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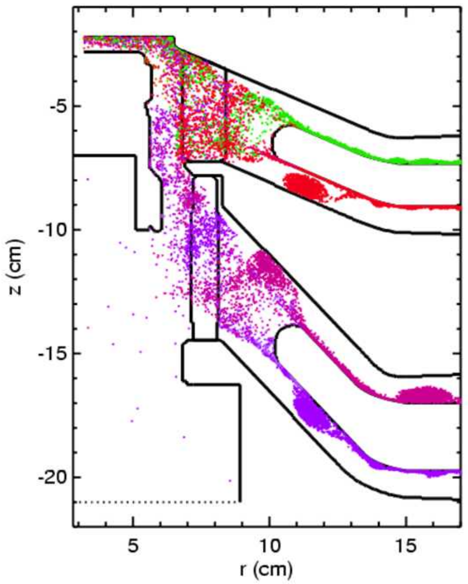

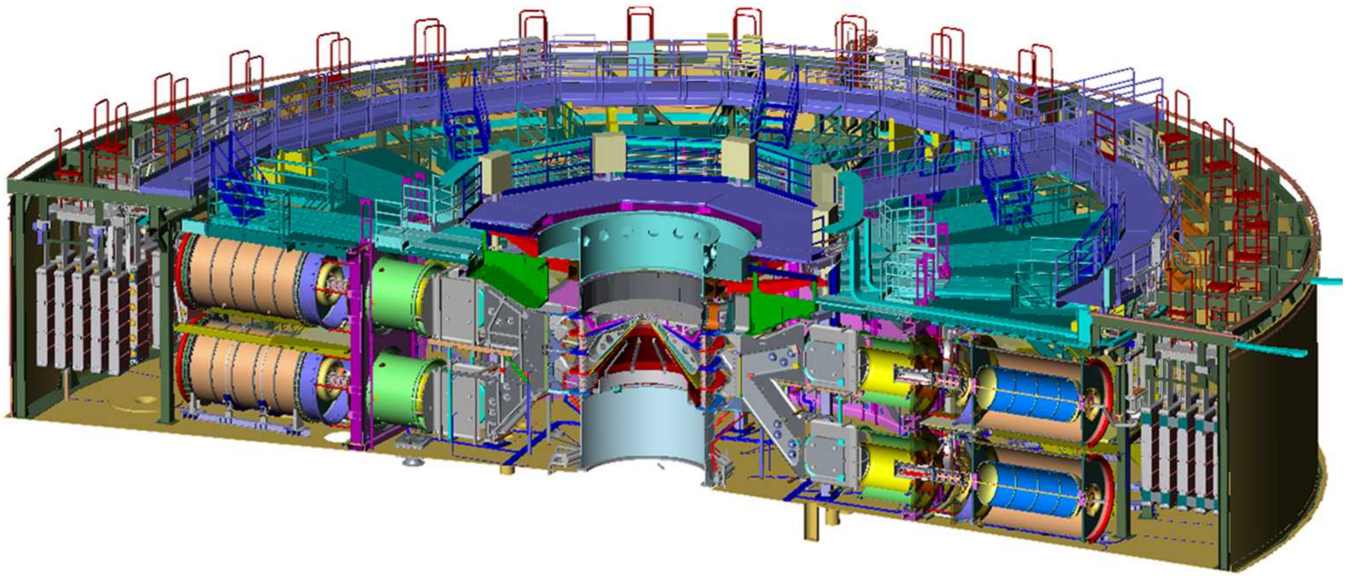

Physics Overview for Modeling Pulsed Power Using Sandia’s codes Quicksilver and EMPHASIS

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U.S. DEPARTMENT OF ENERGY

NNSA National Nuclear Security Administration

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  - Tim Pointon, Keith Cartwright, Becky Coats, Matthew Bettencourt, Chris Moore, Edward Phillips, Richard Kramer, and Ed Love
- Thanks to George Laity for up-to-date Z images

Overview

- What physics is required to model pulsed power flow from Marx bank to load?
  - Relativistic, electromagnetic, kinetic plasma, radiation and neutral transport
  - Volumetric plasma chemistry (collisions between: electrons, ions, neutrals, photons)
    - ionization, excitation, momentum transfer (charge-charge, charge-neutral)
  - Surface physics (neutral, ion and electron emission from surfaces)
    - field emission, thermal emission, desorption, secondary particle emission
- Requirements for credible and practical simulations
  - Particle emission models (space-charge-limited, plasma and/or neutral injection)
  - External circuits for power sources and complicated loads
  - Dynamic particle load-balancing (for efficient parallelization)
  - Implicit algorithms with $\omega_p \Delta t > 1$, $\omega_c \Delta t > 1$, $\Delta x > \lambda_d$
  - Hybrid fluid/kinetic plasma model
  - High fidelity geometric representation (e.g. body fitted boundaries)

Modeling capabilities (past)

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- QUICKSILVER:
  - Structured-mesh particle-in-cell code
    - Parallel with dynamic load balancing
  - Explicit finite-difference EM-PIC (3-D, 2-D)
  - Coupling to transmission line and load models (boundary conditions)
  - Space-charge limited, thermal and secondary particle emission
  - Monte Carlo Collisions (charge-neutral with prescribed neutral background)
  - Coulomb collisions
  - Coupling to ITS for radiation transport
- 30 year history of Pulsed Power applications:
  - Z machine power flow
  - HERMES (and coupling to ITS for rad-transport)
  - Ursa Minor (next-gen radiographic driver)
  - Ion Diodes in the past (PBFA II, SABRE)

Modeling capabilities (present)

- EMPHASIS™ (ElectroMagnetics PHysics AnalySIS):
  - Unstructured finite-element mesh particle-in-cell code
    - Parallel with dynamic load balancing
  - Implicit finite-element EM-PIC (3-D)
  - Coupling to Xyce for external circuit (transmission line and load models)
  - Space-charge limited, thermal, field, and secondary particle emission
  - Monte Carlo Collisions (charge-neutral with prescribed neutral background)
  - Coupling to ITS for radiation transport
  - Drift-diffusion model
    - PIC model coupled to rate equations and conductivity, $\sigma(E)$, and mobility, $\mu(E)$
- Recent applications
  - Optimization of design of dynamic material load geometries on Z
  - Tapered MITL redesigns (e.g. HERMES)

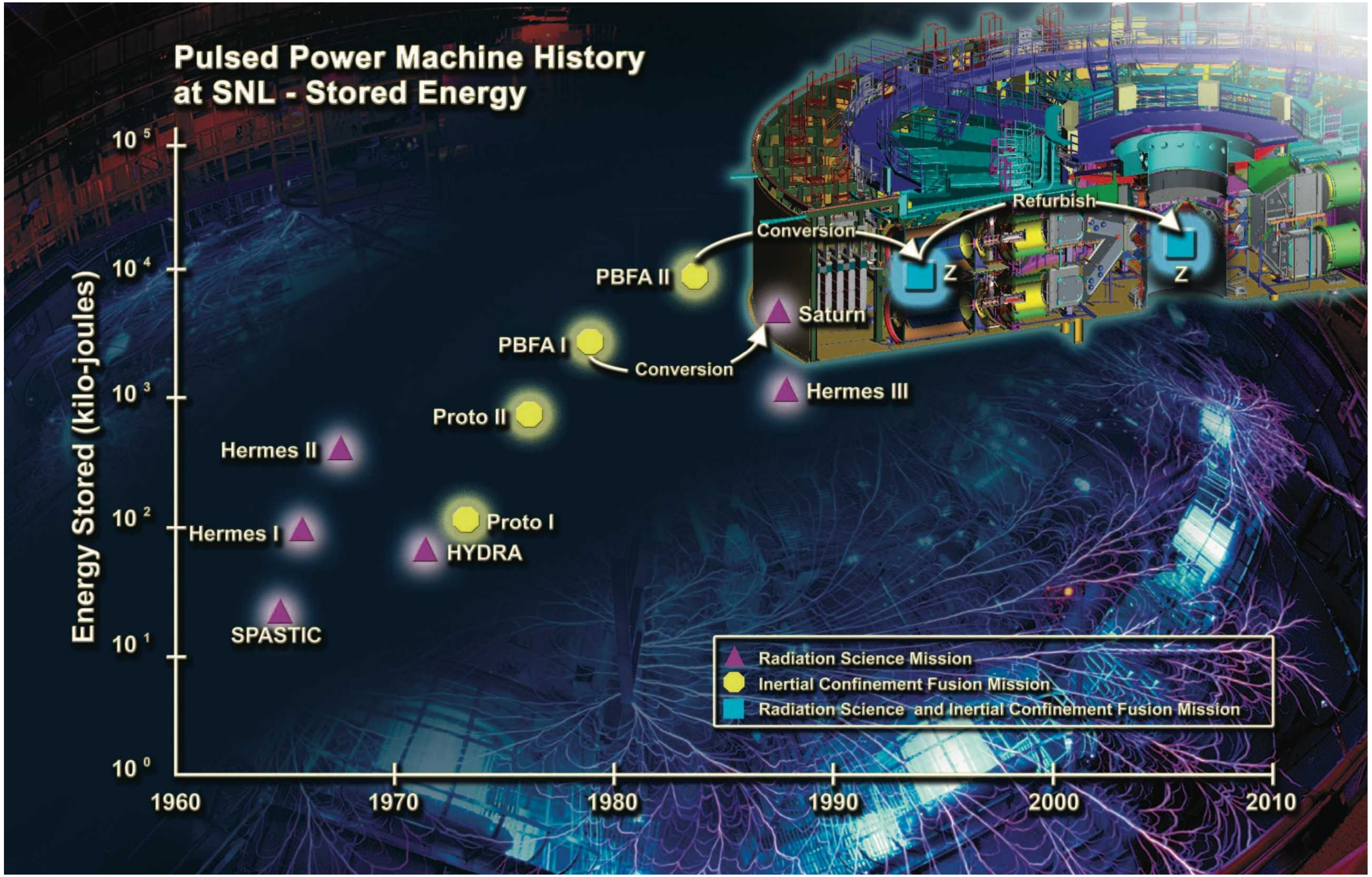
Current Modeling Deficiencies of EMPHASIS

