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Radiation Effects Modeling with the CEPTRE Code

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SAND 2007-???
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Outline

- Sandia Missions
- Overview of CEPTRE
- First- and Second-Order Methods
- Algorithmic Details
- Results
- Summary

Sandia National Laboratories: a Short Introduction

- Started in 1949 as a division of Los Alamos
- Two locations: Albuquerque NM and Livermore CA
- Currently about 7,500 employees
- Diverse mission includes:
  - Ensuring the safety of the nuclear weapons stockpile
  - Energy and infrastructure
  - Nonproliferation
  - Homeland security

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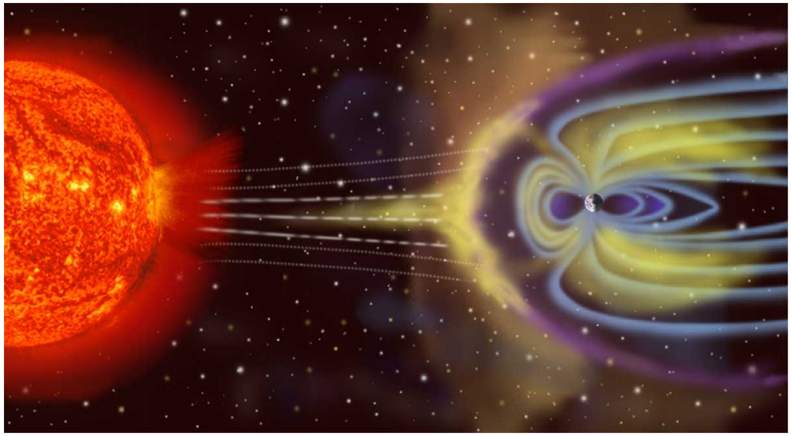
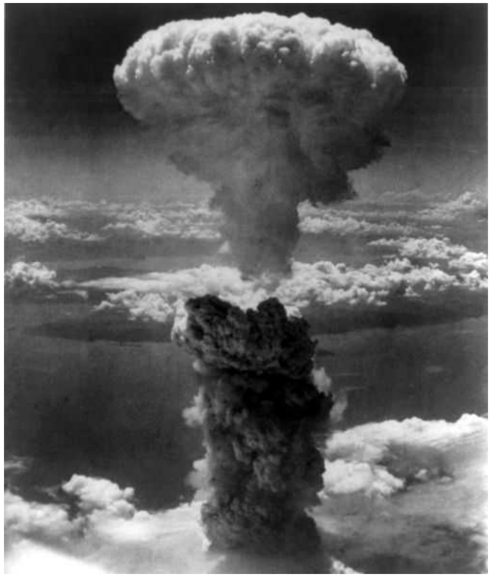
Nuclear and Radiation Science Activities at Sandia

- Radiation effects
  - Experiments
  - Simulation
- Nuclear power systems
  - Advanced power conversion technologies
  - Hydrogen production
  - Spent fuel management (Yucca Mountain)
- Space nuclear power and propulsion
- Inertial fusion energy (Z-pinch)

Protecting Components and Systems in Harsh Radiation Environments





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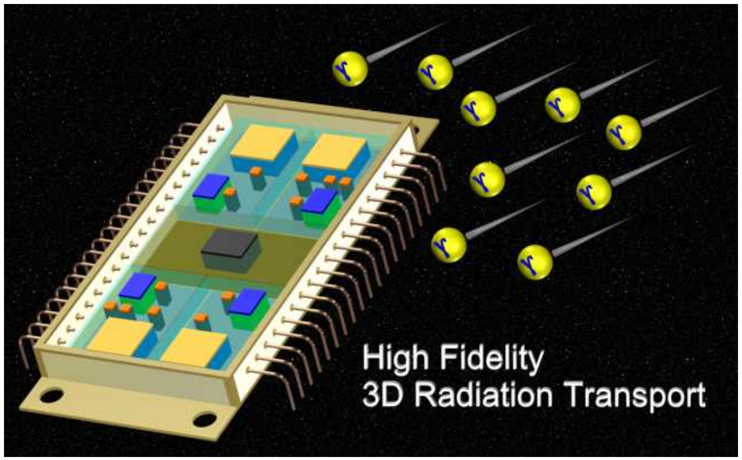
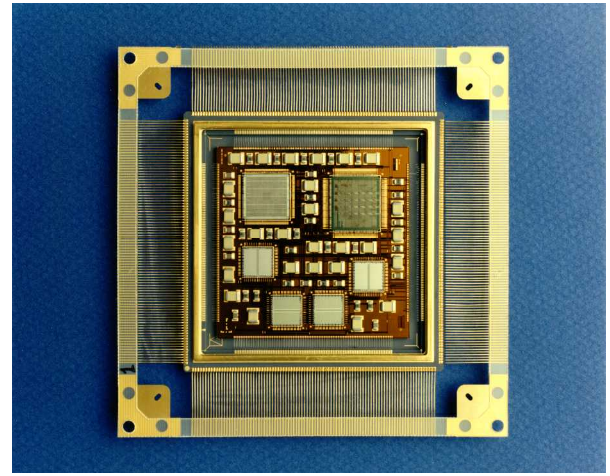
Radiation transport is fundamental to understanding the effects produced in nuclear & space radiation environments



