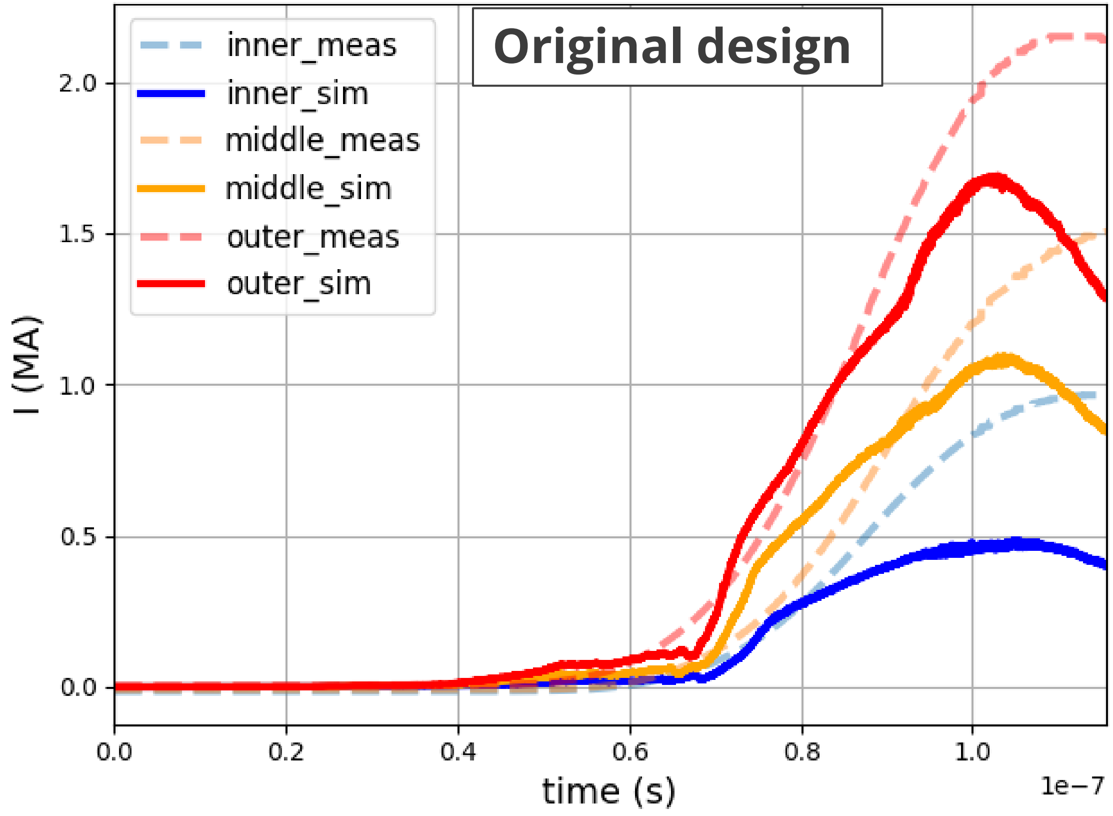
Saturn e-beam re-design mitigates anode damage