- Radiation transport is decoupled from the plasma
  - Time independent radiation transport simulation modulated in time
- Full multi-fluid PIC hybrid
- Evolution of neutral and excited species
- Implicit algorithms with $\omega_p \Delta t > 1$, $\omega_c \Delta t > 1$, $\Delta x > \lambda_d$

Modeling capabilities (future)

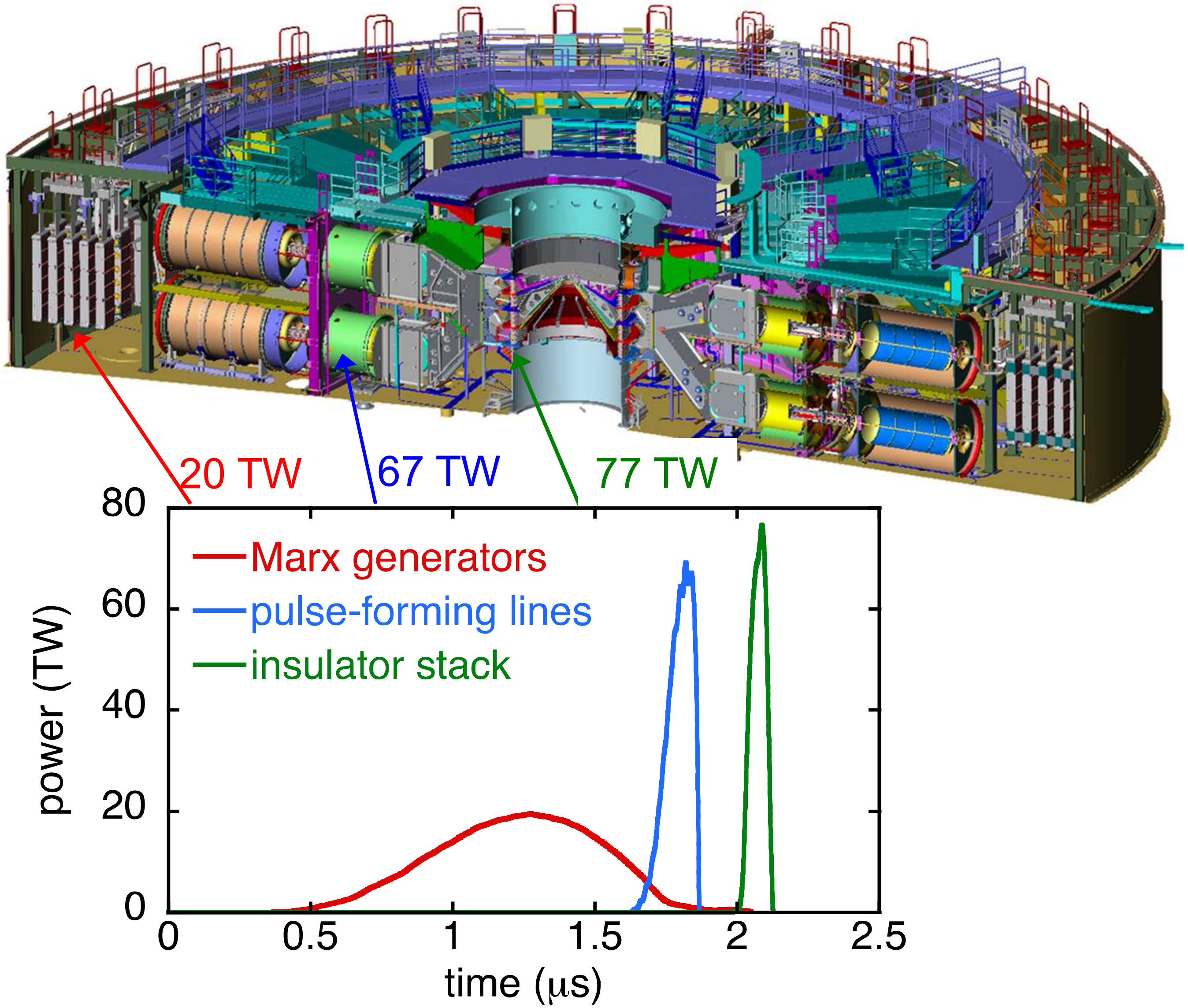
- EMPIRE: ElectroMagnetic Plasma with Integrated Radiation Effects
  - Implicit finite-element EM-PIC (3-D)
  - Hybrid structured/unstructured in-situ meshing
  - Built to operate on next generation platforms
  - Parallel with dynamic load balancing
  - Coupling to Xyce for external circuit (transmission line and load models)
  - Comprehensive emission models
    - Soon to have space-charge limited, thermal beam particle emission
  - Direct Simulation Monte Carlo (DSMC)
    - self-consistent evolution charged, neutral, and excited species
  - Monte Carlo Collisions (MCC)
    - charge-neutral with prescribed neutral background
  - Coupling to ITS for radiation transport
    - Will be replaced with a self consistent time accurate integrated radiation transport
  - Hybrid with full multi-fluid model
- Recent applications
  - Two stream instability
  - Laudau damping
  - Linear plasma waves

Pulsed Power at SNL

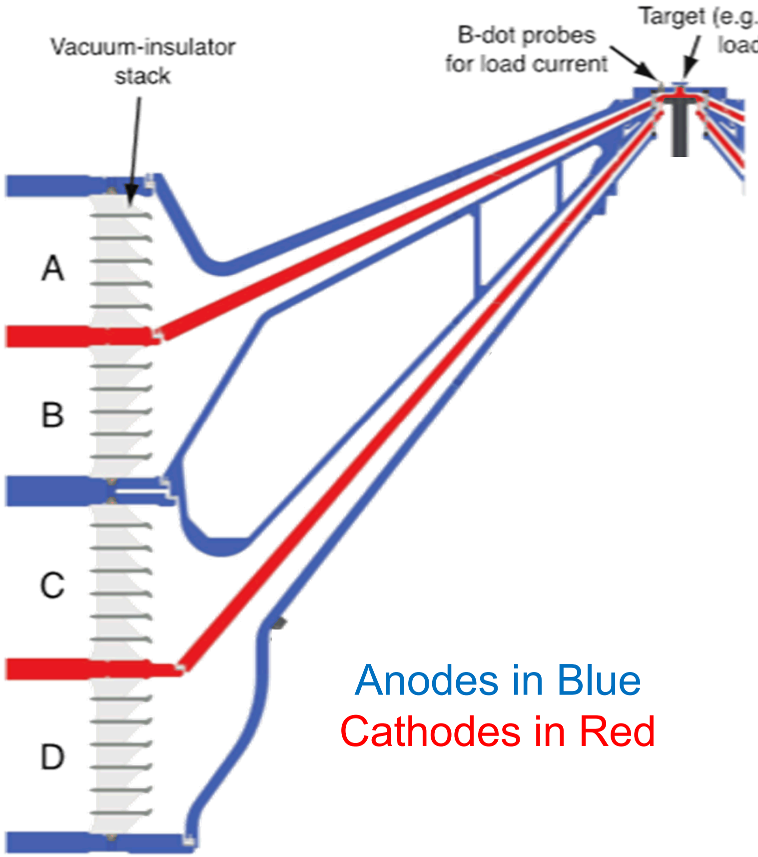


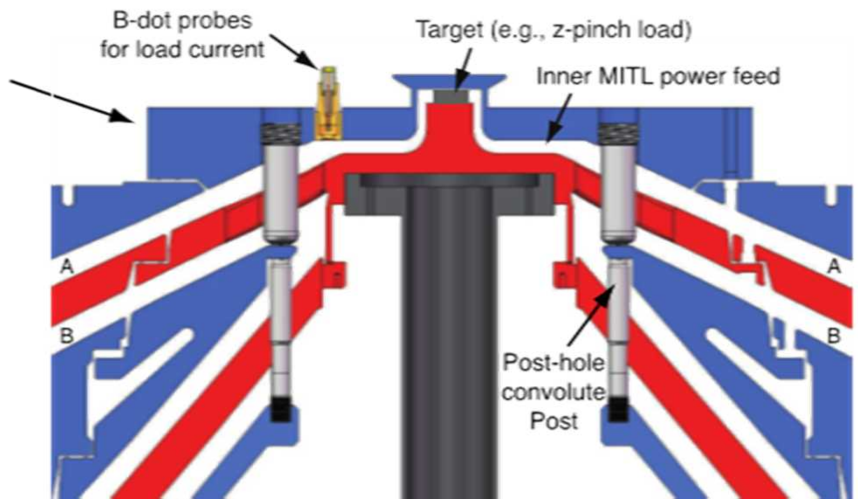
The Z machine Pulsed Power technology

- Marx Generators
- Intermediate storage capacitors
- Laser-triggered gas switches
- Pulse-forming lines
- Self-breaking water switches
- Water convolute
- Vacuum-insulator stack
- Vacuum section