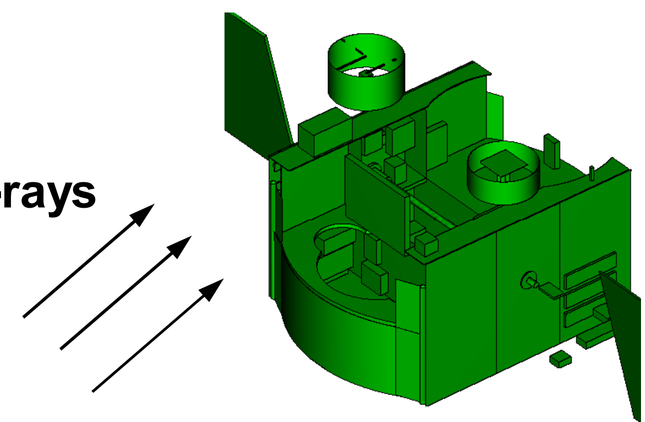
The transport of coupled photon, electron, and positron radiation from 1.0 keV to 20.0 MeV



ICs

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

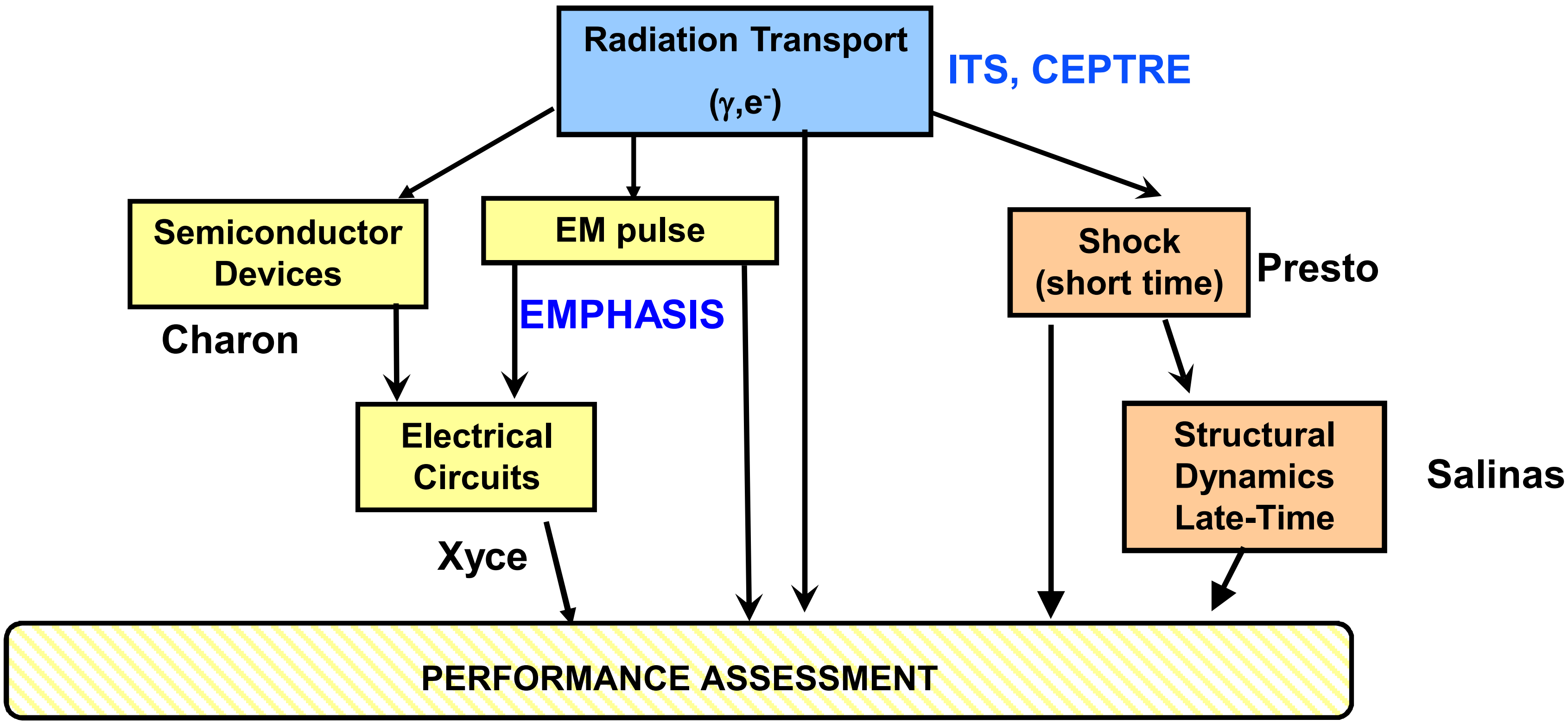
X-rays



Satellite