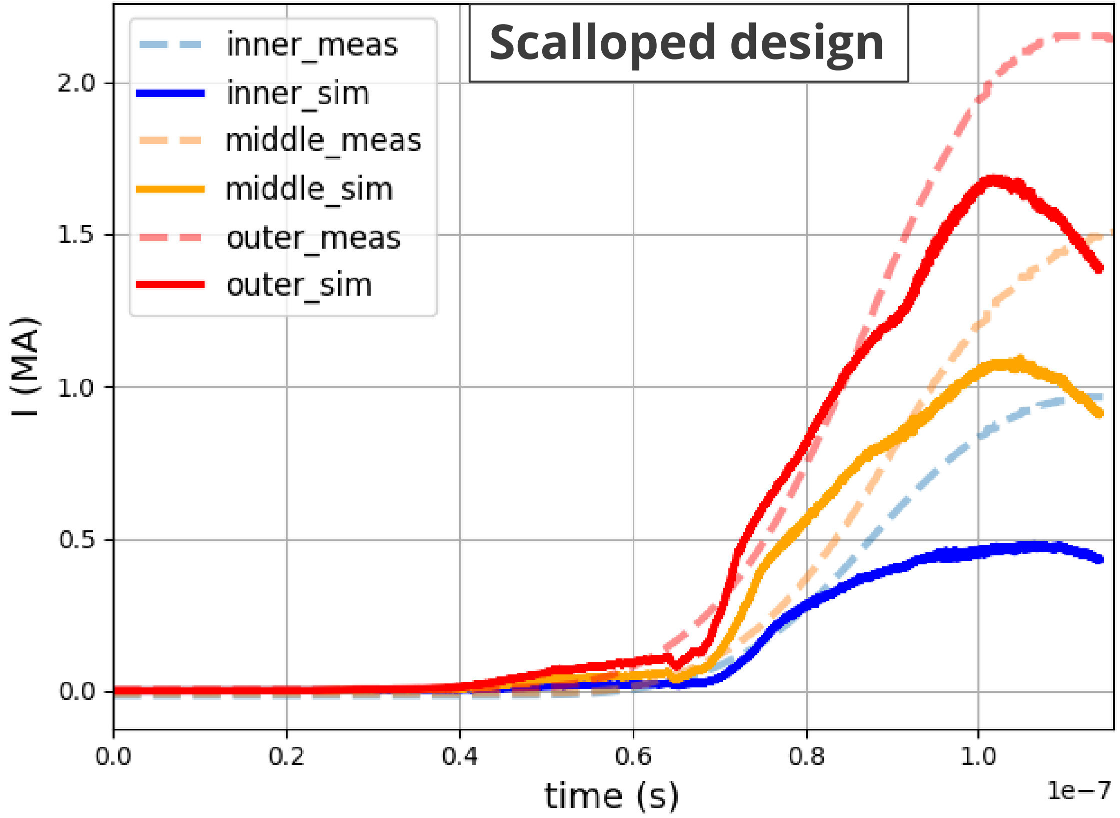
animation

The post hole plates have been redesigned (green) to mitigate hardware damage from electron impacts compared to the original design (teal)