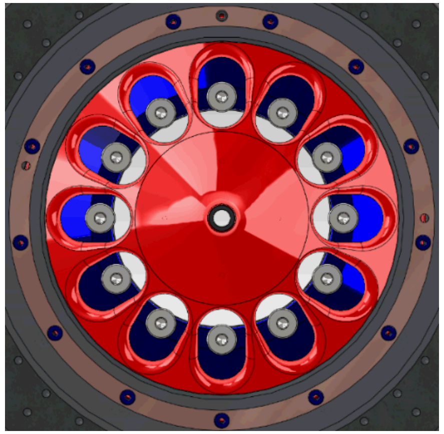


Vacuum Section





Anodes in Blue
Cathodes in Red

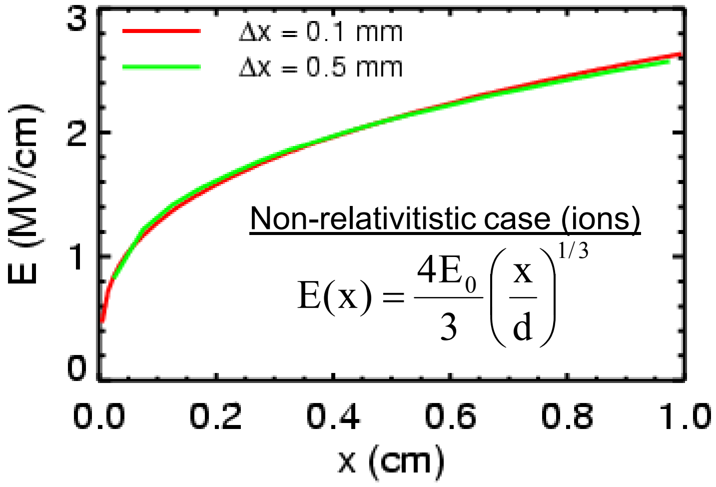


- 4 magnetically insulated transmission lines
- Coupled in parallel with a double post-hole convolute to the inner MITL

Space-charge-limited electron emission

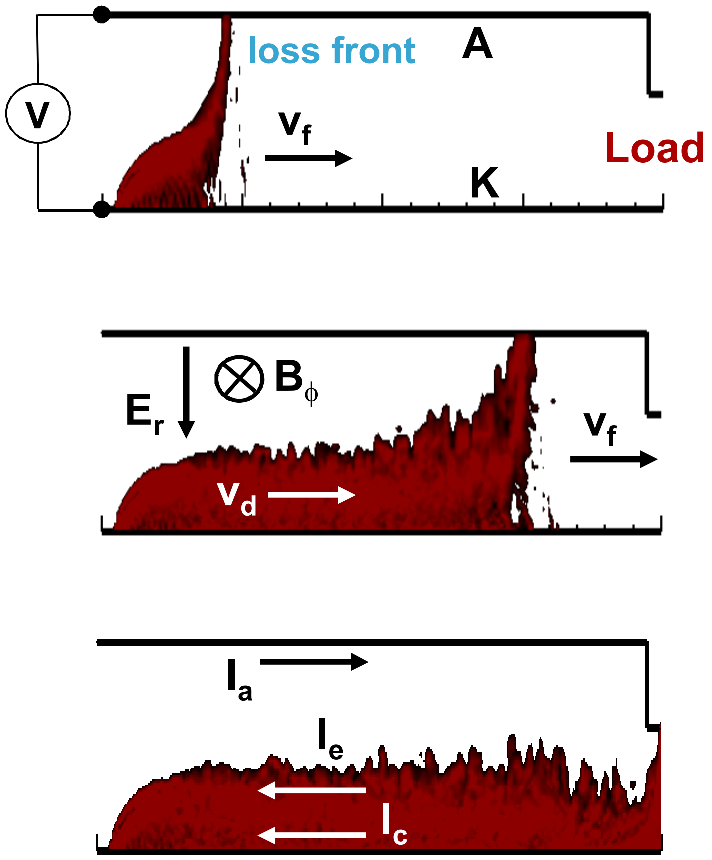
- Electron emission from the cathode when E > ~250 kV/cm
- Electron current reduces E_{normal} at surface, and increases until J_e forces $E_n \rightarrow 0$ -- "space-charge-limited" emission
- Analytic solution for 1-D planar diode:
  - Gap *d*, voltage *V*, particle charge *q*, mass *m*
  - Child-Langmuir current: $J_{CL} = \frac{4\varepsilon_0}{9}\left(\frac{2q}{m}\right)^{1/2}\frac{V^{3/2}}{d^2}$ (non-relativistic)

- Modeling challenge: very steep E-field profile at emission surface
  - Ion diode: d = 1 cm, V = 2 MV; $E_0 = V/d$

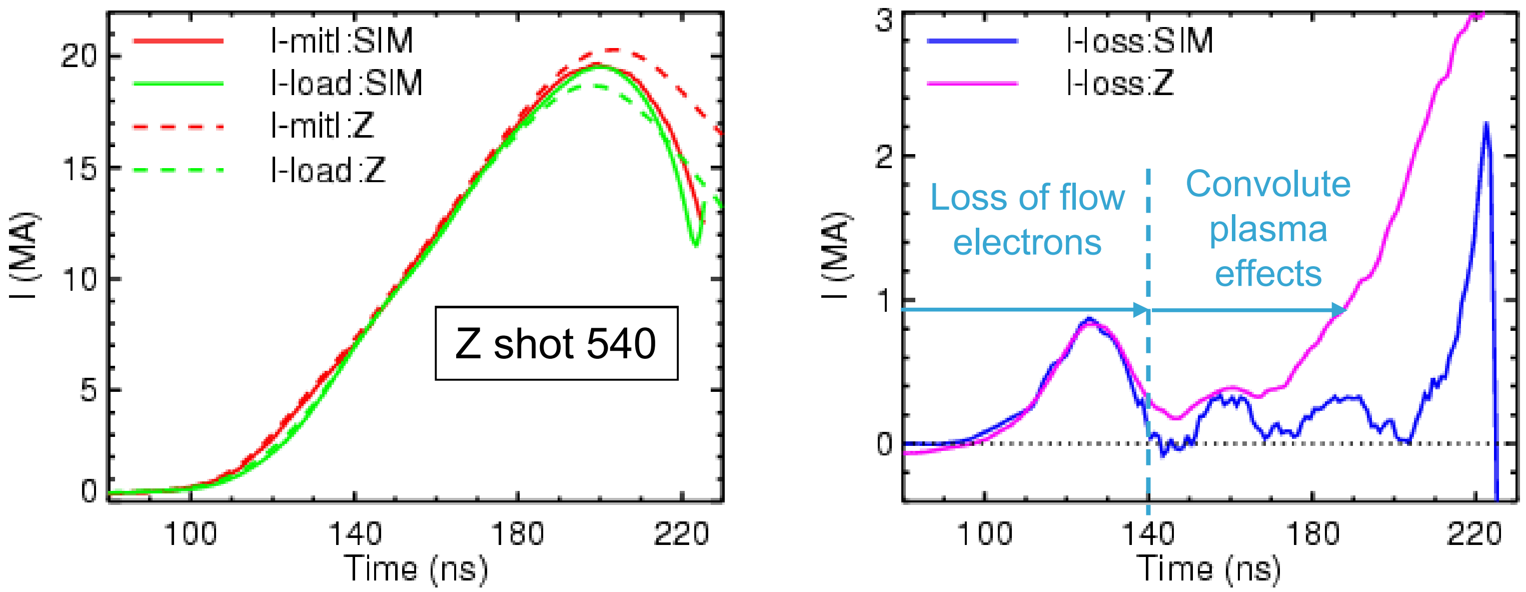


MITLs enable efficient power delivery

- Illustrated with coaxial MITL (courtesy of Steve Rosenthal)
- When emission first starts, electrons go straight across the A-K gap – current loss
- Behind the "loss front", B-field from the current flow can stop electrons from reaching anode – "magnetic insulation"
- Useable current delivered to the load is the cathode current $I_c = I_a - I_e$, where I_e is the current flowing in the electron sheath (typically dumped as a loss elsewhere)
- MITL design is a tradeoff between:
  - Large gap: better insulation, lower flow
  - Small gap: lower inductance