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

ASC Program : Codes & Effects



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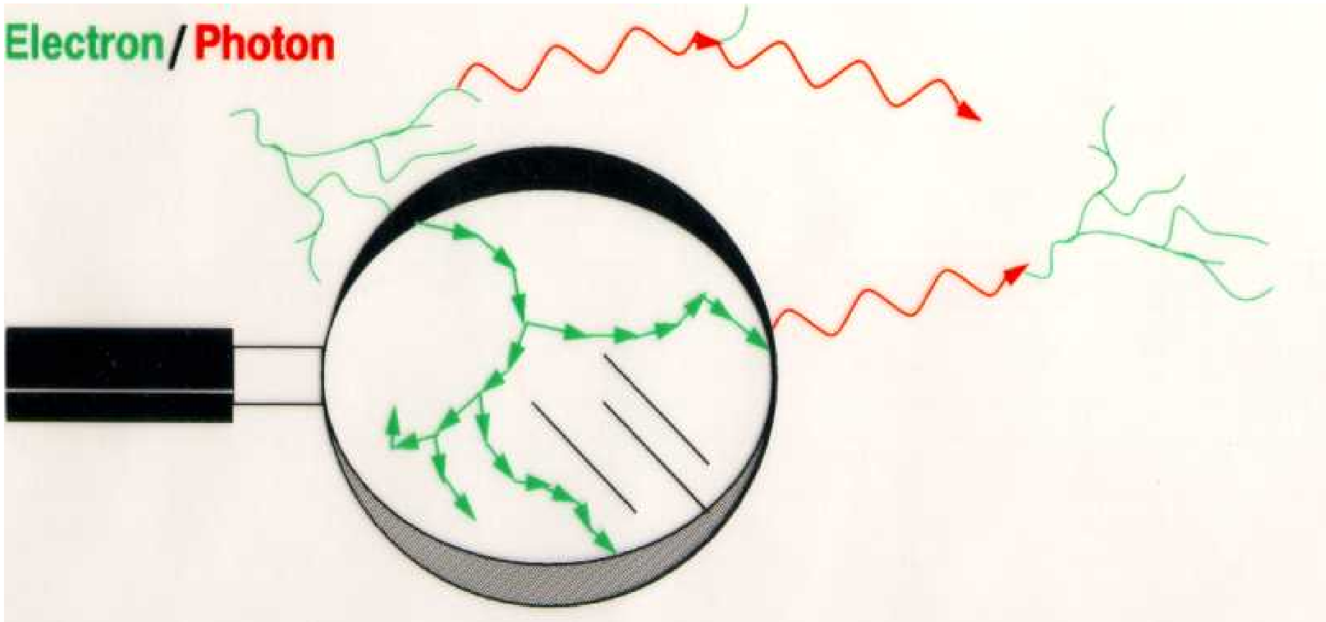
Coupled photon-electron particle cascade



Electrons and photons have radically different transport scales!