Re-design maintains desired power flow characteristics

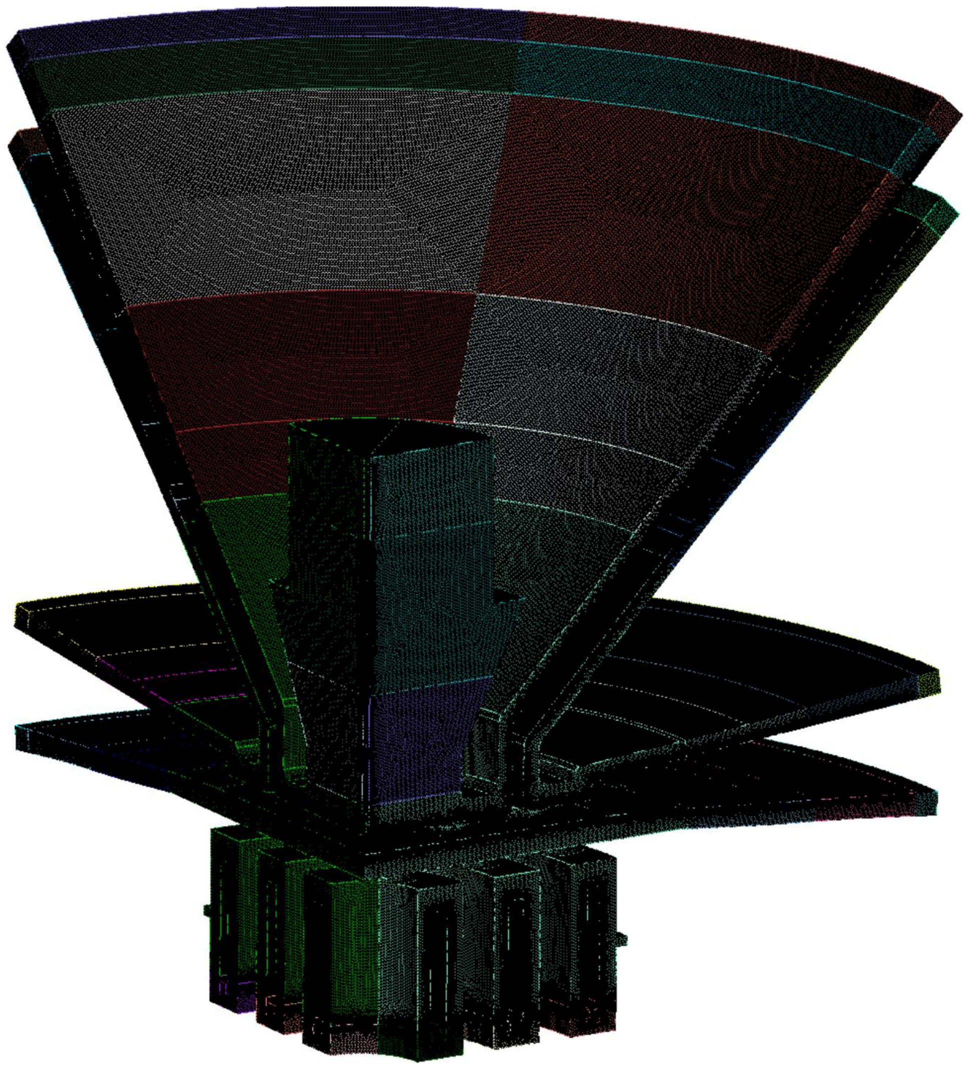




- Simulated currents agree reasonably with measurements given missing physics from model (gap closure)
- *Fact*: Simulations with "everything but gap closure" *typically* undershoot the max diode currents in Saturn by ~ 0.5 MA; this is a reflection of an operating principle which leverages plasma expansion to reach design targets

Next: designing new transitions and feeds to connect the new MITLs to the E-Beam convolute

Near-term: we are planning to run the full 90° periodic geometry on LANL Crossroads



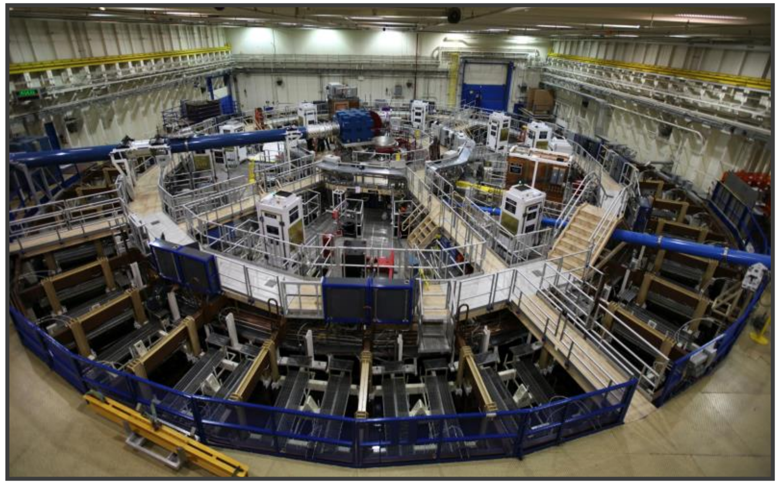
Mesh summary

Number of coordinates per node	=	3
Number of nodes	=	99973185
Number of elements	=	574,370,176
Number of element blocks	=	3
Number of nodal point sets	=	10
Length of node list	=	5878
Length of distribution list	=	5878
Number of element side sets	=	111
Length of element list	=	42794312
Length of node list	=	128382936
Length of distribution list	=	128382936
Number of coordinate frames	=	0

Mesh size = 574M elements + thermal grids ⇒

- 28,728 cpus / 513 nodes ≈ 5.8% of the machine
- 30 wall-hours

RAMSES Simulation Results and Impact to Pulsed Power



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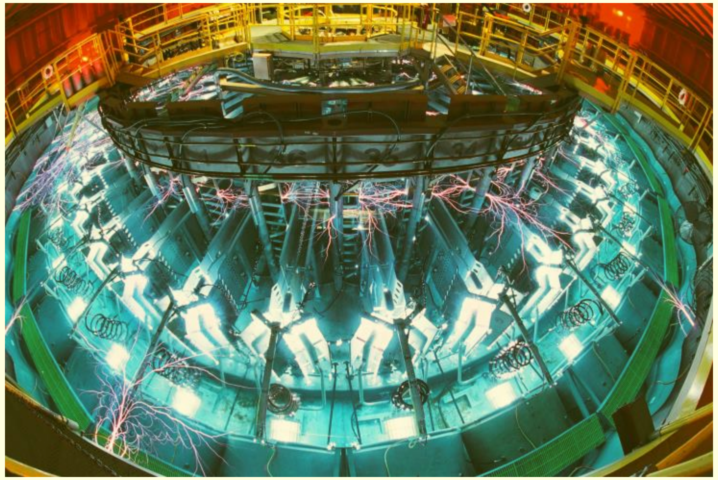
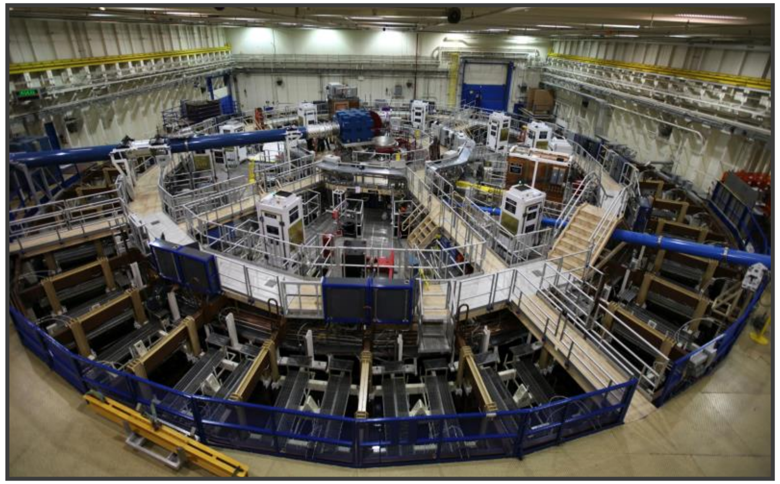


