SAND2021-10284PE

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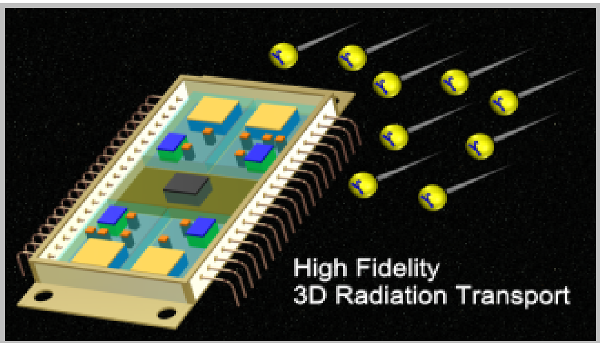
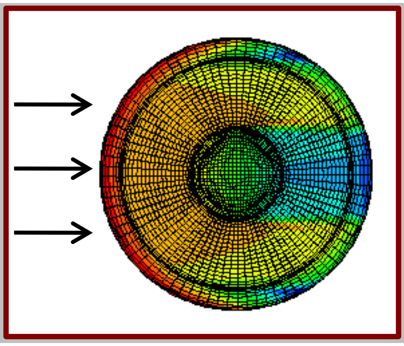


SCEPTRE



Algorithms and Applications of the SCEPTRE Radiation Transport Code

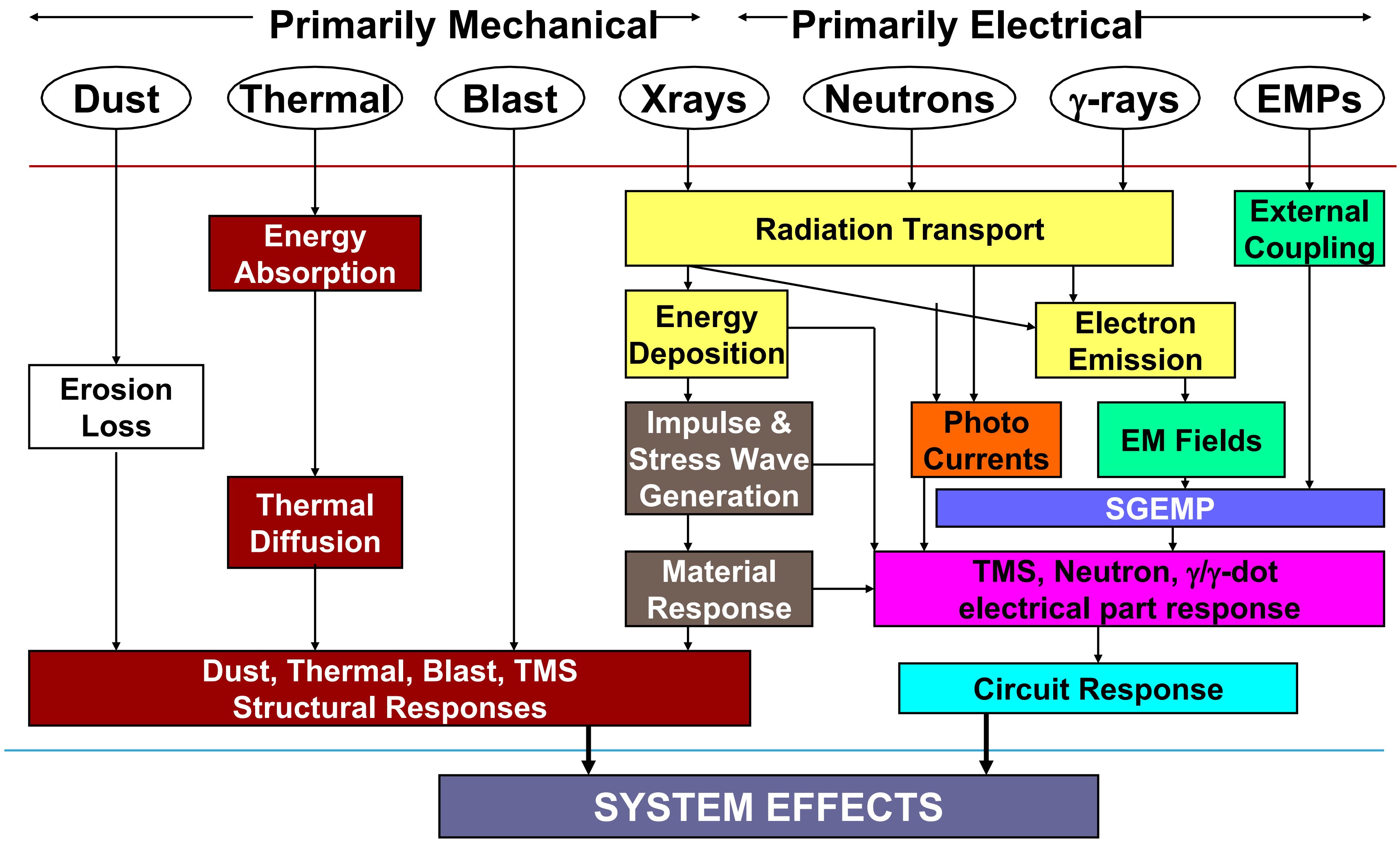
Shawn Pautz

SAND ???

U.S. DEPARTMENT OF ENERGY

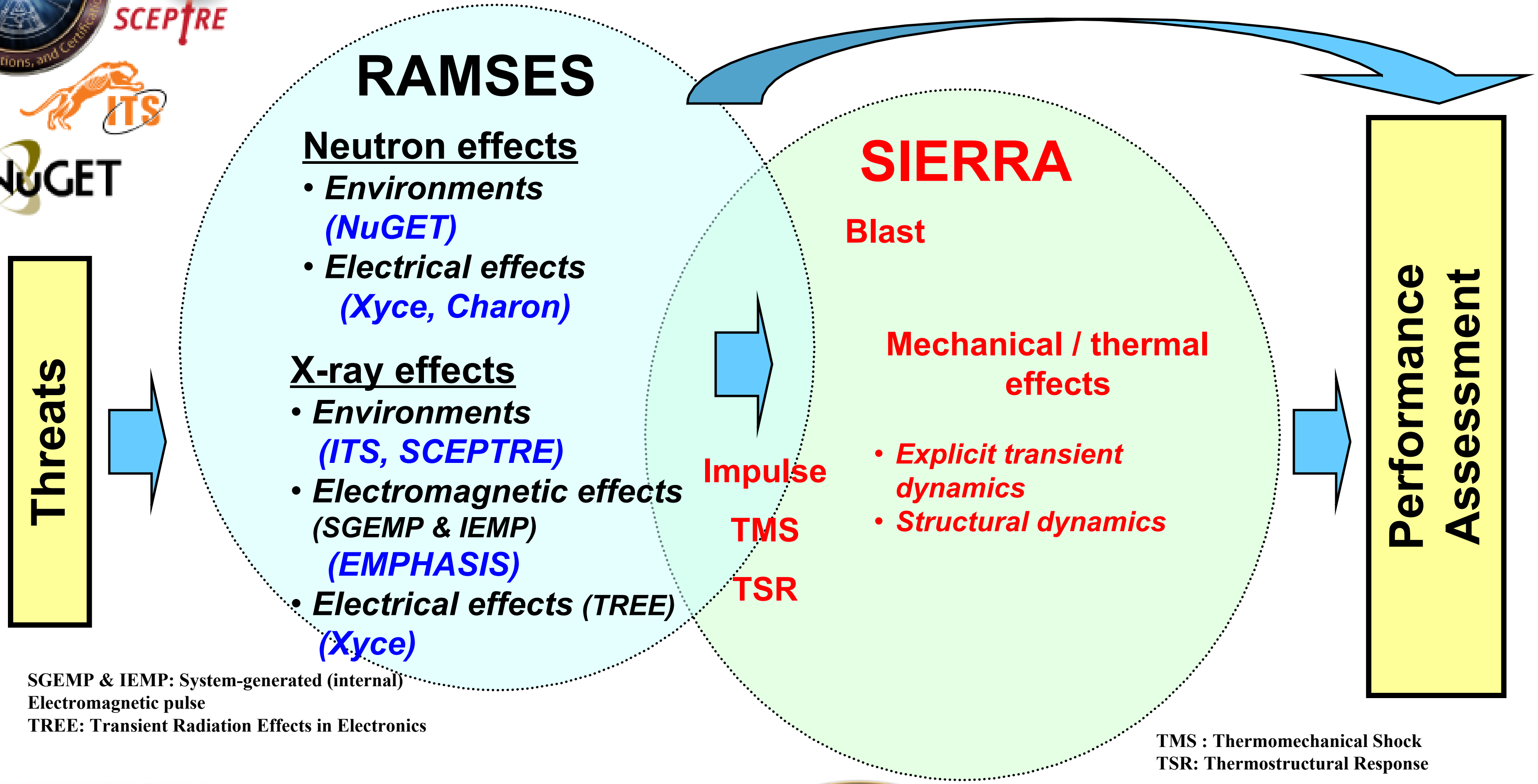
NNSA National Nuclear Security Administration

Physics of Radiation Effects for Nuclear Weapon Effects Assessment



The RAMSES code suite has now been consolidated into 1300 - similar to SIERRA in 1500

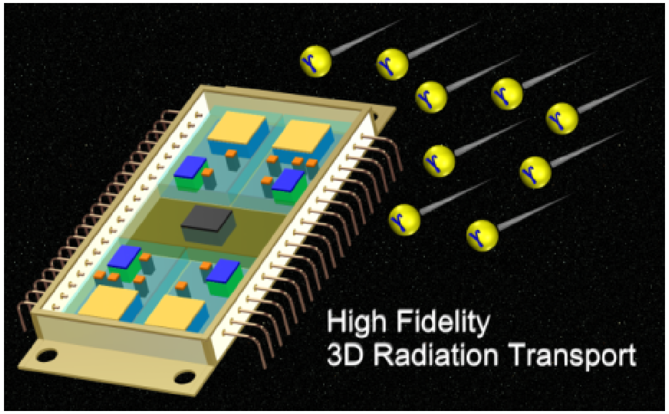
Nuclear Survivability of Non-nuclear Components