Simulation challenge: radically different cross sections for electrons and photons

Particle Energy (keV)	Photon MFP (micron)		Electron MFP (micron)	
	silicon	gold	silicon	gold
100	24,000	100	.03	.006
30	4,000	21	.01	.003

For Monte Carlo, analog simulation of electrons would be prohibitively computationally expensive

- *Solution: Condensed-history models*

For deterministic, proper treatment of electron cross sections would require excessive discretization in energy and angle and would be prohibitively computationally expensive.

- *Solution: Boltzmann-Fokker-Planck (BFP) transport equation*

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

- Runtime limited
  - Memory not generally a limitation
- Complex 3D modeling capability exists
- Efficient for computing integral quantities
  - Total charge crossing a surface
  - Total dose in a region
- Easily adaptable to parallel computers

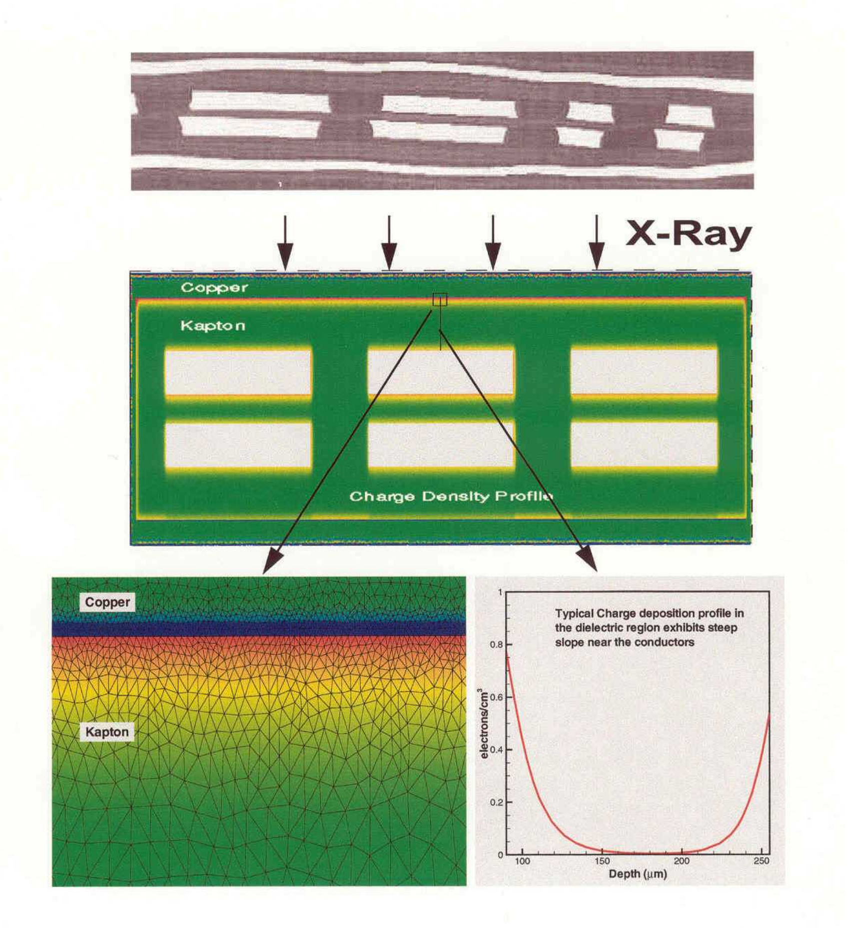
Deterministic Methods (CEPTRE)

Numerical solution of the mathematical equation describing the transport

- Memory and/or runtime limited
- Complex 3D modeling capability is being developed
- Essential for computing differential quantities
  - charge deposition distributions
  - energy deposition distributions
  - space, energy, and angle dependent emission quantities

Cable SGEMP Simulation Needs

- Requires accurate resolution of dose-enhancement and charge profiles near conductor/dielectric interfaces
- Results in extremely small mesh cells near the material interfaces



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CEPTRE

Coupled Electron-Photon Transport for Radiation Effects

- Initial code for SGEMP simulations
- Implemented in Nevada framework
- 2nd-order formulation only
- Even/odd parity, SAAF, LS
- 2D/3D, linear/quadratic elements
- Large matrix solve