Saturn

HERMES-III

- Saturn Refurbishment Project:
  - Machine-scale power flow simulations
  - Bremsstrahlung diode physics
- Saturn Redesign of the e-beam source

RAMSES Simulation Results and Impact to Pulsed Power



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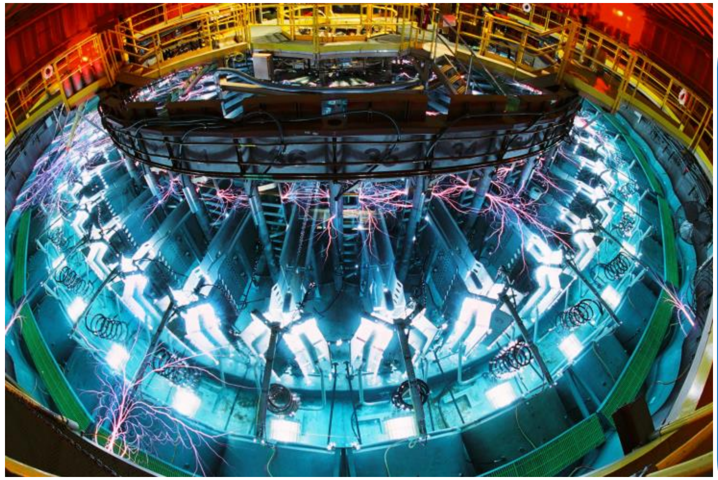