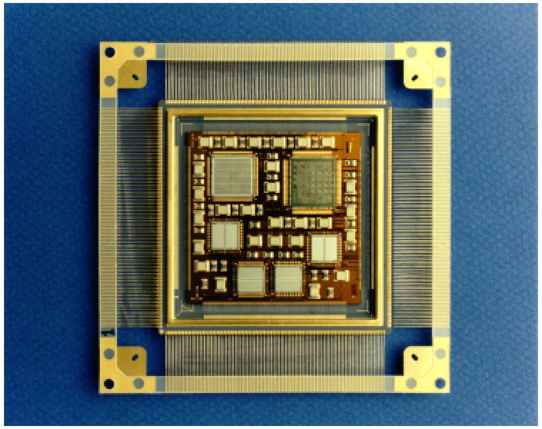
SGEMP & IEMP: System-generated (internal) Electromagnetic pulse
TREE: Transient Radiation Effects in Electronics

TMS : Thermomechanical Shock
TSR: Thermostructural Response

Radiation transport is fundamental to understanding the effects produced in nuclear and space radiation environments

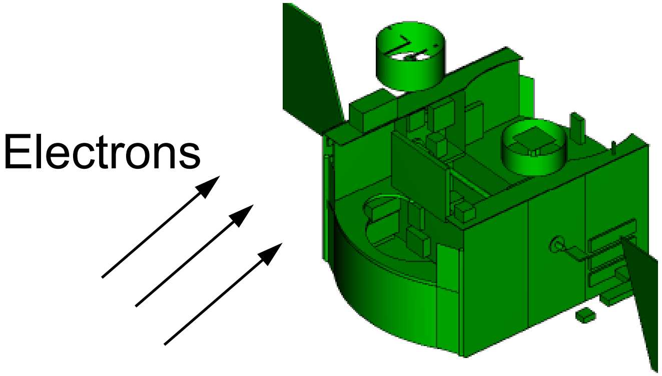


The transport of coupled photon, electron, and positron radiation from 1.0 keV to 20.0 MeV



ICs

Goal: Predict the effect of radiation on electrical components (e.g. ICs, cables)



Satellite

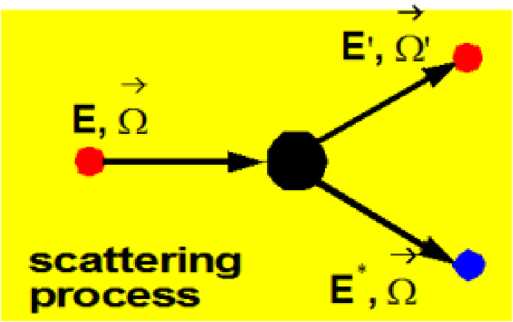
Goal: Predict the effect of radiation on materials and structures (mechanical effects)

Radiation transport fundamentals

Particles (neutrons, photons, electrons,…) described by location r, energy E, and direction of travel (or angle) Ω.

Interactions with matter described by cross sections (or opacities) – the probability per unit path length that a given interaction (including outcome) occurs.

The fundamental goal of radiation transport is to determine the "angular flux density" $\psi(r, E, \Omega)$ - the number of particles per unit volume per unit energy per unit solid angle. Once we know that, we can determine derived quantities like dose.



Two totally different methods are available in computational physics to model radiation transport

Monte Carlo Methods (ITS)

Computer simulation of random walk by statistical sampling

- "Lagrangian" view: what happens to a given particle
- Runtime limited
  - Memory not generally a limitation
- Complex 3D modeling capability
- Efficient for computing integral quantities
  - Total charge crossing a surface
  - Total dose in a region
- Easily adaptable to traditional parallel computers (modern architectures are challenging)

Deterministic Methods (SCEPTRE)

Numerical solution of the mathematical equation describing the transport

- "Eulerian" view: what happens in a phase space element (r, E, Ω)
- Memory and/or runtime limited
- Complex 3D modeling capability
- Essential for computing differential quantities
  - Charge/energy deposition distributions
  - Space, energy, and angle dependent emission quantities
- Parallelizable, but challenging

Applications of SCEPTRE to Radiation Effects

- SCEPTRE: Sandia's Computational Engine for Particle Transport for Radiation Effects
- SCEPTRE provides extensive and distributive information vs. limited information from Monte Carlo
- Characterize and quantify radiation environments
- Convert radiation environment (X-ray, neutron, etc.) to physical quantities for subsequent electrical or mechanical analyses
  - Energy deposition
    - Device response from production of electron-hole pairs
    - Thermal and mechanical responses
  - Charge profile and photo-Compton electron emission
    - Induced electromagnetic pulse in cable, box and cavity

Linear Boltzmann transport equation

SCEPTRE

$$[\vec{\Omega} \cdot \nabla + \sigma_t(r,E)]\psi(r,E,\vec{\Omega}) =$$
$$\int dE' \int d\vec{\Omega}' \sigma_s(r,E' \to E, \vec{\Omega}' \to \vec{\Omega})\psi(r,E',\vec{\Omega}') + q(r,E,\vec{\Omega})$$

$\vec{\Omega} \cdot \nabla$:	"streaming" term
σ_t:	"collision" (total) term
σ_s:	double differential scattering term

Other terms may be introduced to incorporate additional physics:

- Continuous slowing down operator
- Lorentz terms for charged-particle transport in EM fields

Energy differencing: multigroup

If we integrate the energy-dependent Boltzmann equation over an energy range ("group"), we obtain a coupled system of within-group (or monoenergetic) equations, which are typically solved via "outer" (Richardson) iterations:

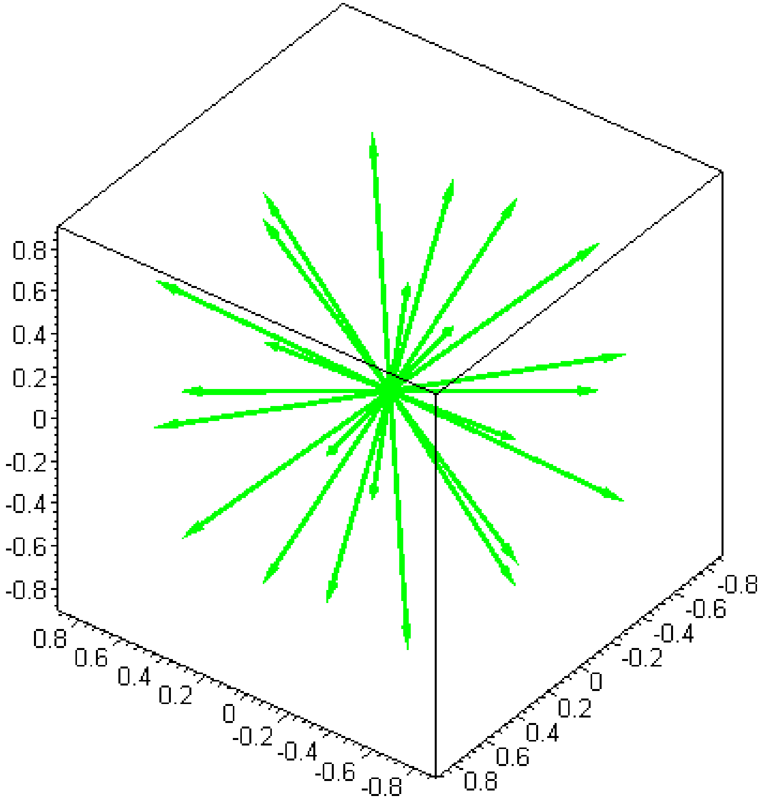
$$[\vec{\Omega} \cdot \nabla + \sigma_{t,g}(r)]\psi_g(r,\vec{\Omega}) =$$
$$\sum_{g'} \int d\vec{\Omega}' \sigma_{s,g' \to g}(r,\vec{\Omega}' \to \vec{\Omega})\psi_{g'}(r,\vec{\Omega}') + q_g(r,\vec{\Omega})$$

Note: assumptions about the spectral shape of the flux are made, which affects the multigroup cross sections. This is notoriously difficult for neutronics due to nuclear resonances. Such cross sections are usually supplied as an external database rather than embedded in the code.

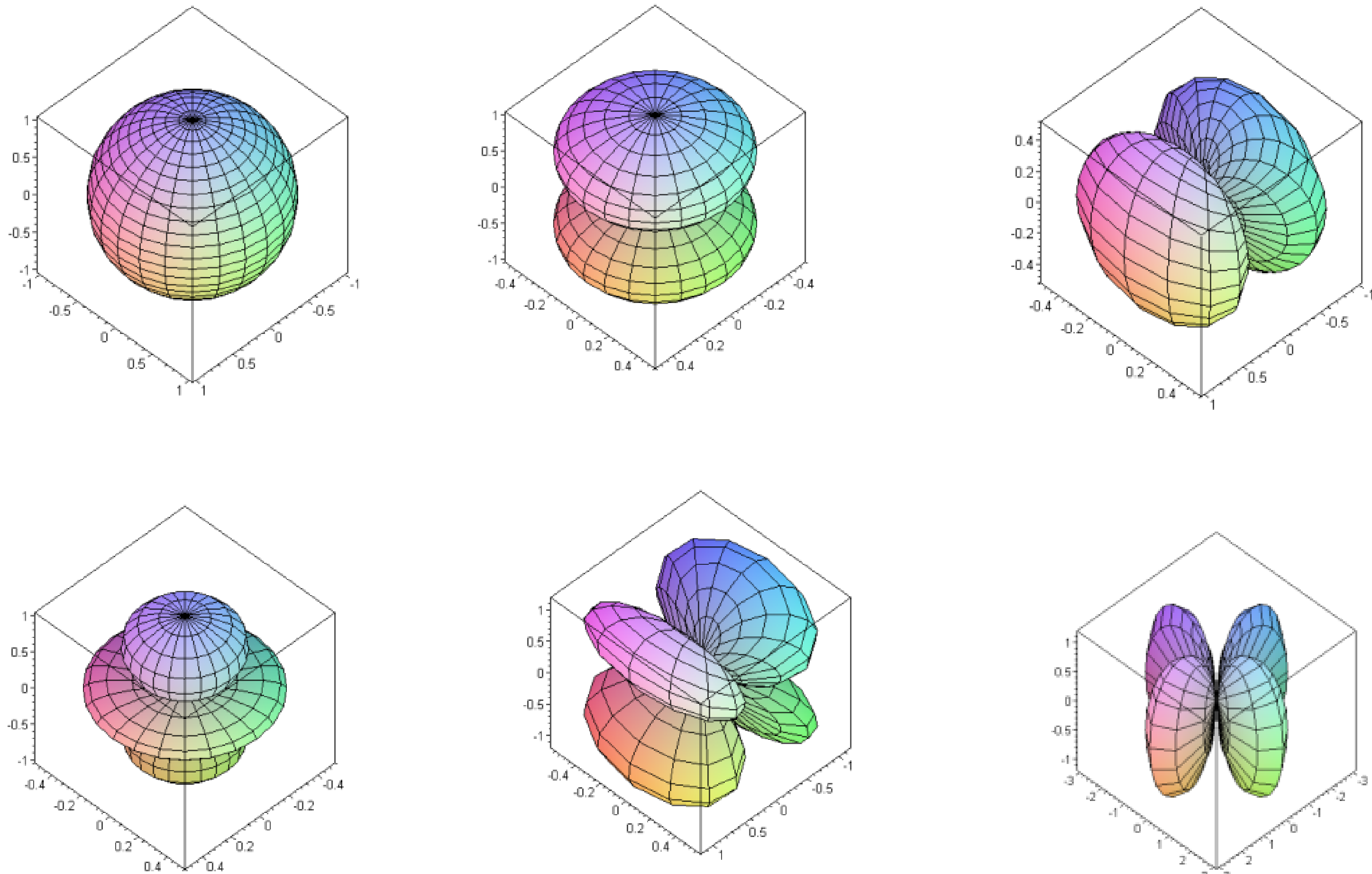
(Takeaway lesson: Codes like Sceptre solve the cross section problem by defining it as someone else's problem.)