SCEPTRE

Sandia's Computational Engine for Particle Transport for Radiation Effects

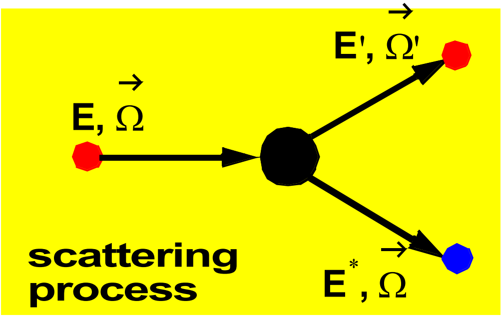
- Second generation code
- Standalone code (no framework)
- 1st- and 2nd-order formulations
- S_n and P_n
- Even/odd parity, SAAF, LS
- 2D/3D, linear/quadratic elements
- Large matrix solve or source iteration

SCEPTRE Status

- Many components and subsystems complete and functional
- Some notable holes remain
- Lots of unit tests

CEPTRE/SCEPTRE Details

- Time-independent, deterministic, coupled electron-photon transport code on unstructured meshes
- Numerical solutions to the Boltzmann transport equation which describes the particle distribution in phase space (r, E, Ω)
- Physics of particle-media interactions properly characterized by cross sections
- Discretization of Phase Space
  - *Multigroup* approximation in energy along with Legendre expansion of scattering cross sections
  - *Discrete-Ordinates (*also *Spherical Harmonics)* approximation in direction
  - *Finite-Element* approximation in space



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Forms of Boltzmann Transport Equation

First-order:

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

Second-order:

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

The continuous forms are equivalent, but their discretized forms have different properties

Multigroup energy differencing

Integrate the continuous-energy Boltzmann equation over an energy band ("group"):

$$\int_{E=E_g}^{E_{g+1}} dE\left(\;\right)$$

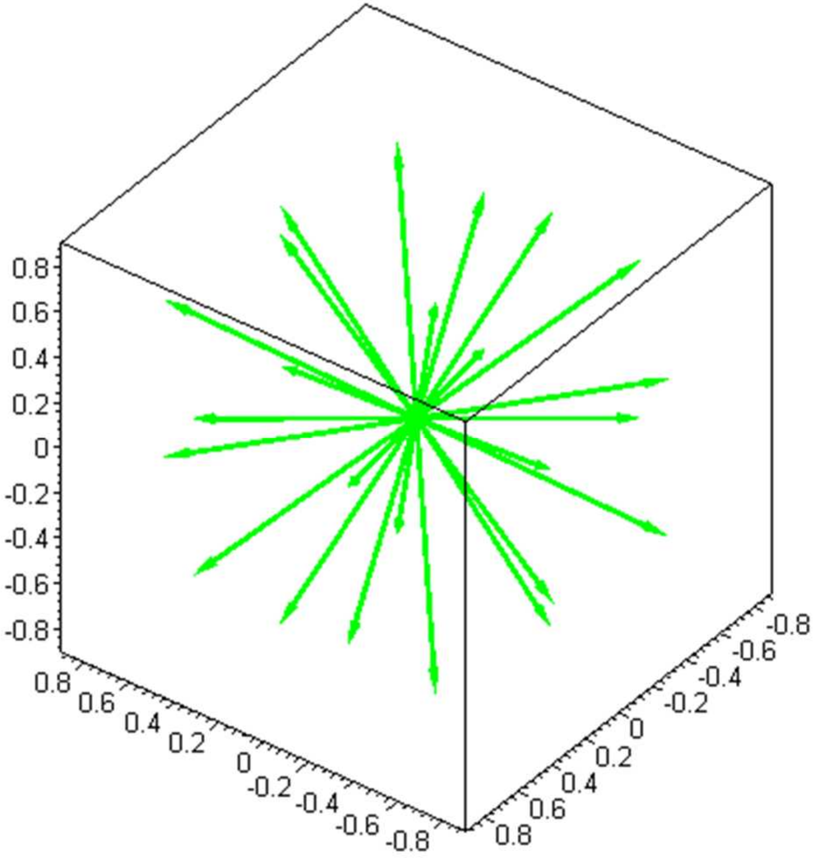
↓

$$\left[\Omega\cdot\nabla+\sigma_{t,g}\right]\psi_g\left(r,\Omega\right)=$$

$$M\Sigma_{g\to g}D\psi_g\left(r,\Omega\right)+\sum_{g'\neq g}M\Sigma_{g'\to g}D\psi_{g'}\left(r,\Omega\right)+Q_g\left(r,\Omega\right)$$