Saturn

HERMES-III

- Rapid optimization of Bremsstrahlung Diode

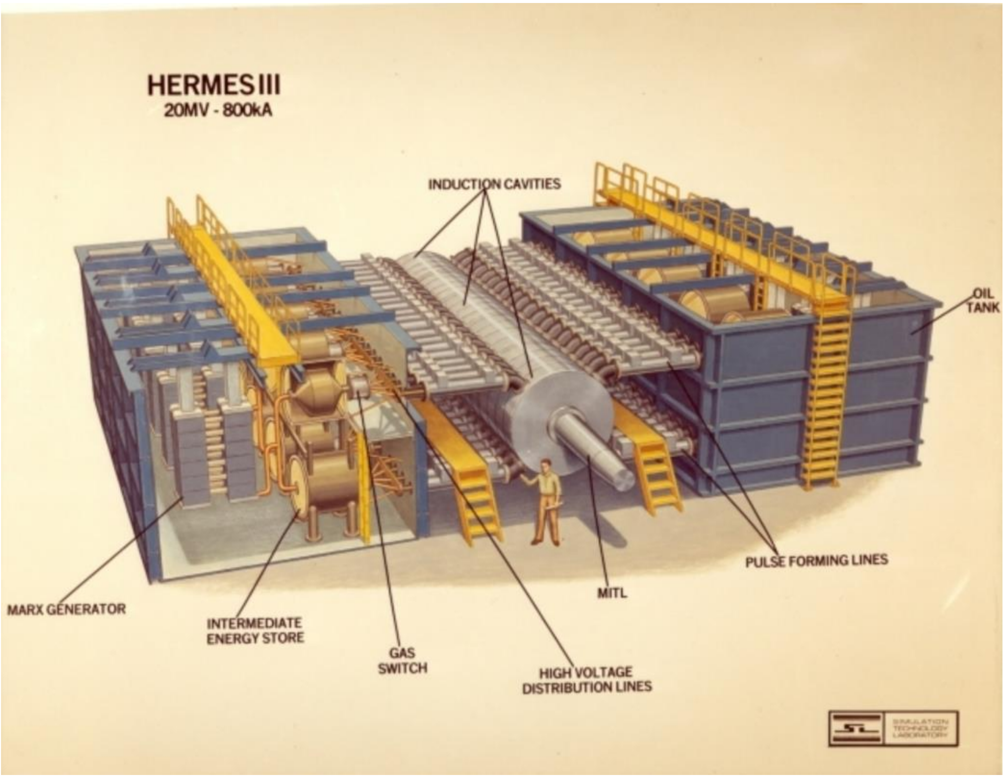
System overview: HERMES-III accelerator

A 12 TW pulsed-power accelerator used to produce high energy X-rays

Figure: HERMES-III Extended MITL (2019)[1]

15 m

Figure: Artist rendering[2] of HERMES-III



Pulsed-power driver:

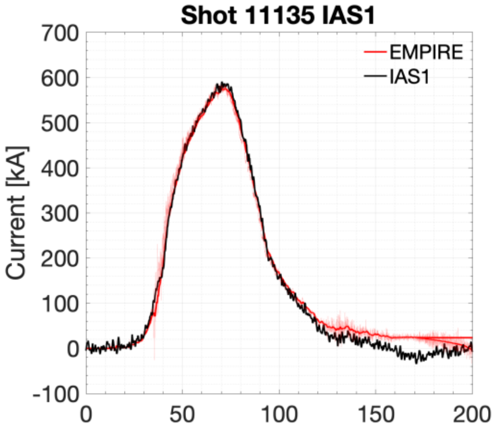
- Marx generator/Inductive Voltage Adder approach
- 10 Marx banks, 1.56 MJ total[2] → 20 MV, 600 kA
- 40 ns power pulse delivered to diode

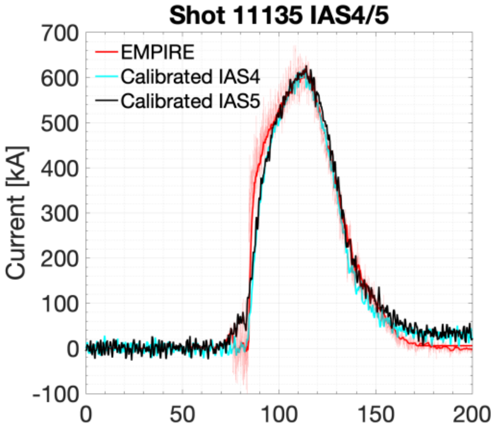
[1]Progress in Modeling the 2019 Extended Magnetically Insulated Transmission Line (MITL) and Courtyard Environment Trial at HERMES-III. Cartwright, K. et al. SAND report, Sept. 2022. SAND2022-13172.

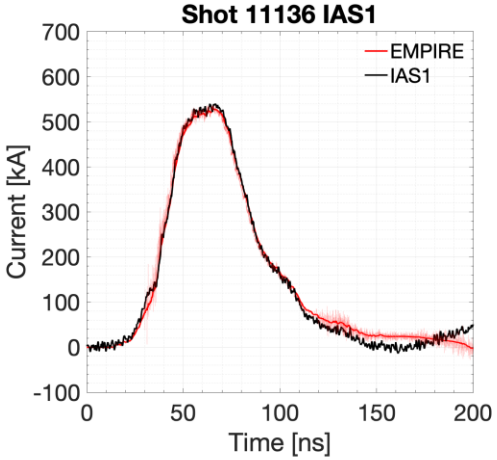
[2]Characterization of an Improved MITL Extension for the HERMES III Accelerator. Grabowski, T. et al. Presented at the 23rd IEEE International Pulsed Power Conference (virtual), December 12-16, 2021. 2021SAND2021-14770C

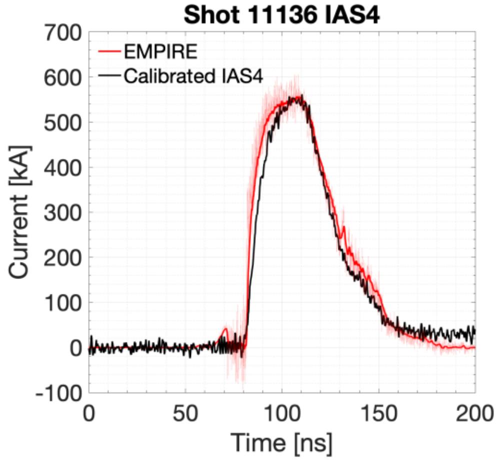
HERMES-III: Extended MITL Validation of shot 11135[1,2]