Angular discretization: discrete ordinates (S_n)

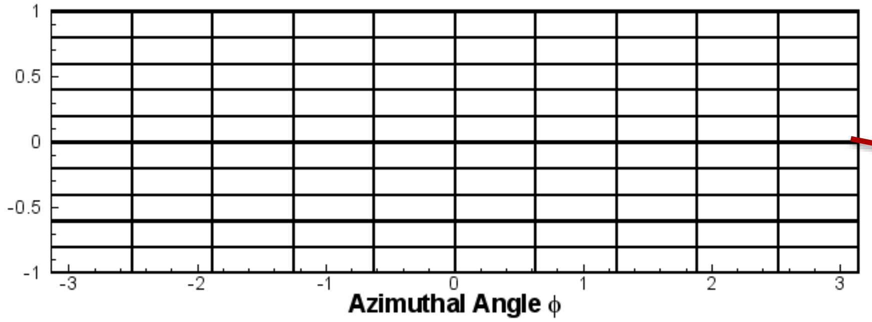
- Collocation in angle
- Compute solution in discrete directions
- Use numerical quadrature to compute angular integrations



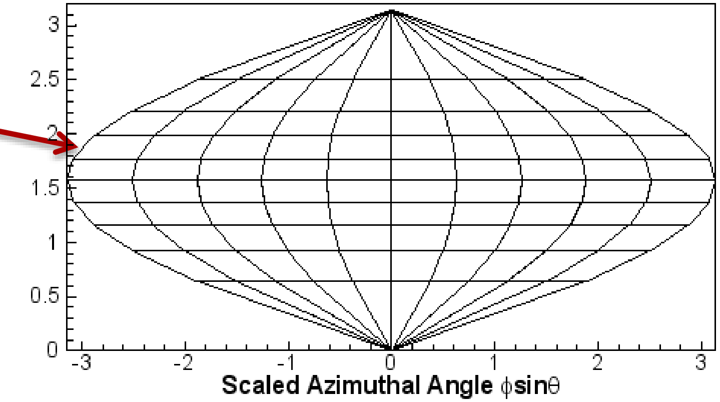
Angular discretization: spherical harmonics (P_n)



Angular discretization: finite elements

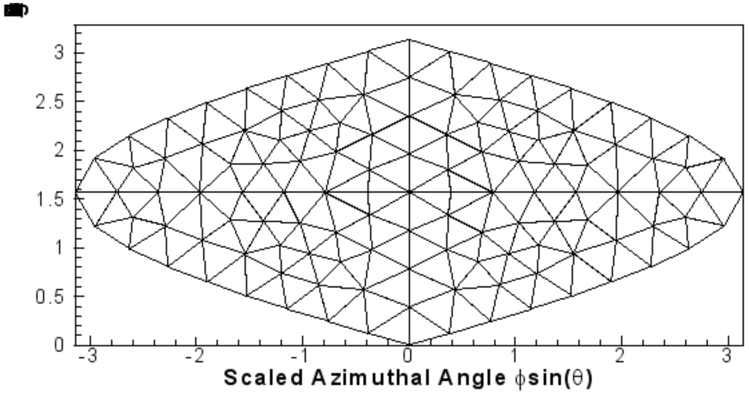


Regular mesh in μ-ϕ space



Mapped from μ-ϕ space mesh

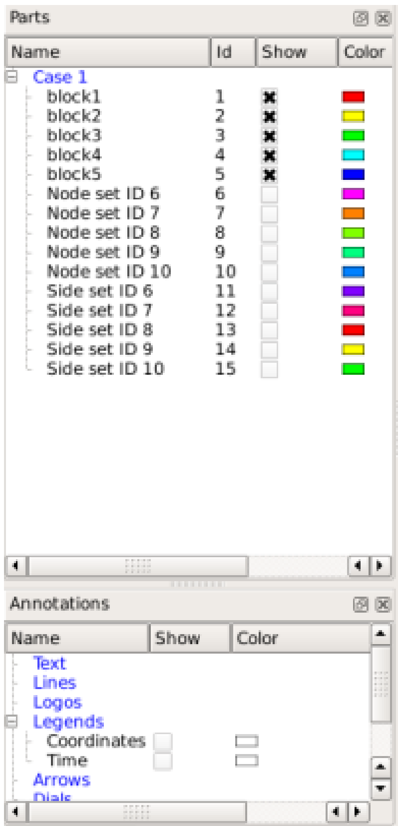
- Problems with meshing μ-ϕ space:
  - Elements mapped to a single point at the poles
  - Non-uniform mesh
- Alternative: use sinusoidal projection and then mesh

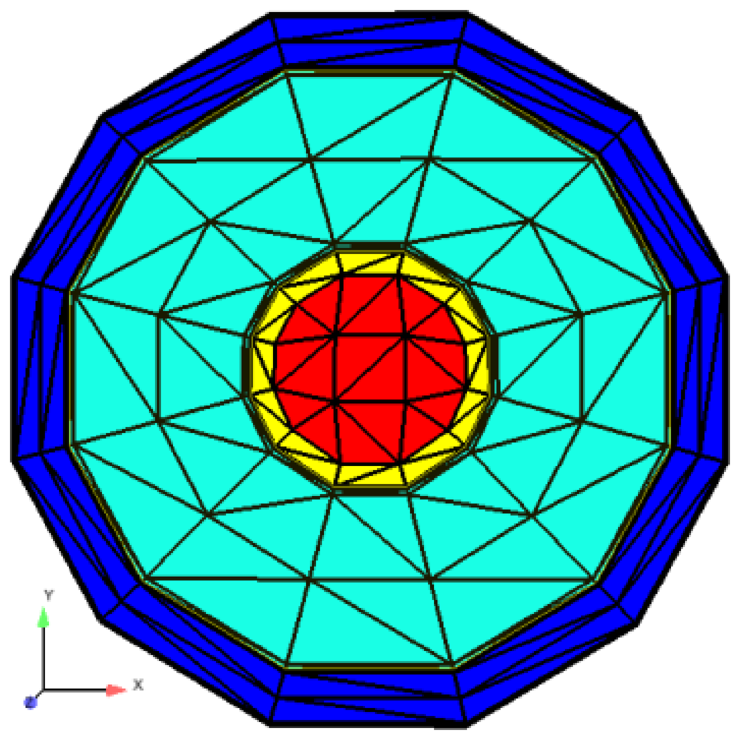


Mesh of sphere mapped to planar region

Spatial discretization: finite elements

- 1D, 2D, and 3D unstructured Cartesian meshes
- Continuous and discontinuous finite elements
- Linear or quadratic basis functions





Forms of (monoenergetic) Boltzmann equation

First-order: $$\left[\Omega \cdot \nabla + \sigma_t\right]\psi(r,\Omega) = M\Sigma D\,\psi(r,\Omega) + Q(r,\Omega)$$

Second-order:

$$\left[-\Omega \cdot \nabla \Re^{-1} \Omega \cdot \nabla + \Re\right]\psi(r,\Omega) = Q(r,\Omega) - \Omega \cdot \nabla\left[\Re^{-1} Q(r,\Omega)\right]$$

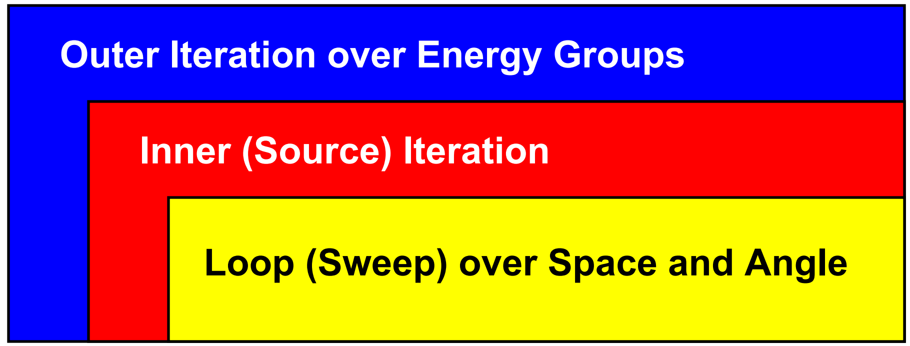
The two continuous forms above are equivalent.