Angular differencing: discrete ordinates

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



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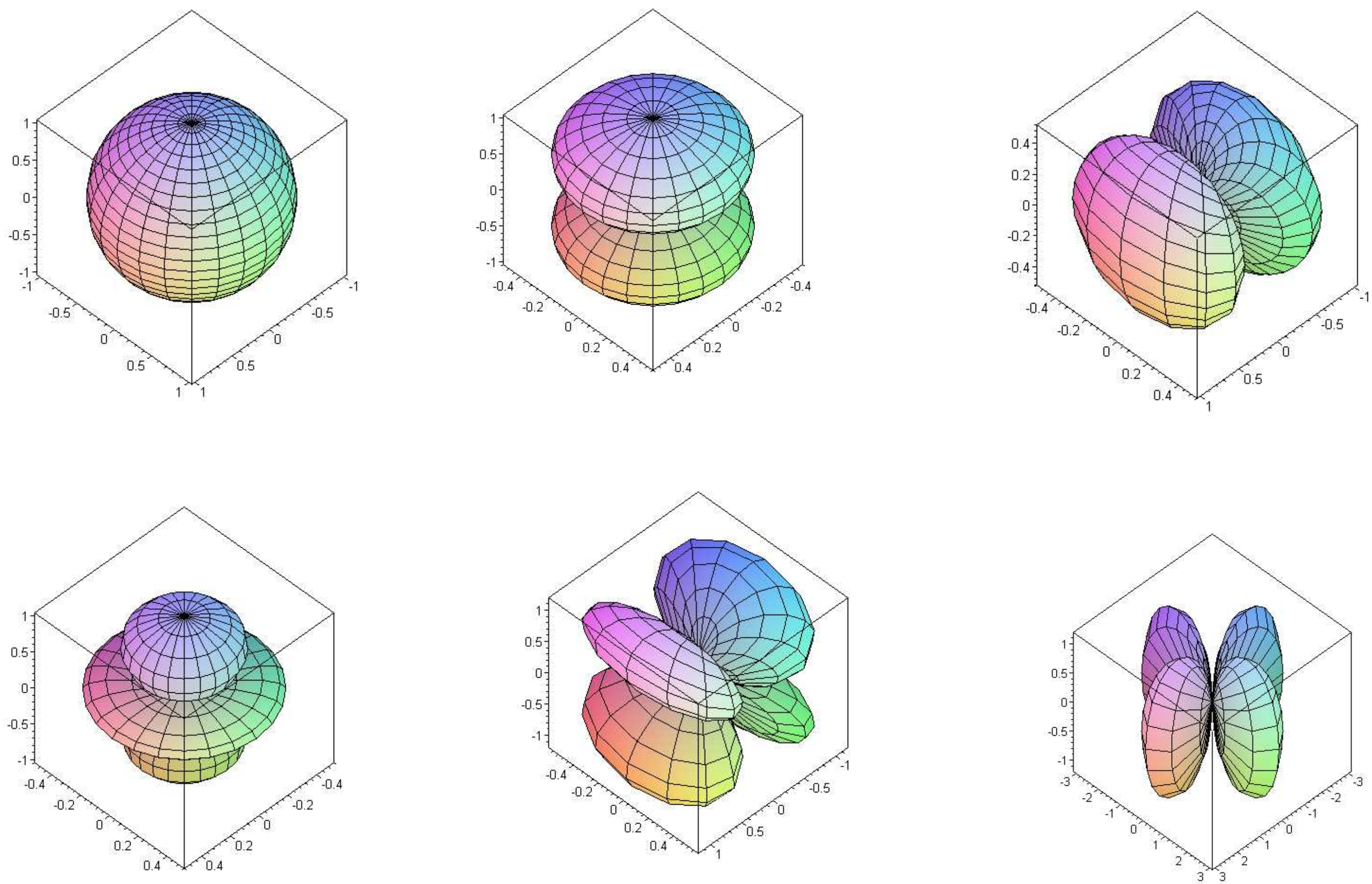
Angular differencing: spherical harmonics