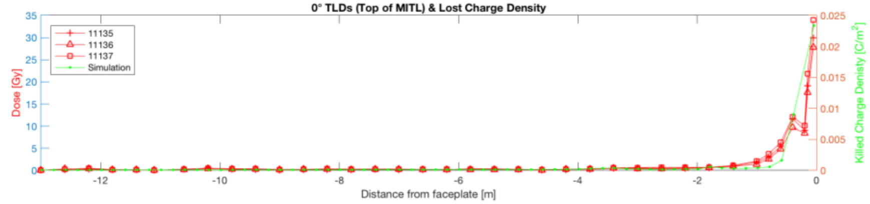
In the April 2018 tests of the legacy extended MITL and the July 2019 tests of there designed extended MITL, a series of TLDs were laid out along the length of the MITL anode outer surface

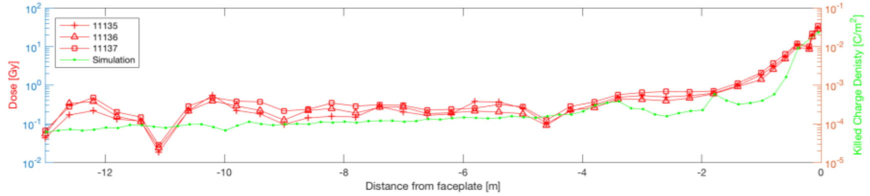


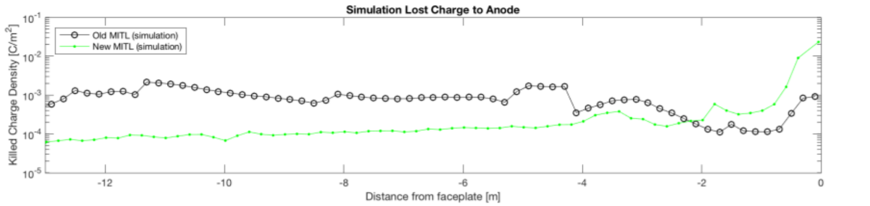


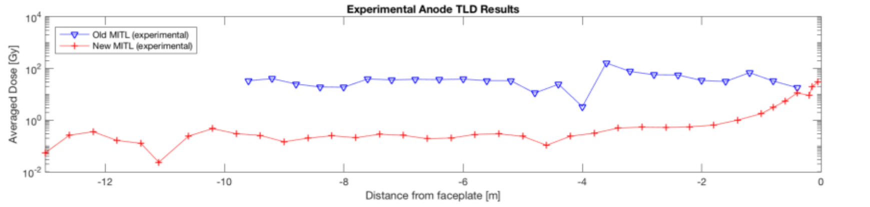


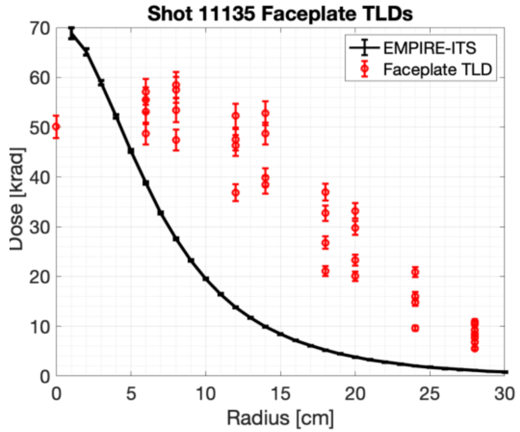


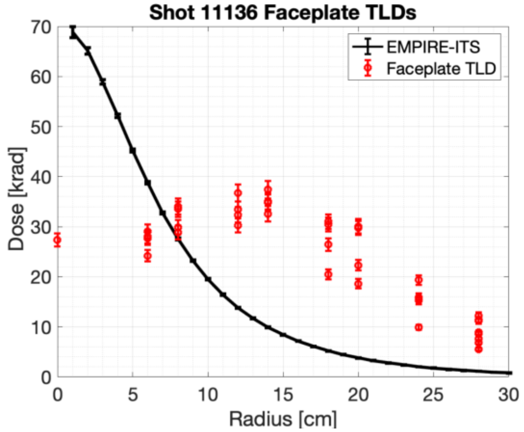










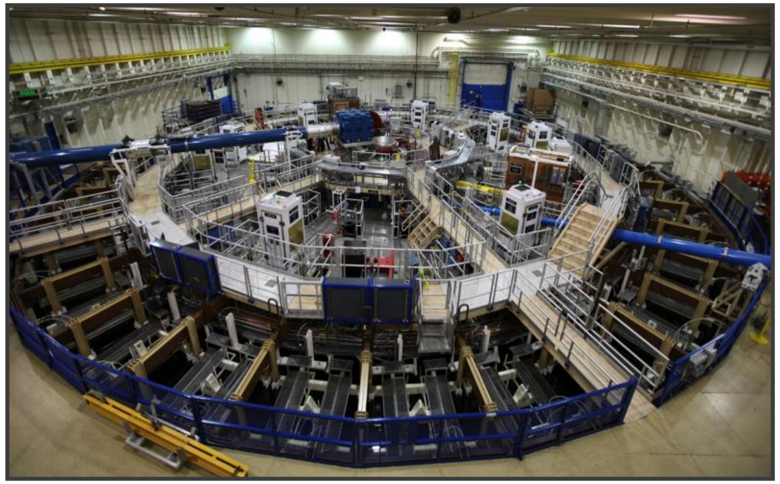


[1]Powell, T. *Theory, Simulation, and Experiments on a Magnetically Insulated Transmission Line Terminated by a Bremsstrahlung Diode*. PhD dissertation. May 2023.
[2]Cartwright, K. et al. *Progress in Modeling the 2019 Extended Magnetically Insulated Transmission Line (MITL) and Courtyard Environment Trial at HERMES-III*. SAND report, September 2022. SAND2022-13172.

Outline

- RAMSES' role in SNL's mission space
- Code overviews: ITS, Empire
- Pulsed power at Sandia
- RAMSES Simulation Results and Impact to Pulsed Power