Discretizations, however, yield different properties:

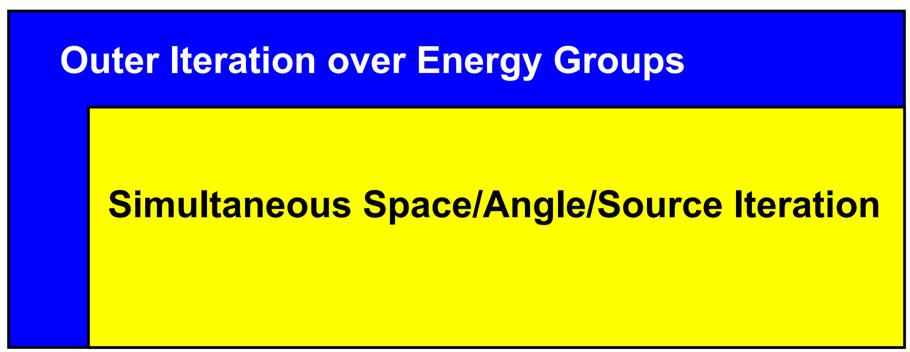
Solutions
Solvers

Iterative approaches for different solvers

First-order:



Second-order:



Iterative solution strategies

First-order:

Source iteration – fix source, solve streaming-plus-collision term, update scattering source, repeat

Advantages: Lower triangular system, small(er) memory

Disadvantages: Scalability, no canned solvers

Second-order:

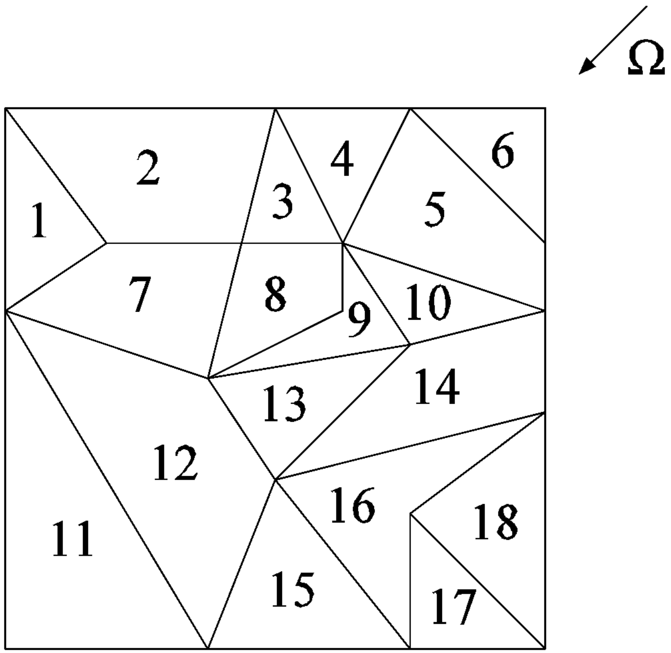
Large matrix solve

Advantages: SPD matrix, Trilinos solvers

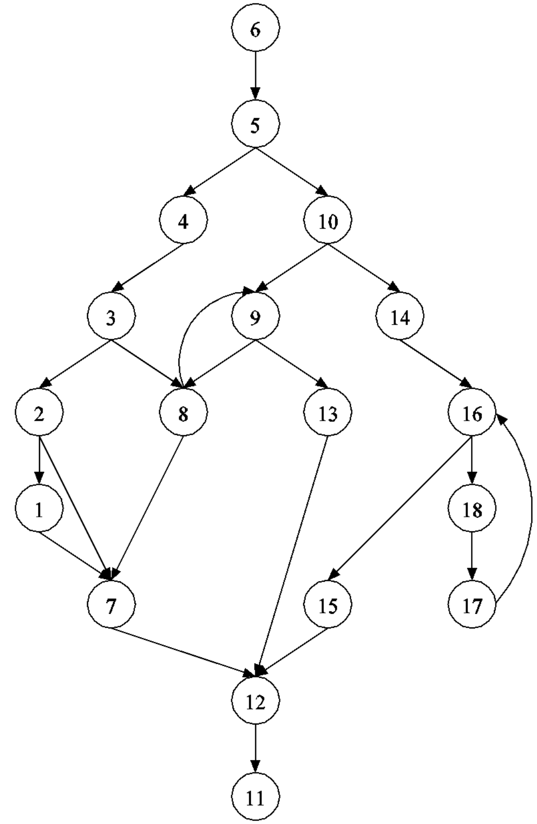
Disadvantages: Large memory requirements, problems with vacuum regions

First-order sweeps: directed task graph

mesh



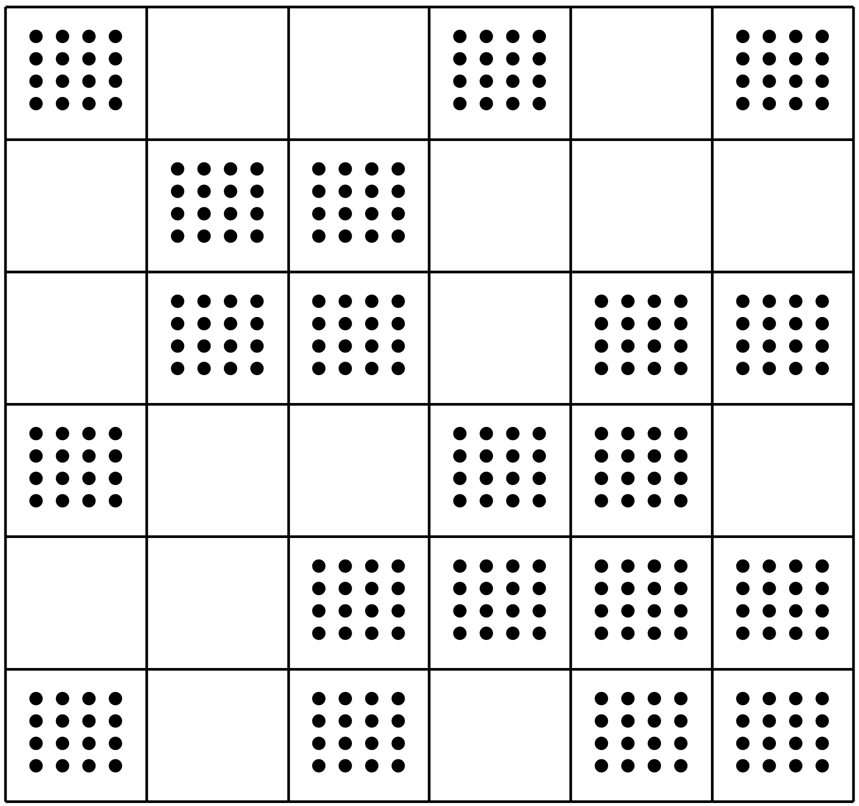
sweep graph



The first-order approach produces a huge number of very small linear systems to solve: one for every angle/element/energy/iteration

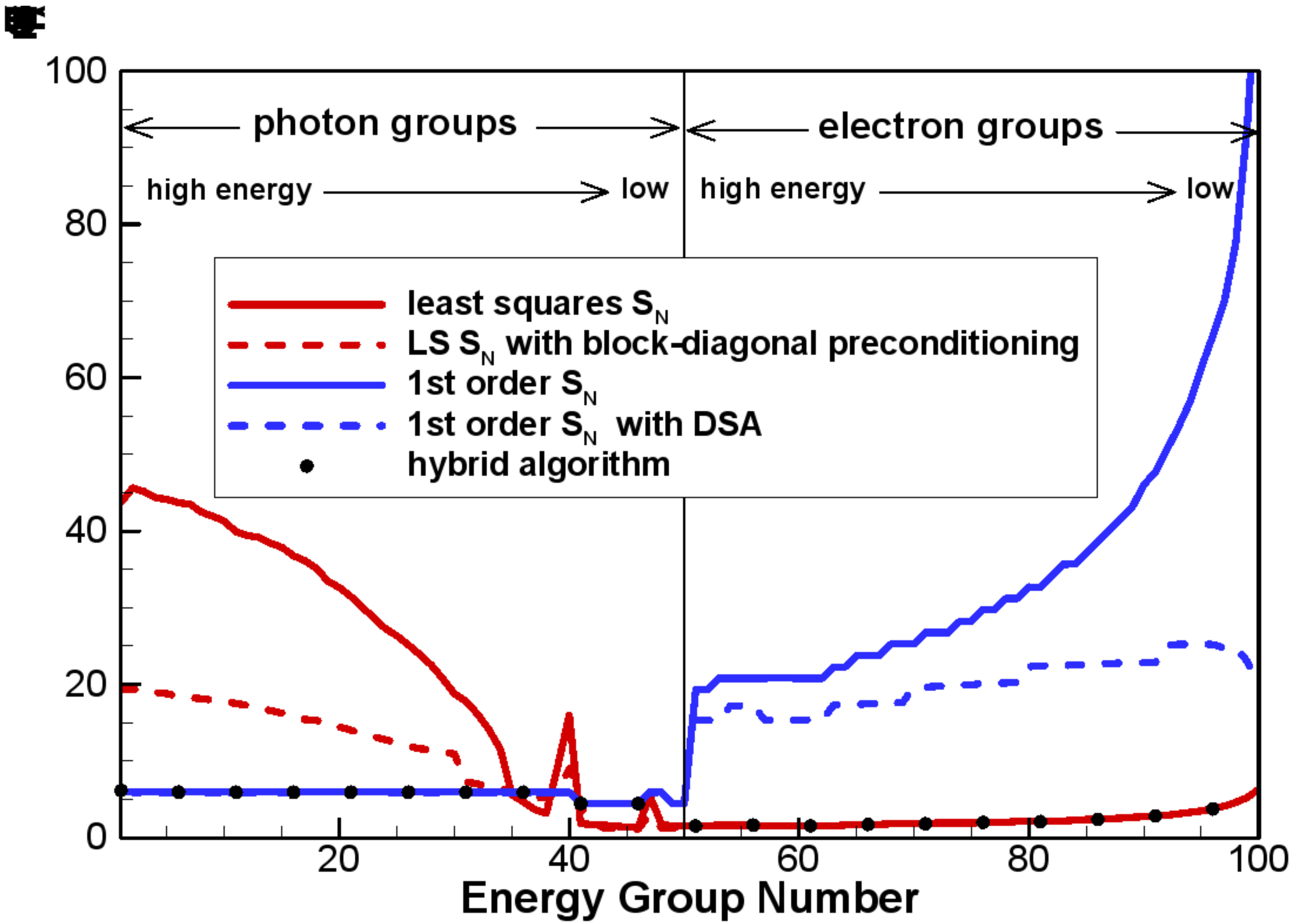
Second-order Transport Methods Result in a Sparse-Block Matrix Structure