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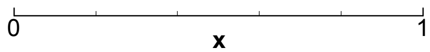
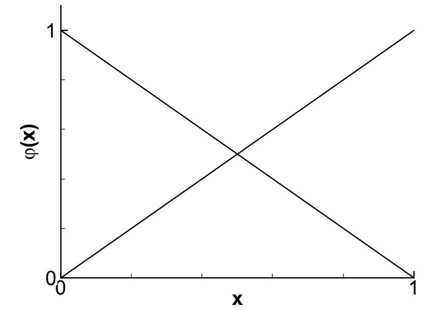
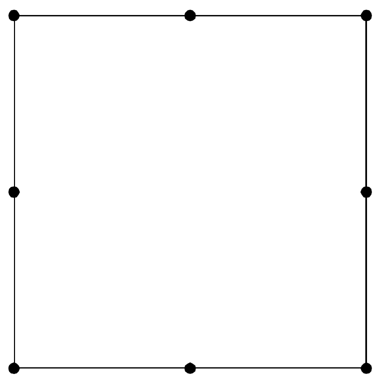
Spatial differencing: finite element method

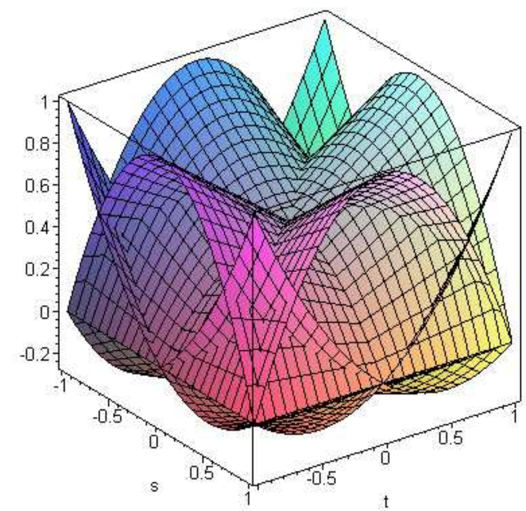
1D
Linear





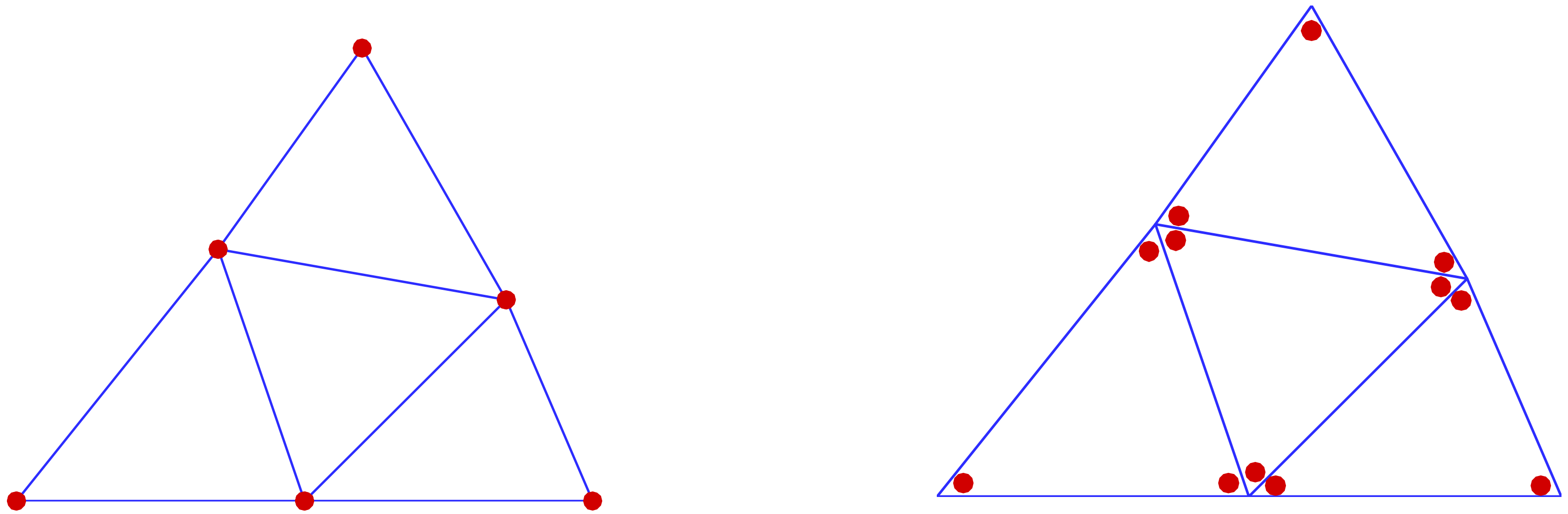
Quadratic
Quadrilateral





Continuous vs. Discontinuous FEM Representations

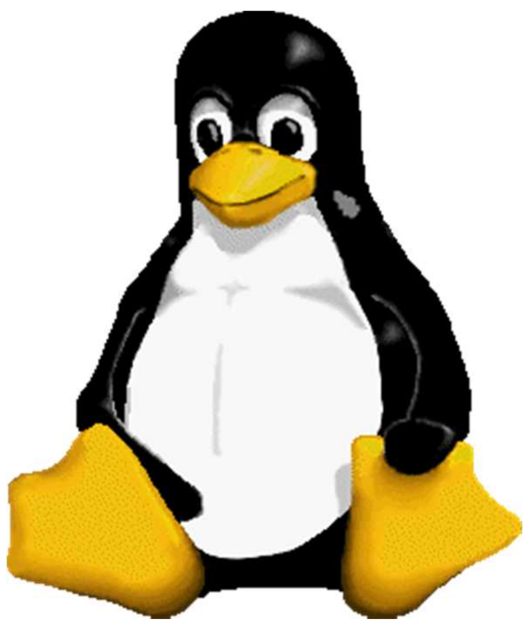