- Outlook and Future Impacts

RAMSES impact to Pulsed Power at Sandia



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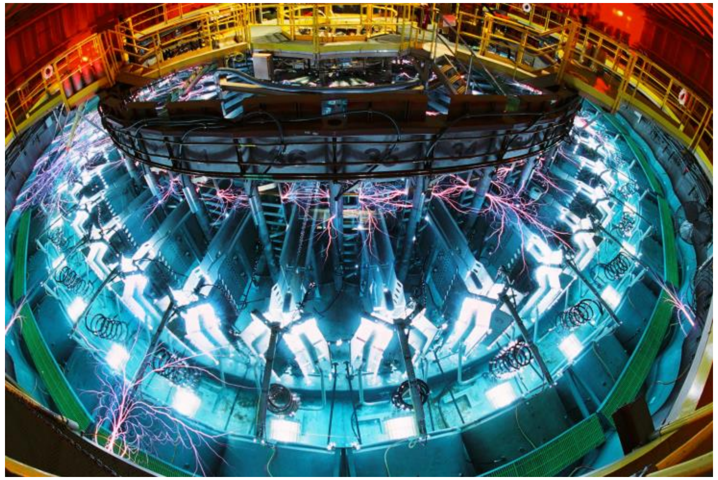


Saturn

HERMES-III

Outlook and future impacts

We envision RAMSES taking on an increased role in Sandia's pulsed-power apparatus, delivering progressively higher fidelity (and faster turnaround) simulations to meet program objectives, including (but not limited to) impacting decisions pertaining to accelerator design, refurbishment, and used as a tool to meet agile needs more broadly (informing shot proposals, diagnostics viability and decisions).

Thank you for your attention! Questions?

Title slide photo credits and descriptions

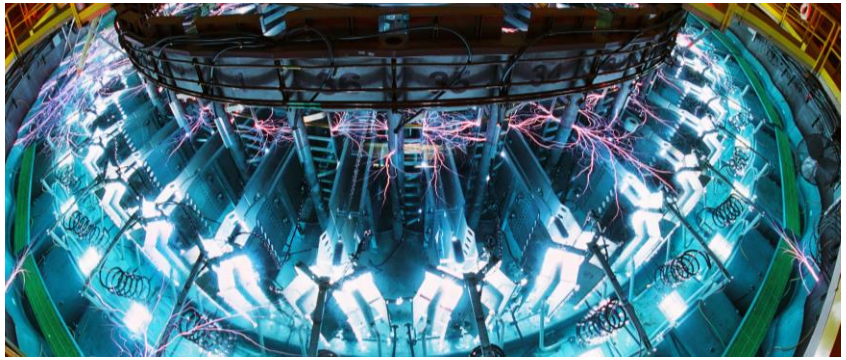
SNL's Attaway HPC

"Water flows through flexible tubes and pipes visible through glass panels above two rows of Attaway's compute racks. At the end of the racks, cooling distribution units control water flow and rates. Image Credit: Sandia."