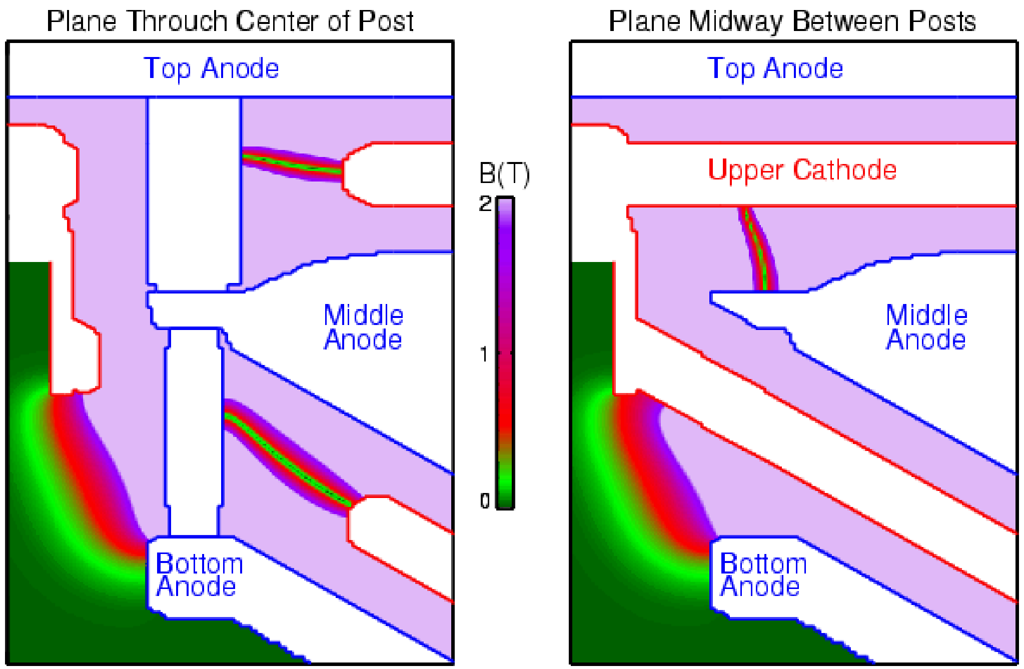


Quicksilver can accurately predict early-time losses

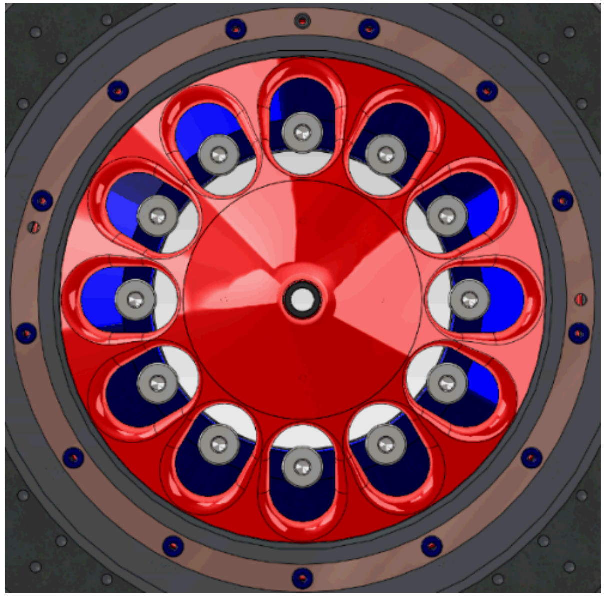


- Simulations with SCL emission on all cathode surface
- Early-time loss: MITL flow electrons lost to the anode ("loss front")
- Extra late-time loss is due to expanding electrode plasmas in the convolute
  - Experimental results in M.R. Gomez, *et al.*, Phys Rev ST-AB **20**, 010401 (2017)
  - Simulations with LSP [D.V. Rose, *et al.*, Phys Rev ST-AB **11**, 060401 (2008)].

Magnetic nulls in the convolute

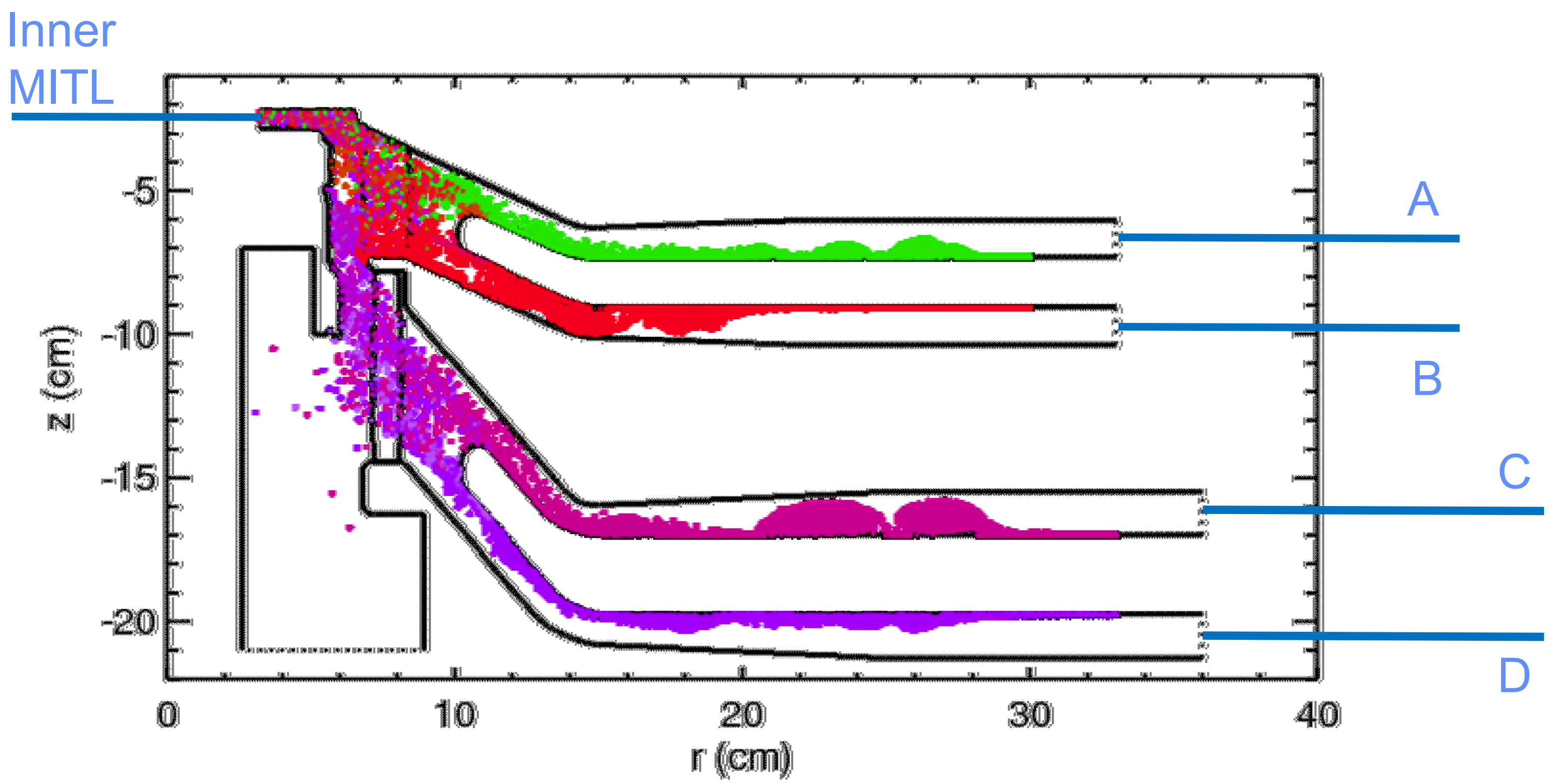


Convolute top view



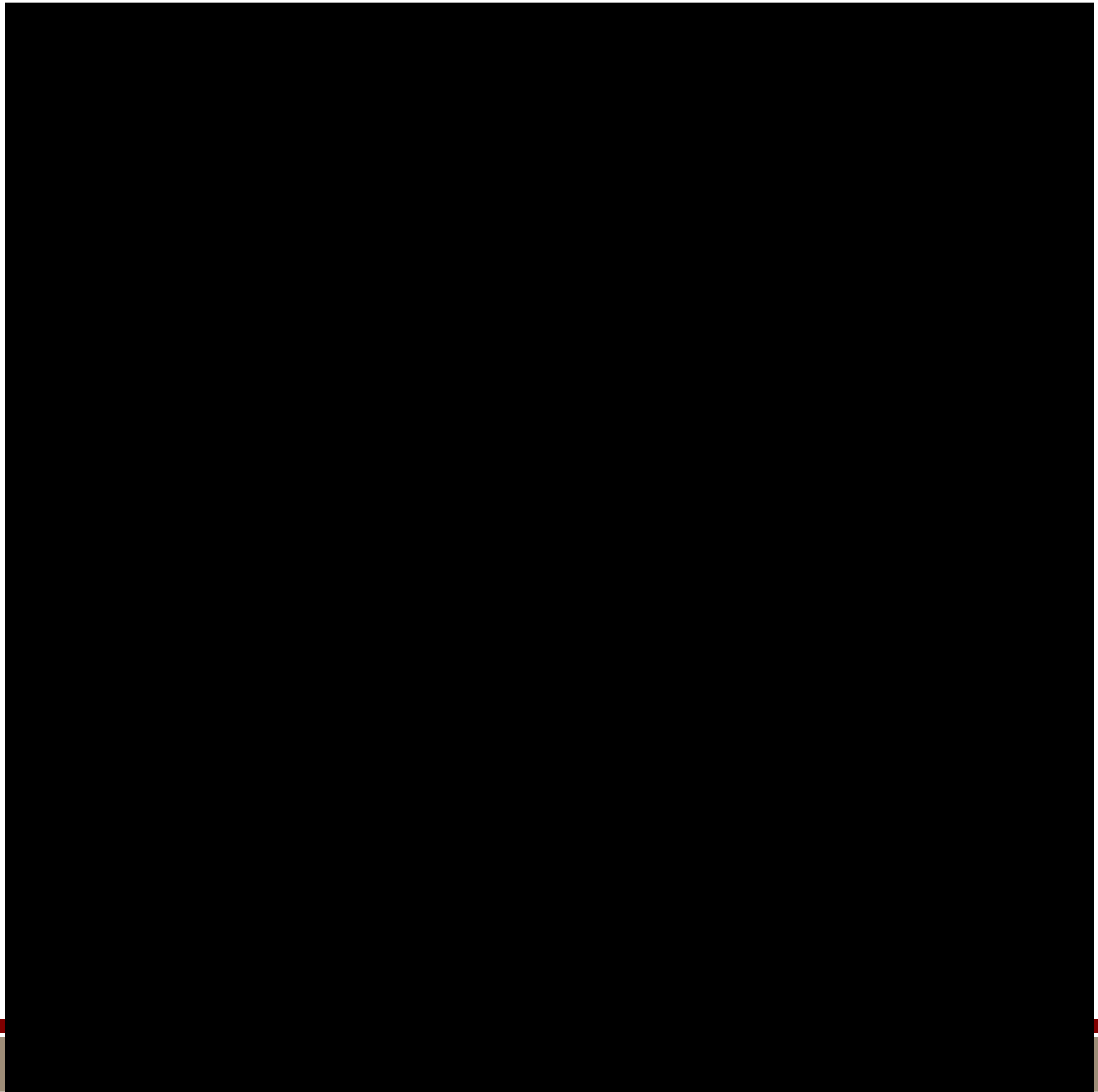
- Electrons flow into the convolute from the feed MITLs
  - Complicated by non-uniform impedance of feed MITLs, $Z \sim d/r$
- There will be electron losses at the nulls: “loss of magnetic insulation”
  - How much? How fast does the anode surface heat?