A=

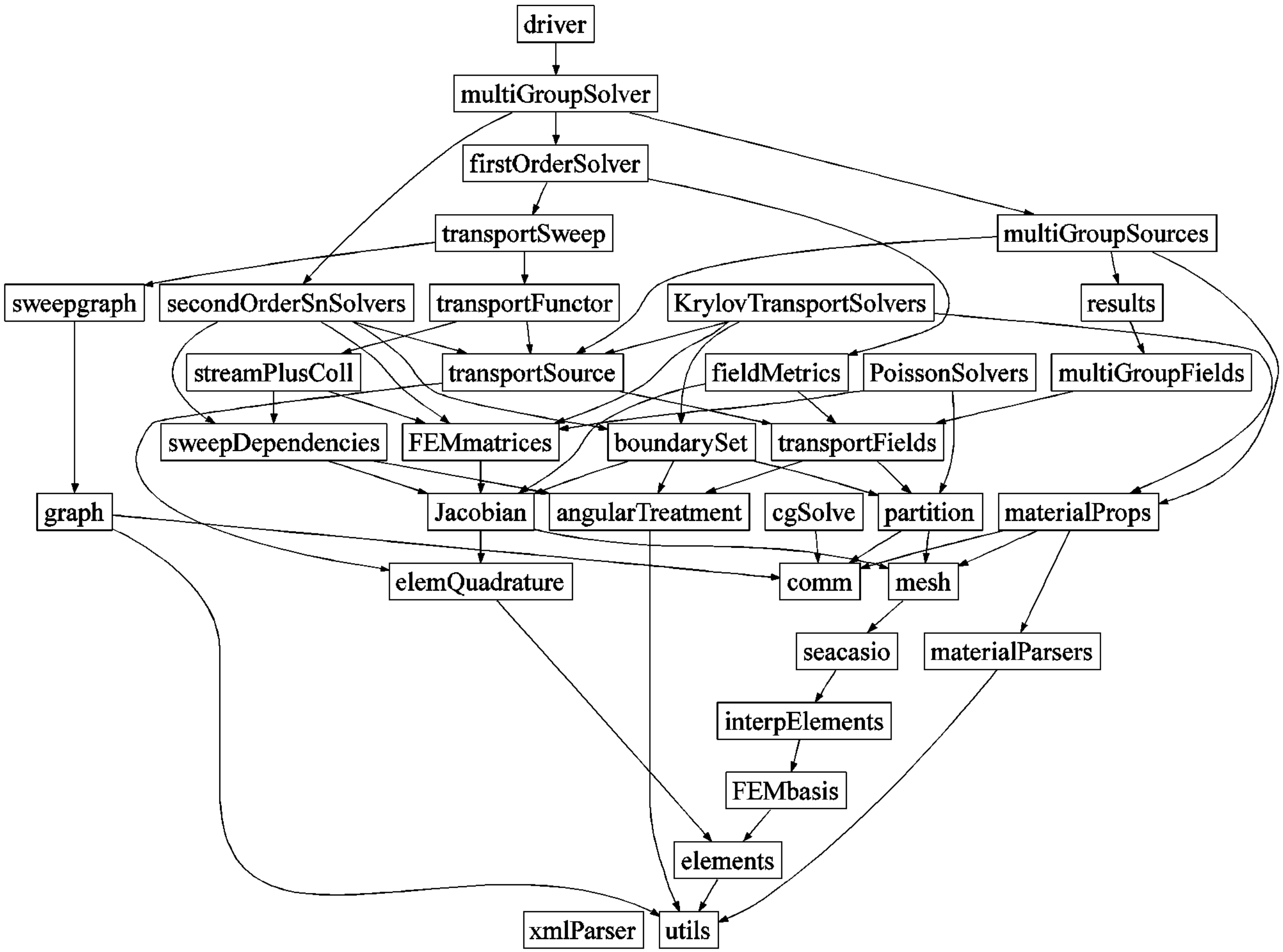


- Limited success achieved in preconditioning linear system
- Out-of-the-box Trilinos preconditioners (ML, IFPack) at best ~2 speedup
- Transport-specific preconditioner (using uncollided flux solution as preconditioner) better
- Others proposed (e.g. use first-order sweep solve as preconditioner)
  - Hybrid first-order/second-order transport methods

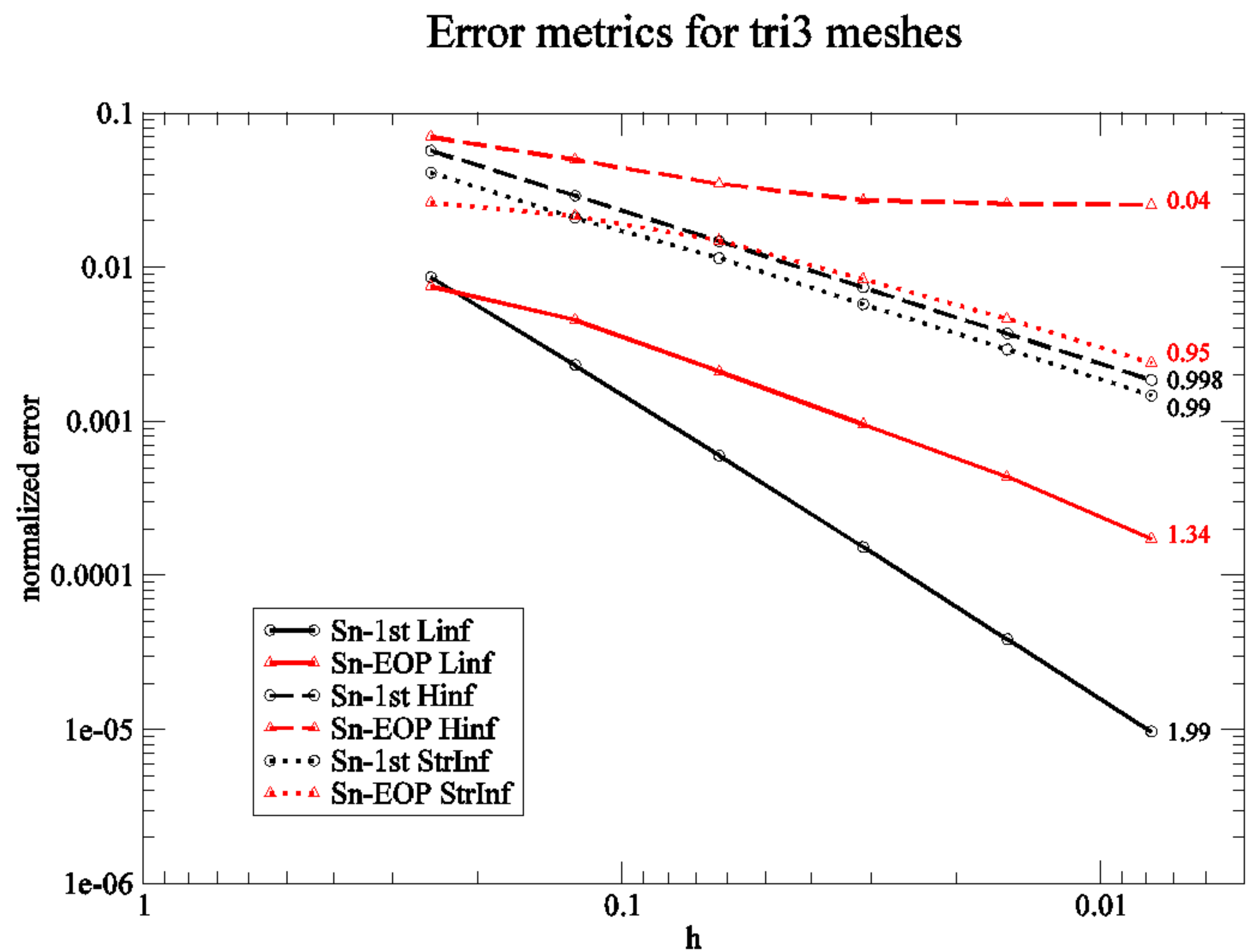
Hybrid Solver



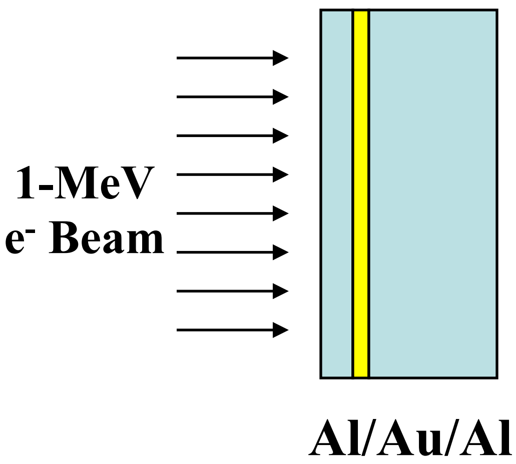
Sceptre levelized design promotes testability, adaptability