Federal Energy Management Program, Department of Energy. July 23, 2021. "Sandia's Liquid-Cooled Data Center Boosts Efficiency and Resiliency" (Press Release). https://www.energy.gov/femp/articles/sandias-liquid-cooled-data-center-boosts-efficiency-and-resiliency

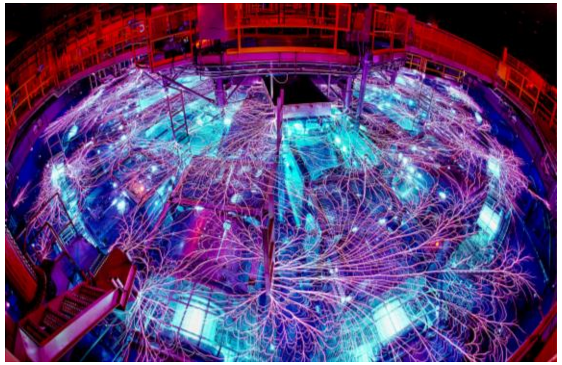
HERMES-III
gamma-ray source

HERMES-III accelerator gallery
https://wp.sandia.gov/radiation-sciences/hermes-iii-accelerator-gallery/



Saturn accelerator
X-ray and e-beam source

Pulsed Power image gallery
https://www.sandia.gov/pulsed-power/image-gallery/



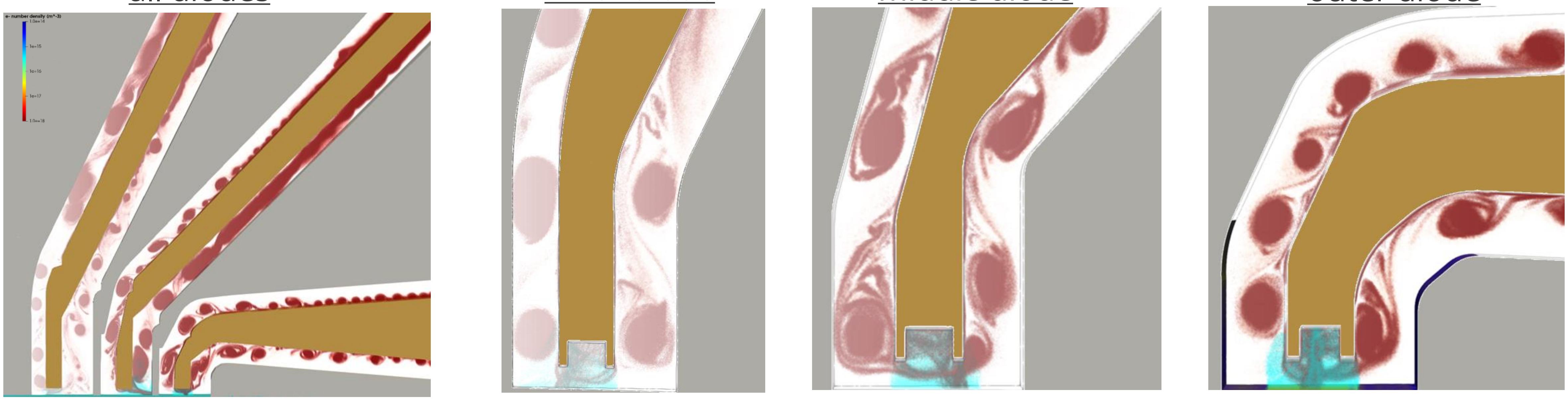
Z machine

Pulsed Power image gallery
https://www.sandia.gov/pulsed-power/image-gallery/

Empire-ITS leveraged to predict radiation field for refurbished geometry design

e^- and H^+ densities near peak power

all diodes | inner diode | middle diode | outer diode



Original geometry | Refurbished geometry

- ✓ Simulated dose from the refurbished hardware proposal (Figure, right) lie within acceptable limits of the original hardware (Figure, left), confirming "do no harm" design principles are upheld
- ✓ Results from different diode gap spacings suggest a weaker dependence on the output radiation dose