Time-accurate Quicksilver simulations of Z MITL/Convolute

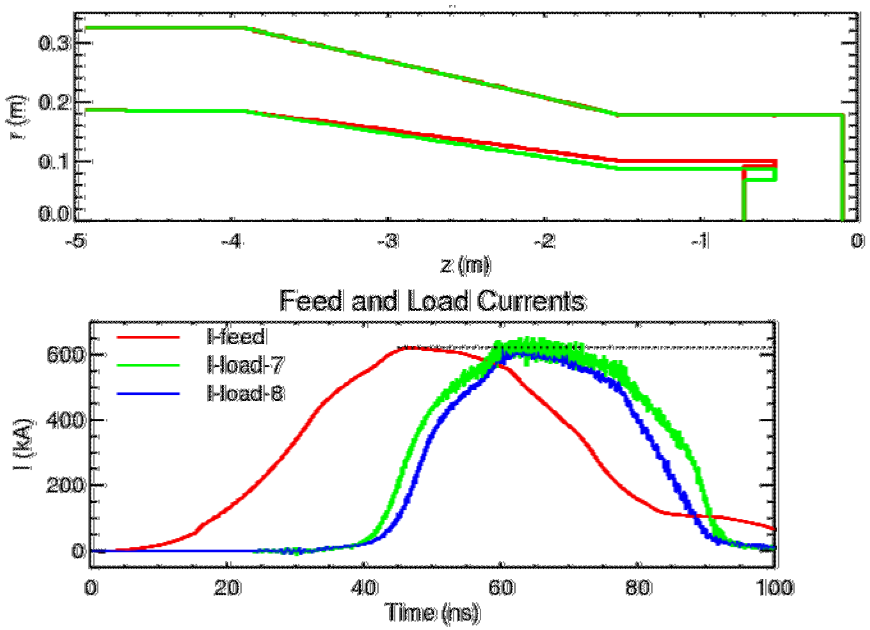


- Only possible with extensive use of 1-D transmission lines
- Reduces the 3-D system size – only emit electrons out to r ~ 30 cm
- Time-accurate source for all four feed MITLs (out to r ~ 3 m)
- Inner MITL connected to a 1-D TL terminated with a realistic load

Quicksilver MITL Movie



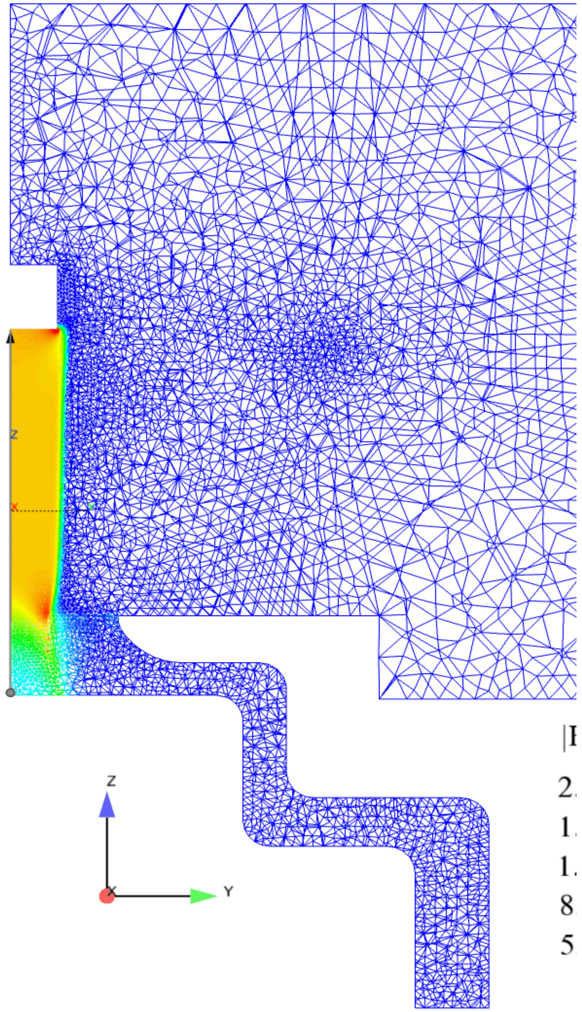
EMPHASIS could help HERMES MITL redesign

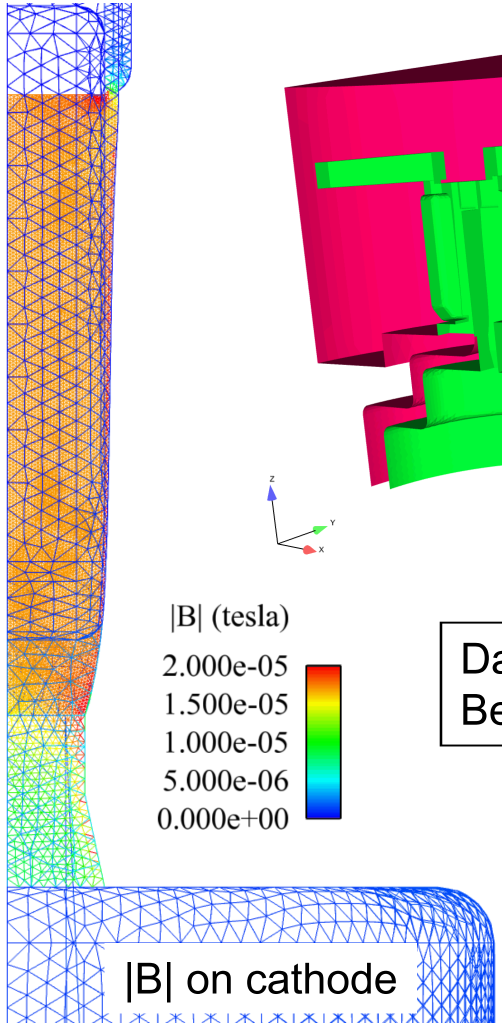


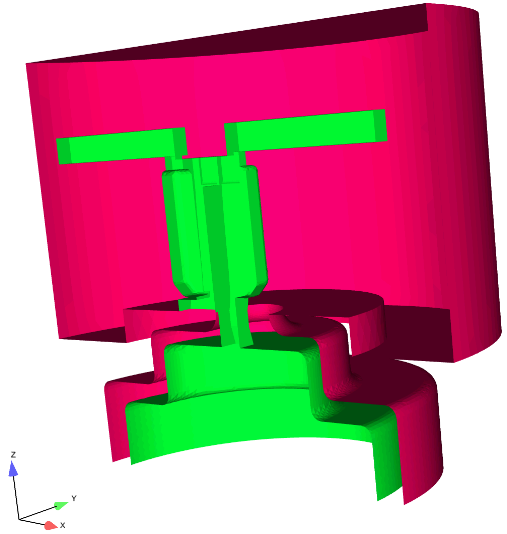
- Extended MITL with constant impedance taper using Quicksilver:
  - Anode: 25.5” → 14”; cathode: 14.5” → 8” diameter
- Reducing downstream cathode diameter to 7” is even better
  - Better mechanical design: larger A-K gap reduces alignment thresholds
  - Actually reduces current loss to zero

… BUT Quicksilver has a numerical instability caused by the stair-stepped cathode

EMPHASIS Simulation of ICE stripline geometry



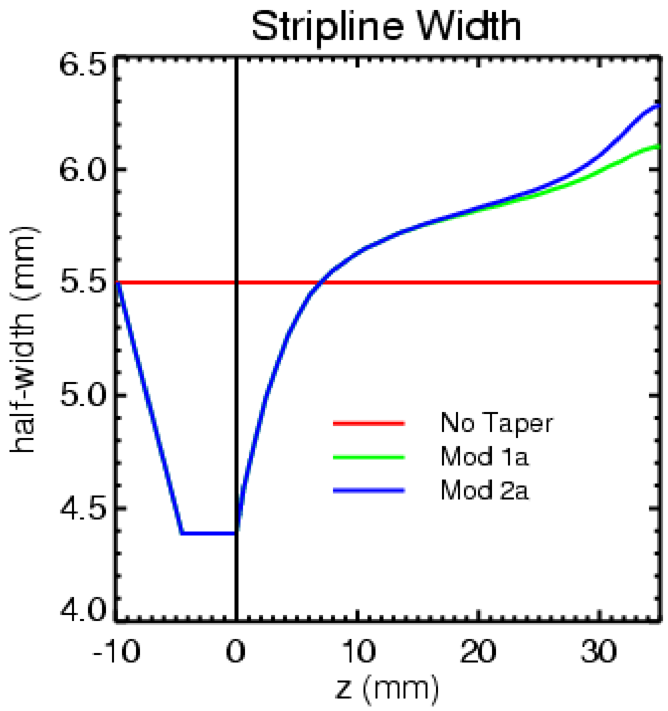


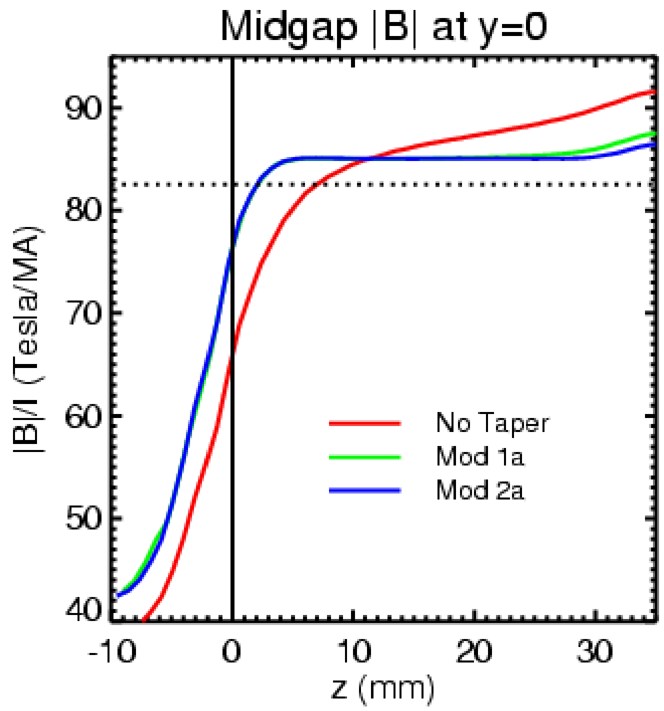


Dave Seidel,
Becky Coats

Goal: Improve B-field uniformity on the cathode (< 1% variation)