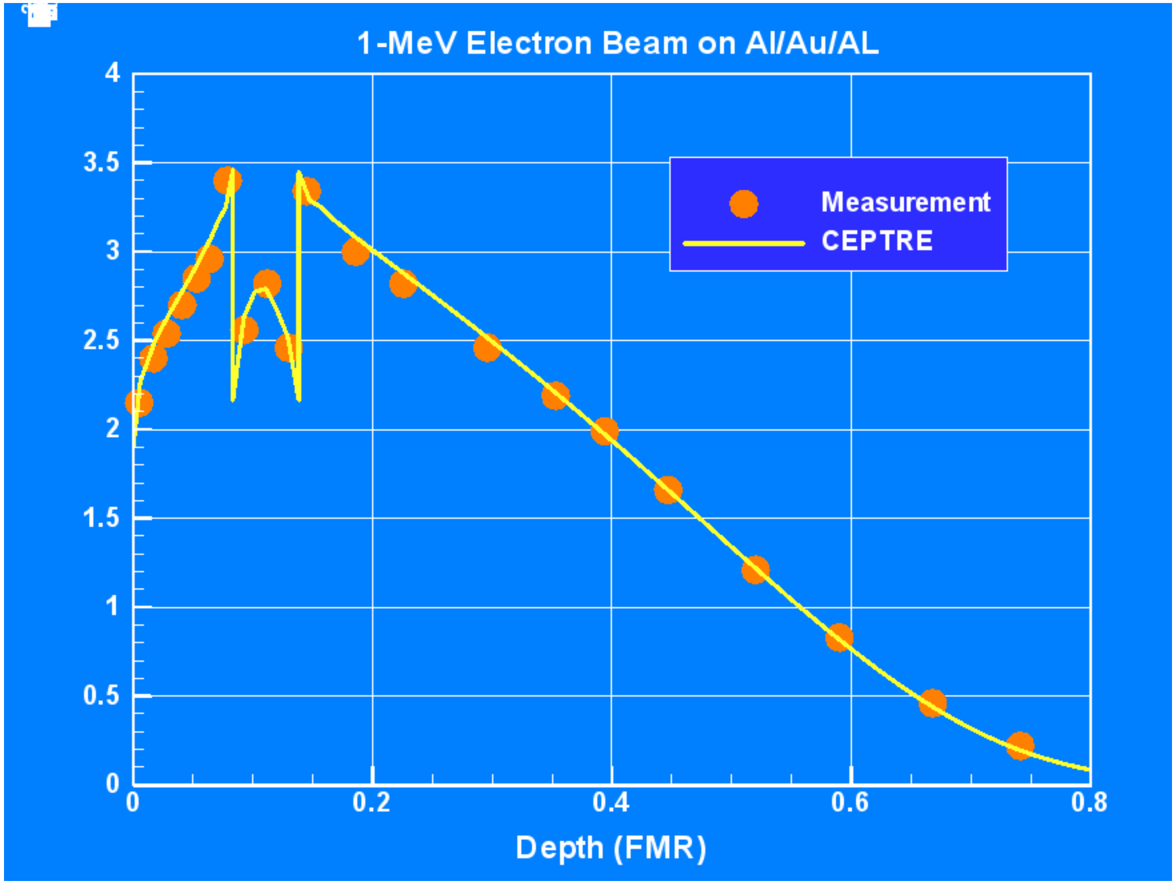


Verification: order of convergence



SCEPTRE Validation: Energy Deposition 1-MeV Electron Beam on Al/Au/Al



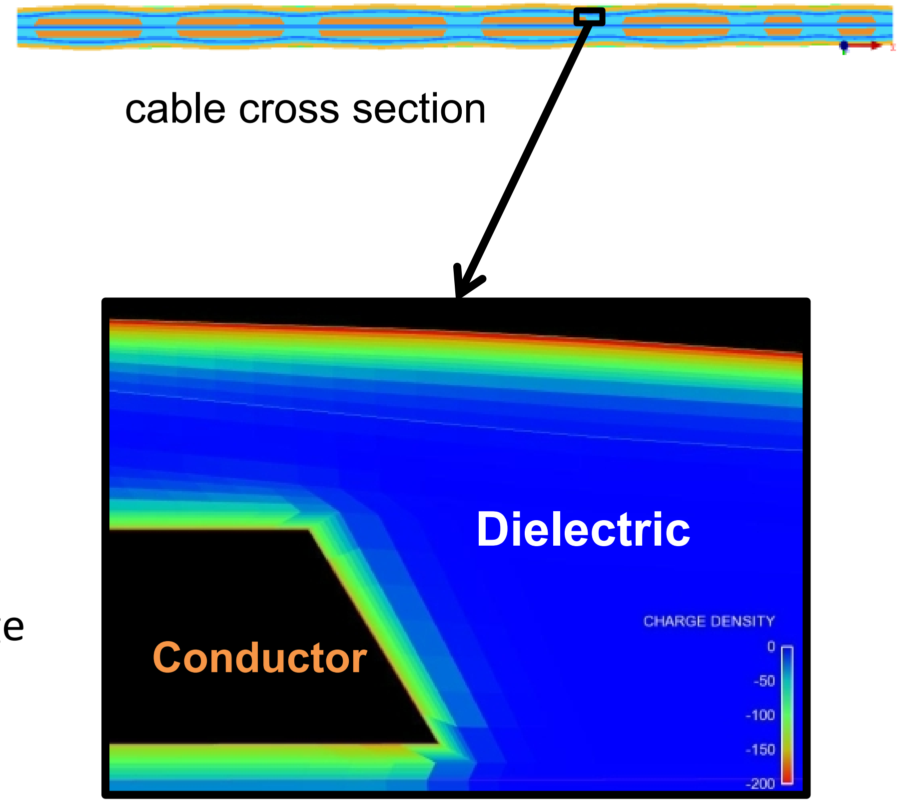


G. J. Lockwood, et al, "Calorimetric Measurement of Electron Energy Deposition In Extended Media," SAND79-0414 (1980)

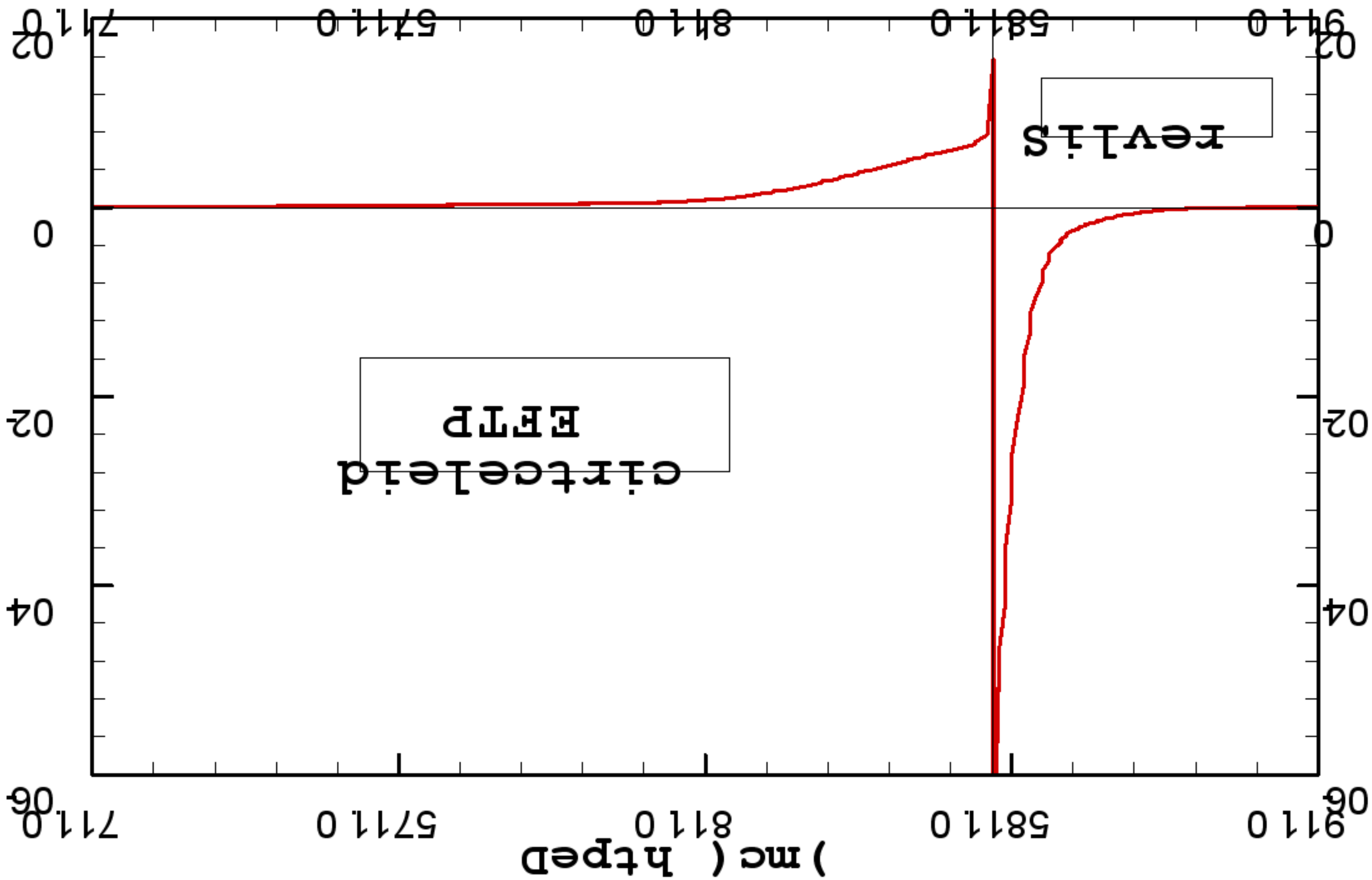
Application: Cable SGEMP

System-Generated Electromagnetic Pulse in Cable

- Photo-Compton interactions produce charge separations near conductor/dielectric interfaces, and induce electromagnetic pulse on the conductors
- Cable SGEMP can potentially upset/burnout downstream electronics
- Extremely difficult to compute
  - Charge injection is the difference between knock-on and induced charge which are similar in magnitude for a rad-hard cable
  - Mean-Free-Path for photon and electron differ by orders of magnitude
- 2.5–D model using SCEPTRE and EMPHASIS