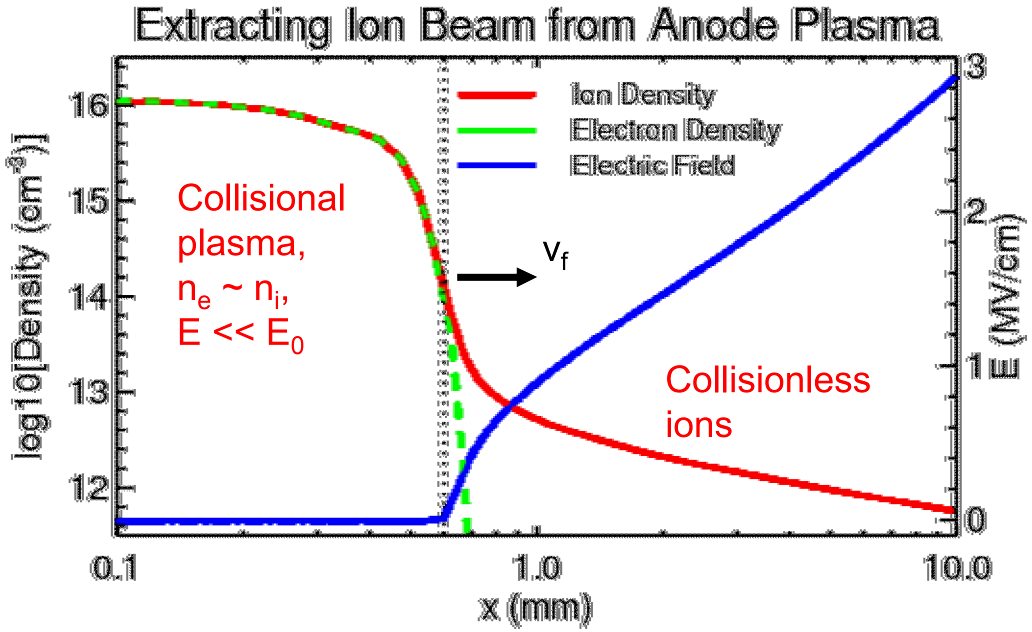
Optimize axial uniformity of |B| in stripline





- Cut “notch” in width of the stripline below the sample area
- Vary width as a function of z above the notch
- Uniformity of B(z) profile over the samples is greatly improved

Electrode plasmas



1D multi-fluid simulation of an ion diode

V = 2 MV
d_0 = 1 cm
E_0 = 2 MV/cm

- Typical plasma parameters: n = 10^{16} – 10^{18} cm^{-3}; T = 1 – 10 eV
  - Debye length λ_{De} ~ 100 nm; Plasma frequency ω_{pe} ~ 10^{13} s^{-1}
- Expansion velocity of plasma front, v_f ~ 1 – 20 cm/μs
- Dynamic effective anode-cathode gap: $d_{eff}(t) = d_0 - v_f t$
  - A decreasing A-K gap is almost always bad

Modeling electrode plasmas is very difficult

- Clearly, must operate at $\Delta x/\lambda_{De} >> 1$
  - Possible with energy-conserving PIC: stable, but no guarantee of accuracy
- Large E-fields introduce a new, <u>severe</u> constraint: $eE\Delta x/T_e <\sim 1$
  - A significant fraction of the plasma electrons and ions must be able to cross a cell against the E-field to sustain expansion
  - For d = 1 cm, V = 2 MV, T_e = 1 eV, need $\Delta x \sim 1\ \mu m$
- Cathode plasma expansion is harder to model than anode plasma
  - Less drag from Coulomb collisions as electrons accelerate ($\nu_{ei} \sim 1/v^3$)
- Only path forward seems to be a hybrid fluid-PIC model
  - Fluids for dense plasma with plasma-front tracking scheme
  - Creation of PIC particles at the front

Summary

- Quicksilver has had success modeling many pulsed power systems
  - PBFA II, SABRE, Z, Ursa Minor, HERMES, and many more
- Key enabling capabilities
  - Massively parallel with dynamic load balancing
  - Particle emission models
  - External circuits (1-D transmission lines or Xyce)
- Unstructured mesh capabilities of EMPHASIS and EMPIRE can address key geometry issues not possible with legacy structured EM-PIC
  - Work needed on emission models and external circuits (Xyce)
- Development of advanced plasma emission models are necessary to simulate late-time current loss on Z (and impedance collapse in other devices)
  - A very difficult problem

Backup slides

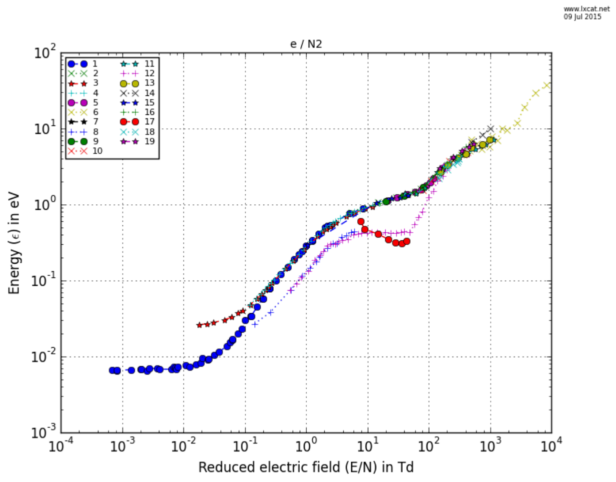
Surface Plasma Generation Models

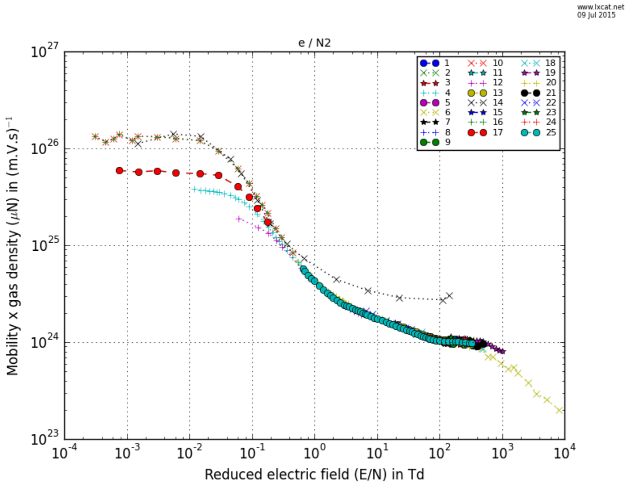
Emission Model	Incident Particle	Secondary Particle	Thermal Dependence
Desorption (Hertz-Knudsen-Langmuir)(Sanford et.al.)	None	Neutral	Yes
Thermo-Field Emission (Murphy & Good)	None	Electron	Yes
Space Charge Limited Emission (limit of thermo-field emission for high voltage) (Shiffler)	None	Electron	No
Secondary Emission (Lin and Joy)	Electron	Electron	No
Secondary Emission (Raizer 1991)	Ion	Electron	No
Associative Desorption (Lieberman and Lichtenberg)	Ion/Neutral	Ion/Neutral	Yes
Sputtering (Langley)	Ion	Ion/Neutral	Weak
Stimulated ion emission	Electron	Ion	Weak

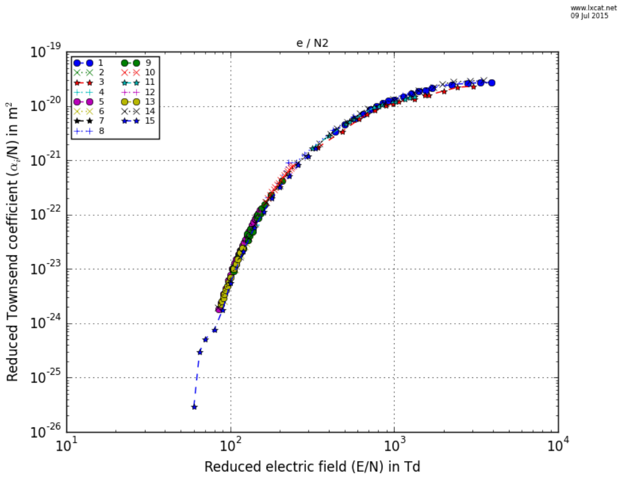
It is necessary to couple the desorption and thermo-field emission to a thermal solve on the electrodes to accurately model surface plasma generation

Modeling

- EMPHASIS EM/PIC
  - EM field solve
- Conductivity Model
  - Mobility/conductivity as a function of electric field and density
  - One can write the time update as one big matrix,
    - Use Ohms law for the current



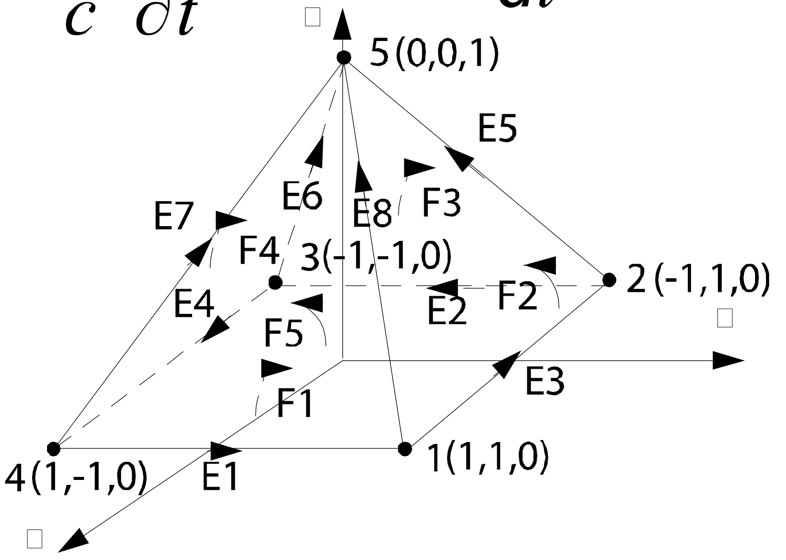




Hagelaar and Pitchford 2005

Second Order EM Formulation

$$\nabla\times\left(\frac{1}{\mu_r}\nabla\times\bar{E}\right)+\frac{\varepsilon_r}{c^2}\frac{\partial^2}{\partial t^2}\bar{E}+\mu_0\sigma\frac{d}{dt}\bar{E}+\mu_0\bar{E}\frac{d\sigma}{dt} = -\mu_0\frac{\partial}{\partial t}\bar{J}$$



$$[T]\frac{d^2 E}{dt^2}+[B]\frac{\partial E}{\partial t}+[S]E+F] = 0$$

Newmark time integration

$$[T]\frac{E^{n+1}-2E^{n}+E^{n-1}}{\Delta t^{2}}+[B]\frac{E^{n+1}-E^{n-1}}{2\Delta t}+[S]\left(\alpha_1 E^{n+1}+\alpha_2 E^{n}+\alpha_3 E^{n-1}\right)+F]=0$$

Second order accuracy $\alpha_1+\alpha_2+\alpha_3=1$

Unconditional stable $\alpha_2^2=4\alpha_1\alpha_3$

Energy conserving (symplectic) $\alpha_1=\alpha_3$

Leads to $\alpha_1={}^{1}/_{4}, \alpha_2={}^{1}/_{2}$, and $\alpha_3={}^{1}/_{4}$

Godfrey update

$$E^{n+1} - 2E^{n} + E^{n-1} +$$

$$4\Delta t \frac{([B] + (2\alpha_1 + \alpha_2)\Delta t[S])E^{n} + (-[B] + (1 - (2\alpha_1 + \alpha_2))\Delta t[S])E^{n-1} + \Delta t F])}{4[T] + 2\Delta t[B] + 4\alpha_1 \Delta t^2 [S]} = 0.$$

[B] and [S] are updated as the conductivity changes

Fill time is on the order of the solve time

Rate Equations

$$\frac{\partial \boldsymbol{n}}{\partial t} + \boldsymbol{\nabla}\left(n\boldsymbol{u}\right) = G - L$$

Secondary Electron Rates

$$\frac{\partial N_e}{\partial t} = S_e + \left(\nu_i(E) - \nu_a\right) N_e - \alpha_{ei}(E) N_e N_+ \tag{5.1}$$

N_e is the electron density

N_+ is the positive ion density

N_- is the negative ion density

S_e is the photoelectrons created by the primary electrons

ν_i is the rate of production of the secondary electrons by collisions between secondary electrons

ν_a is the attachment rate of the electrons to neutral air atoms

α_{ei} is the recombination between electrons and positive ions

Ion Rate equations

Positive Ion Rate

$$\frac{\partial N_+}{\partial t} = S_e + \nu_i(E)N_e - \alpha_{ei}(E)N_eN_+ - \alpha_{ii}N_+N_-$$

α_{ei} is the recombination between negitive and positive ions

Negative Ion Rate

$$\frac{\partial N_-}{\partial t} = \nu_a N_e - \alpha_{ii}N_+N_-$$

Conductivity

$$\sigma = \mu_e N_e + \mu_+ N_+ + \mu_- N_-$$

$$\nabla\times\left(\frac{1}{\mu_r}\nabla\times\bar{E}\right) + \frac{\varepsilon_r}{c^2}\frac{\partial^2}{\partial t^2}\bar{E} + \mu_0\sigma\frac{d}{dt}\bar{E} + \mu_0\bar{E}\frac{d\sigma}{dt} = -\mu_0\frac{\partial}{\partial t}\bar{J}$$

Fluid to Drift-Diffusion

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$$mn\left(\frac{\partial \boldsymbol{u}}{\partial t} + (\boldsymbol{u}\cdot\boldsymbol{\nabla})\,\boldsymbol{u}\right) = qn\left(\boldsymbol{E} + \boldsymbol{u}\times\boldsymbol{B}\right) - \boldsymbol{\nabla}\cdot\boldsymbol{\Pi} + f|_c$$

$$\frac{\partial}{\partial t} \equiv 0,\ \boldsymbol{B} = 0,\ (\boldsymbol{u}\cdot\boldsymbol{\nabla})\,\boldsymbol{u} \text{ is zero}\quad \boldsymbol{\nabla}\cdot\boldsymbol{\Pi} = \boldsymbol{\nabla}p,\ \text{isothermal relation } p = nkT$$

$$f|_c = -\sum_\beta mn\nu_{m\beta}\left(\boldsymbol{u} - \boldsymbol{u}_\beta\right) - m\boldsymbol{u}\left(G - L\right)$$

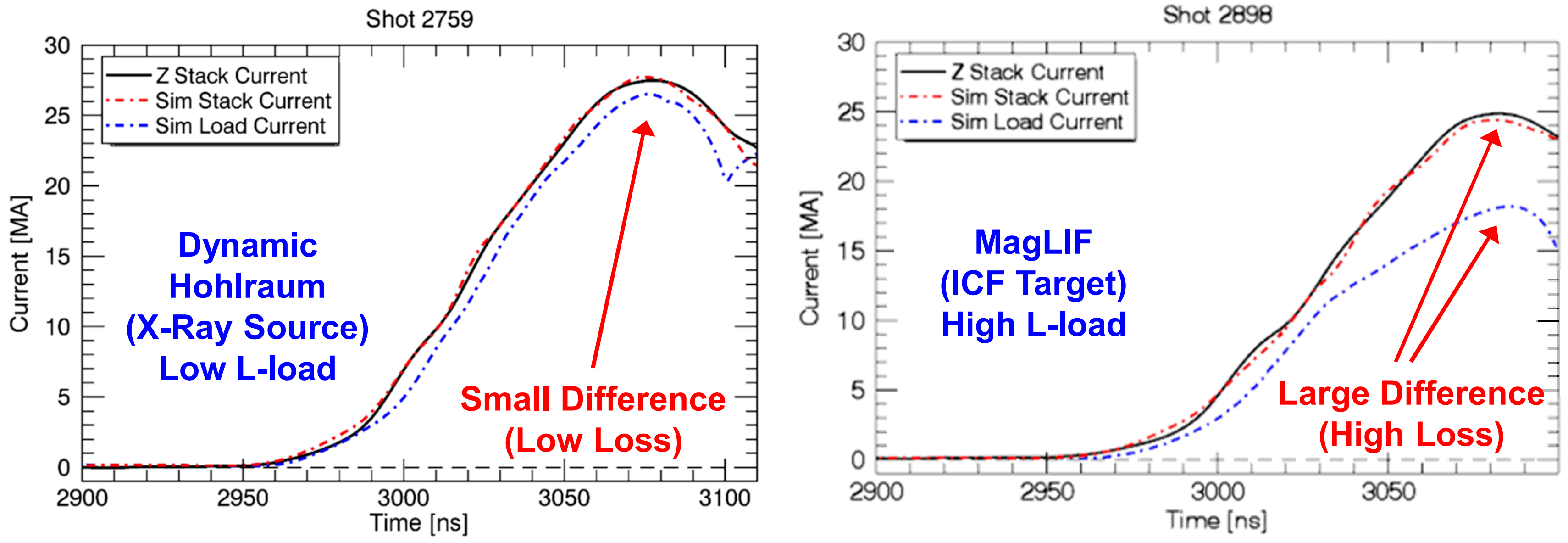
$$f|_c \approx -nm\boldsymbol{u}\nu_m$$

$$0 = qn\boldsymbol{E} - \boldsymbol{\nabla}p - mn\nu_m\boldsymbol{u}$$

$$\boldsymbol{J} = \frac{q^2 n}{m\nu_m}\boldsymbol{E} - \frac{q}{m\nu_m}\boldsymbol{\nabla}p$$