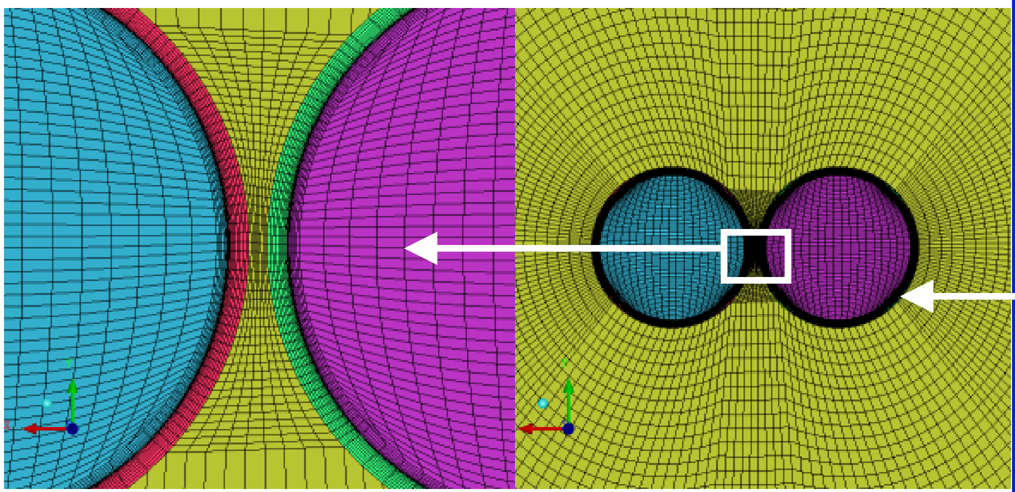


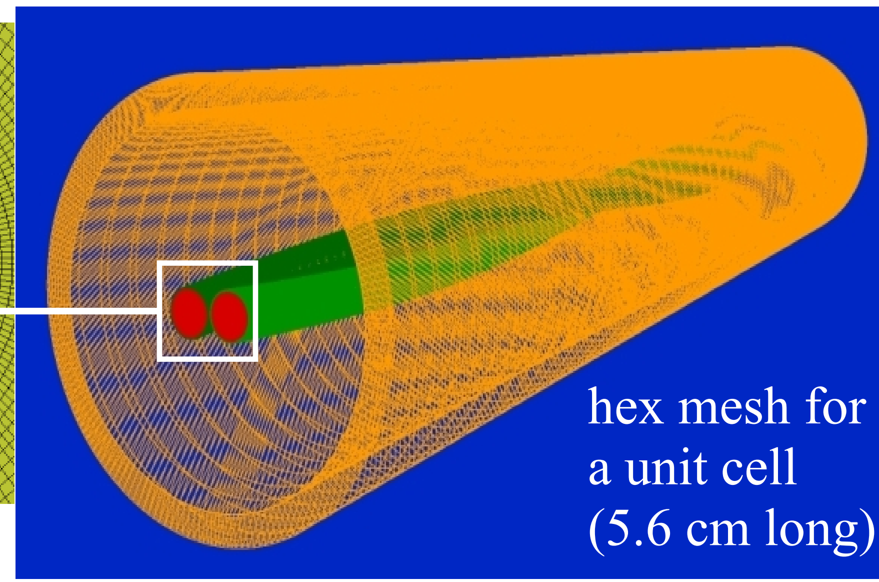
Resolving SGEMP boundary layers



Cable SGEMP

hex mesh cross sections



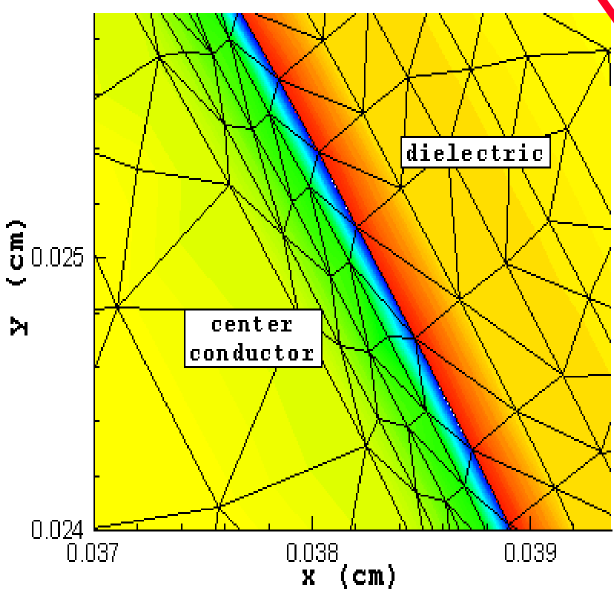


Resolving steep gradients in charge requires µm-size elements near the center conductors

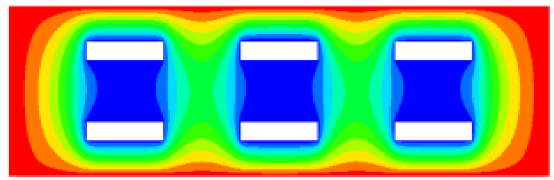
Application: Cable SGEMP

Deterministic (SCEPTRE)

Charge density, currents, & energy deposition at given time



Electric field intensity



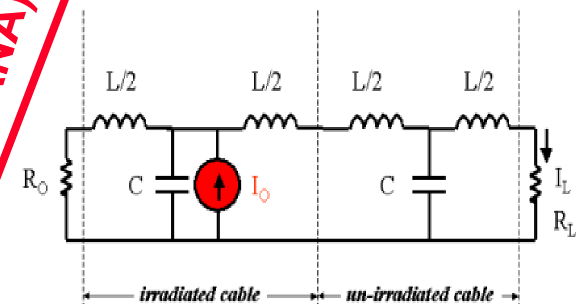
Electrostatics solved simultaneous with lumped circuit model of cable

Drive current as a function of time

(CABANA)

2D quasi-electrostatic solver with radiation-induced conductivity models

Circuit analysis module (SPICE)

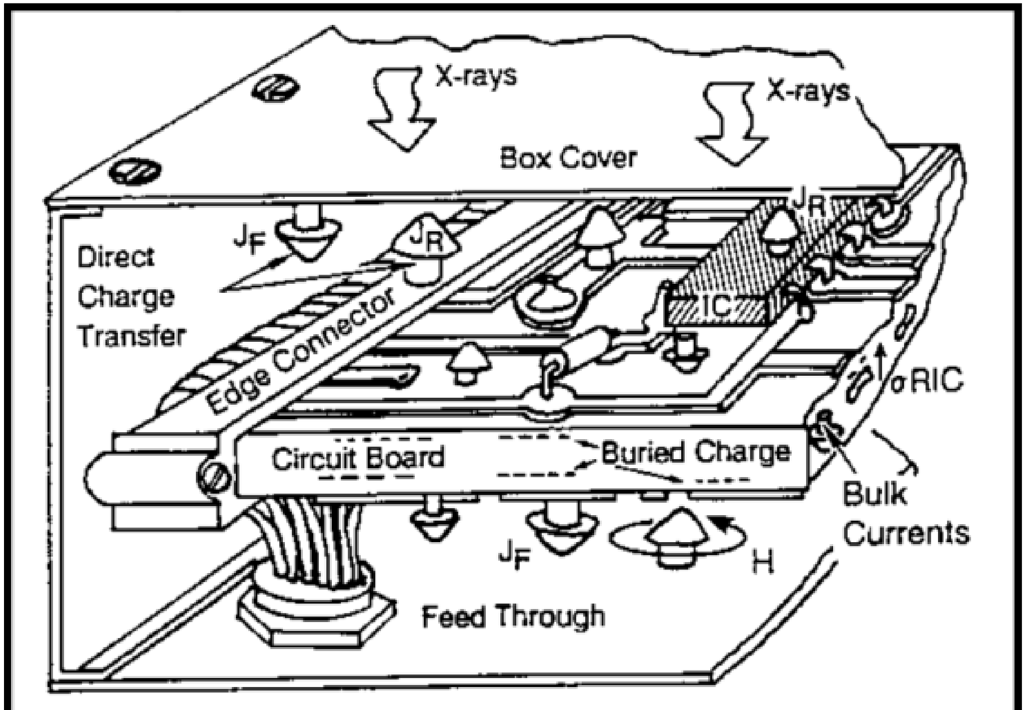


I_0 is the radiation induced current source

Transmission line effects and circuit termination response

Application: Box IEMP

Internal Electromagnetic Pulse in Electronic Box

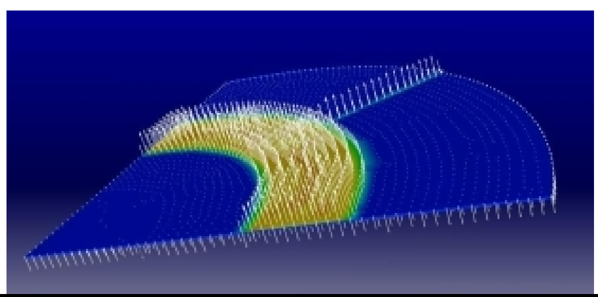


Courtesy of Burr Passenheim, "How to do Radiation Tests"

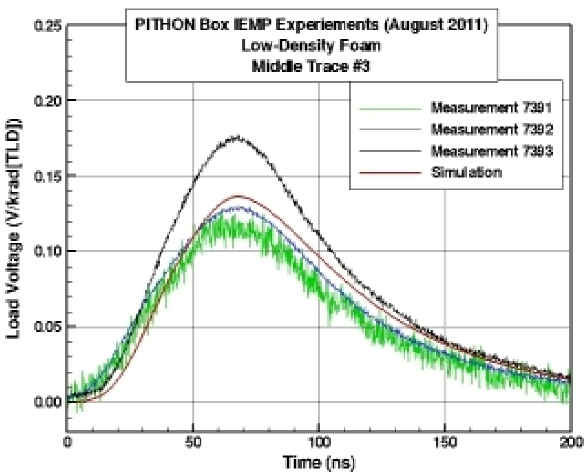
Box IEMP

- **Similar phenomena to Cable SGEMP**
  - **Ground/Power Plane ⇔ Outer Shield**
  - **Connector/Trace ⇔ Internal Conductor**
  - **Board ⇔ Dielectric Filling**
- **Box IEMP can potentially upset/burnout downstream electronics**
- **Mesh generation can be difficult (if not impossible) due to complex geometry and element-size requirement**
- **Full 3D coupling between SCEPTRE and EMPHASIS**

PITHON Experiment with a Cylindrical Box
Multiple-Layer Board with Multiple Traces



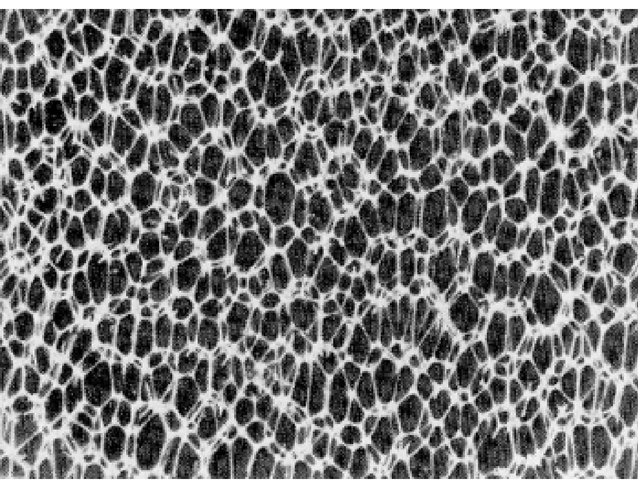
Current Density Profile Near the Middle Trace Above the Ground Plane



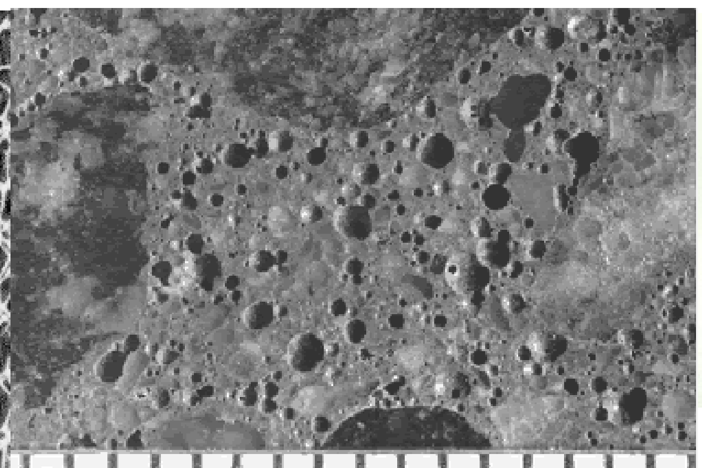
Transport in stochastic media

Some materials are mixtures whose distribution is known in only a statistical sense, and/or are too complicated to directly model.