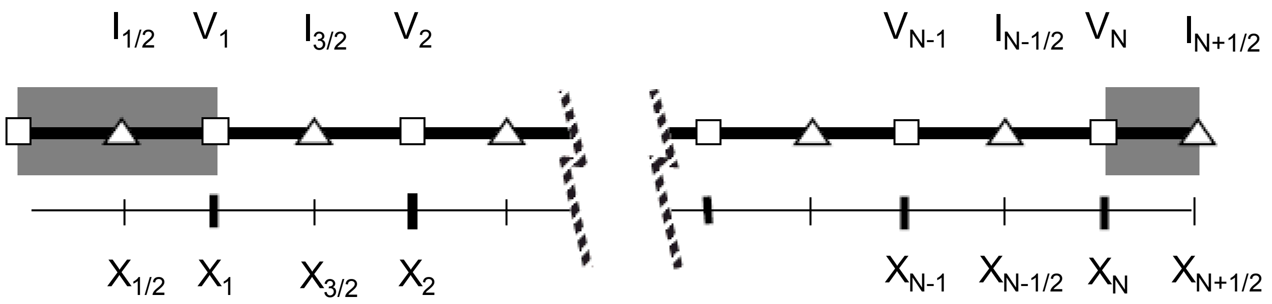
$$\boldsymbol{J} = qn\mu_m\boldsymbol{E} - \mu_m\boldsymbol{\nabla}p$$

Z is modeled with the Bertha circuit code



- POC: Brian Hutsel
- Empirical and physics-based models for all components
  - PIC simulations provide guidance for the vacuum section
- Can simulate entire pulse (~3 μs) in < ~1 minute

Quicksilver 1-D transmission lines

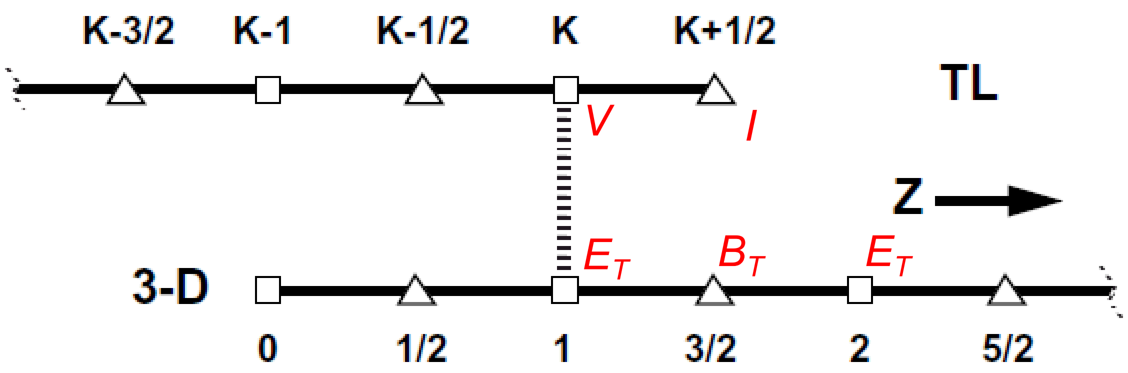


- Telegrapher's equations: $\frac{\partial V}{\partial t} = -\frac{1}{C_l}\frac{\partial I}{\partial x}$; and $\frac{\partial I}{\partial t} = -\frac{1}{L_l}\frac{\partial V}{\partial x}$
- Discretize in space and time: $V_i^n = V(x_i, n\Delta t)$; $I_{i+1/2}^{n-1/2} = I(x_{i+1/2}, (n-1/2)\Delta t)$
- $C_l(x_{i+1/2})$ and $L_l(x_{i+1/2})$ constant in each "full grid" cell: $[x_i, x_{i+1})$
- Leapfrog time advance:

$$V_i^n = V_i^{n-1} - \gamma_i (I_{i+1/2}^{n-1/2} - I_{i-1/2}^{n-1/2}); \text{ where } \gamma_i = \frac{2\Delta t}{\Delta x_{i-1/2}\left[C_l(x_{i-1/2}) + C_l(x_{i+1/2})\right]}$$

$$I_{i+1/2}^{n+1/2} = I_{i+1/2}^{n-1/2} - \lambda_i (V_{i+1}^n - V_i^n); \text{ where } \lambda_i = \frac{\Delta t}{\Delta x_i L_l(x_{i+1/2})}$$

Connect 1-D TLs to 3-D system at “TLports”



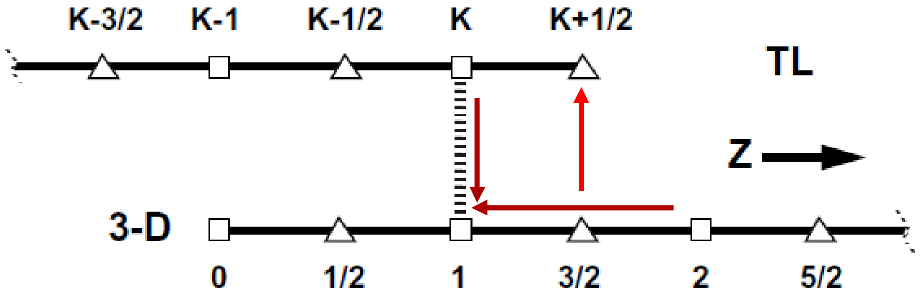
Connection of a TL to a z-normal port (lower z boundary)

- A *TLport* is a rectangular region on a boundary face of a 3-D block, with two conductors separated by a vacuum gap
  - Parallel plates, coaxial lines, more complicated cross-sections
- No interpolation needed in time or normal ordinate (*z* here) to match:
  - Transverse $\boldsymbol{E}_T = (E_x, E_y)$ with *V* at boundary plane
  - Transverse $\boldsymbol{B}_T = (B_x, B_y)$ with *I* half a cell inside

TEM voltage and current in the 3-D system

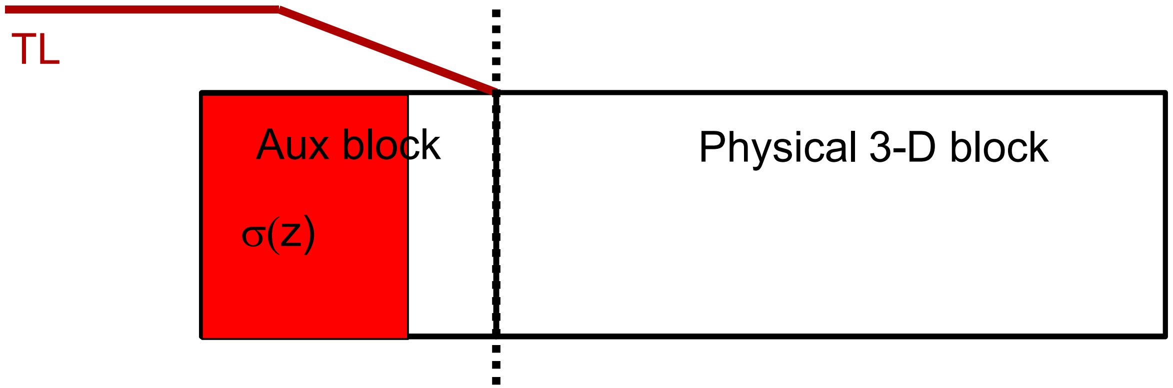
- Solve a 2-D Poisson solution for TEM E-field in the port plane:
  - $\nabla_T^2 \phi = 0$, with BCs $\phi = 0$ on cathode, and $\phi = V_0$ (1 Volt) on anode
  - "Poisson E-field": $E_p = -\nabla \phi$
- QS computes $\boldsymbol{E_p}$ for arbitrary port geometry at t = 0
- $\boldsymbol{E_p}$ is orthogonal to any non-TEM mode profile $\boldsymbol{E_{NT}}$: $\int E_p \bullet E_{NT} dA = 0$
- **Filtering out the non-TEM fields is crucial to stability**
  - TEM voltage: $V = \frac{\varepsilon}{C_l V_0^2} \int E_p \bullet E_T dA, \text{ where } C_l = \frac{\varepsilon}{V_0^2} \int E_p^2 dA$
  - TEM current: $I = \frac{1}{\mu V_0} \int \hat{e}_z \times E_p \bullet B_T dA$

Basic filtered TLport algorithm



- Non-TEM transverse field at k = 1,2 planes: $E_k^{*n} = E_{Tk}^n - (V_{3D,k}^n / V_0) E_P$
- In the port plane, set $E_T^n = (V_K^n / V_0) E_P + E_1^{*n}$
- Compute $E_1^{*n+1} = (1-\delta) E_1^{*n} + \delta E_2^{*n}$; where $\delta = v_{ph} \Delta t / \Delta x$
  - Assumption: all non-TEM waves are travelling upstream with same v_{ph} *(usually c)*
- Use $B_{T,3/2}$ to set boundary value $I_{K+1/2}$ for V_k on next timestep
- Usually works fine for inlet power feeds

“Auxiliary block” TLport algorithm



- Filtered TLport algorithm failure modes:
  - Electrostatic fields from non-TEM structure too close to the port
  - Particles flowing through the boundary
- Solution: add auxiliary field block with conductivity to port boundary
  - For the field solver, this is a “parallel load” with the transmission line
    - TEM fields coupled to the transmission line *V* and *I*
    - non-TEM fields coupled to the aux-block
  - Particles drift ballistically into the aux-block (never come back)
    - Decay particle charge and absorb in conductivity region

Pulsed Power boundary conditions for TLs

- Thevenin equivalent source: $V_{oc}(t)$ and source impedance R_s
- Series RLC circuit for driving system with charged capacitors
  - Variable *R(t)* acting as the switch (start high, then fall)
- T-junctions and multi-line junctions
- Time-dependent inductive loads (dynamic material shots on Z)
- Z-pinch loads:
  - Thin shell $r_w(t)$, height *h*, mass *M*, return current radius *b*
  - Time-dependent inductance: $L(t) = L_h \ln\left(\frac{b}{r_w(t)}\right)$, where $L_h = \frac{\mu_0 h}{2\pi}$
  - Force on the wire array: $M\ddot{r}_w = -\frac{L_h I^2}{2r_w}$
  - Small set of non-linear ODEs to determine boundary *V* and *I*