We have implemented the Levermore-Pomraning (LP) model for transport in stochastic media and perform research in this area.



Photomicrograph of polyurethane foam. Image from National Research Council

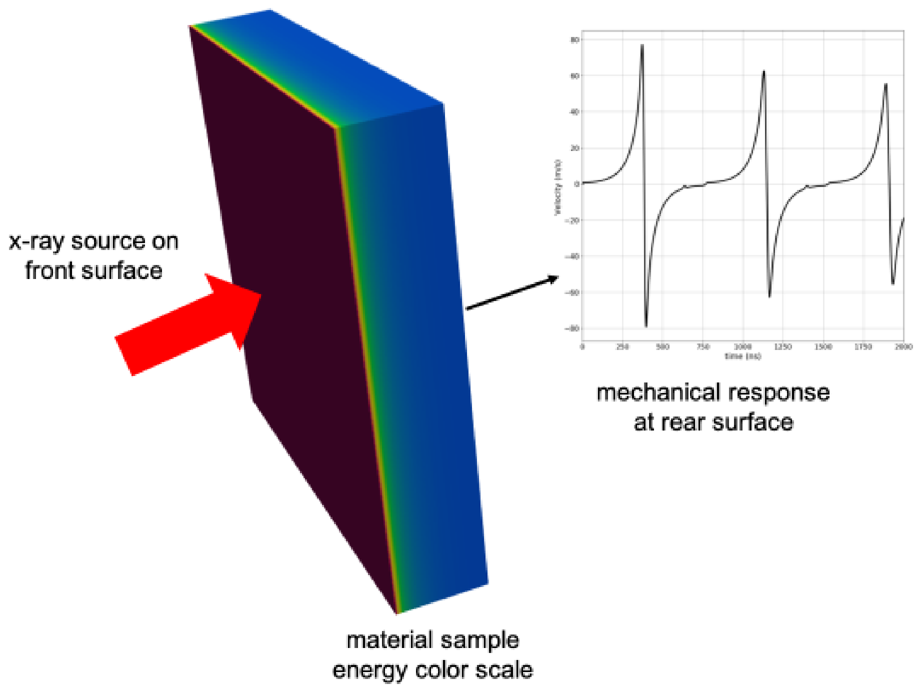


Cross section of concrete. Image from Federal Highway Administration.

Printed circuit board. Image from FreeFoto.com under Creative Commons license.

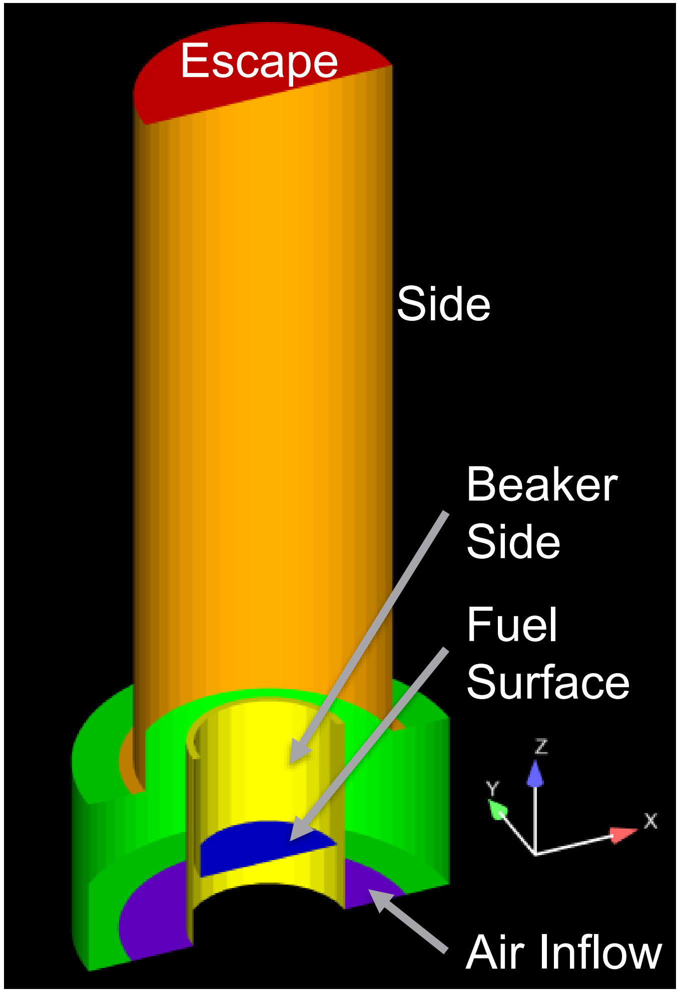
Code Coupling: SCEPTRE/ALEGRA for material response

- MPMD coupling between codes
- SCEPTRE computes energy deposition
- ALEGRA computes mechanical response



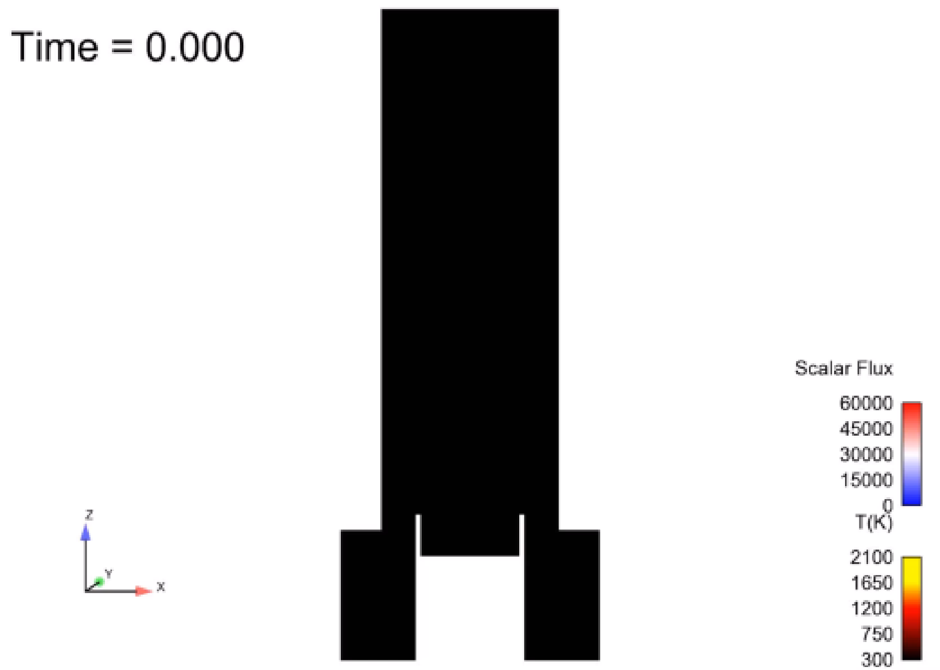
Code coupling: SCEPTRE/Fuego for thermal/fire modeling

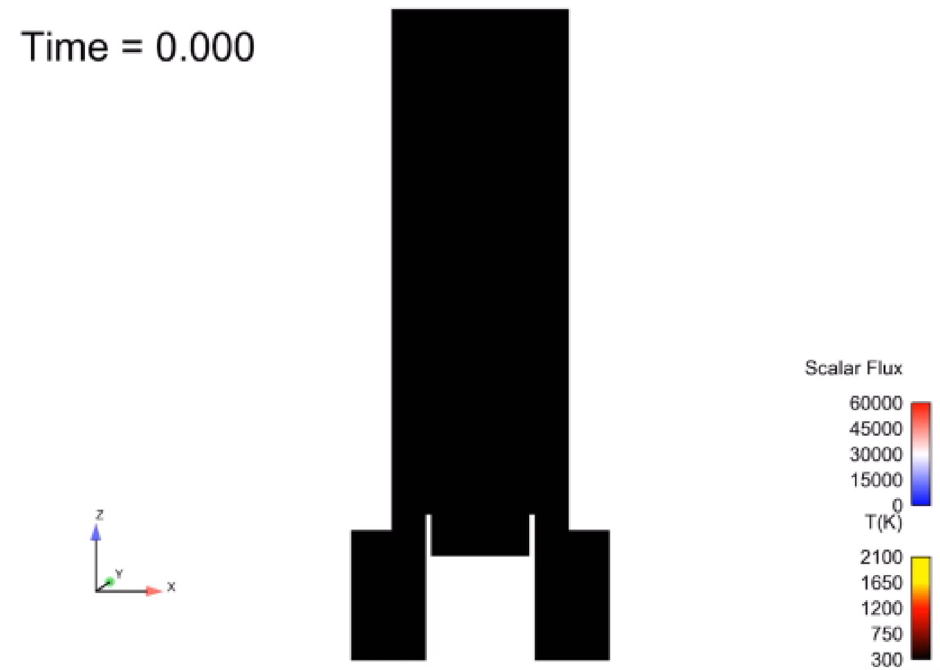
- Fluid
  - Fuel Inflow
  - Combustion (EDC model)
  - Thermal radiation transport (Discrete Ordinates)
- Particles
  - Lagrangian w/ 2 way coupling to fluid
  - Momentum
  - Heat
  - Mass
  - Species



Code coupling: SCEPTRE/Fuego for thermal/fire modeling

SCEPTRE





- Flame Cross Section
- Scalar Flux isosurface with radiative flux vectors