- Solution may be continuous or have discontinuities (shadow boundaries)
- Continuous mesh smaller problem size
- Discontinuous elements may be more accurate



Linear-continuous elements

Linear-discontinuous elements

Cartesian representation has limited fidelity



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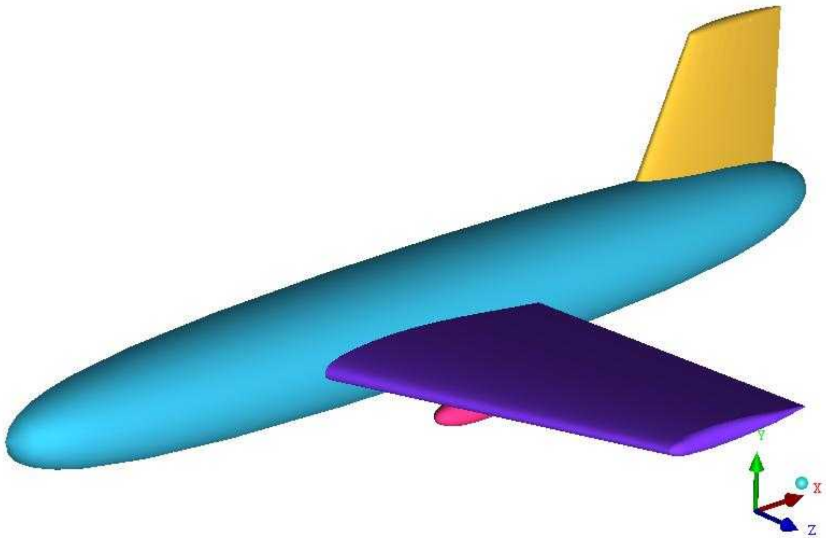
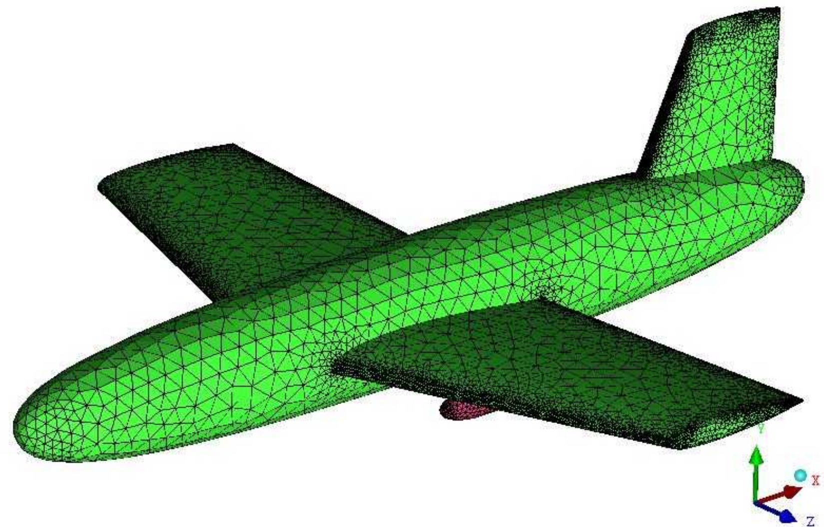
http://www.ericharshbarger.org/lego/penguin.html

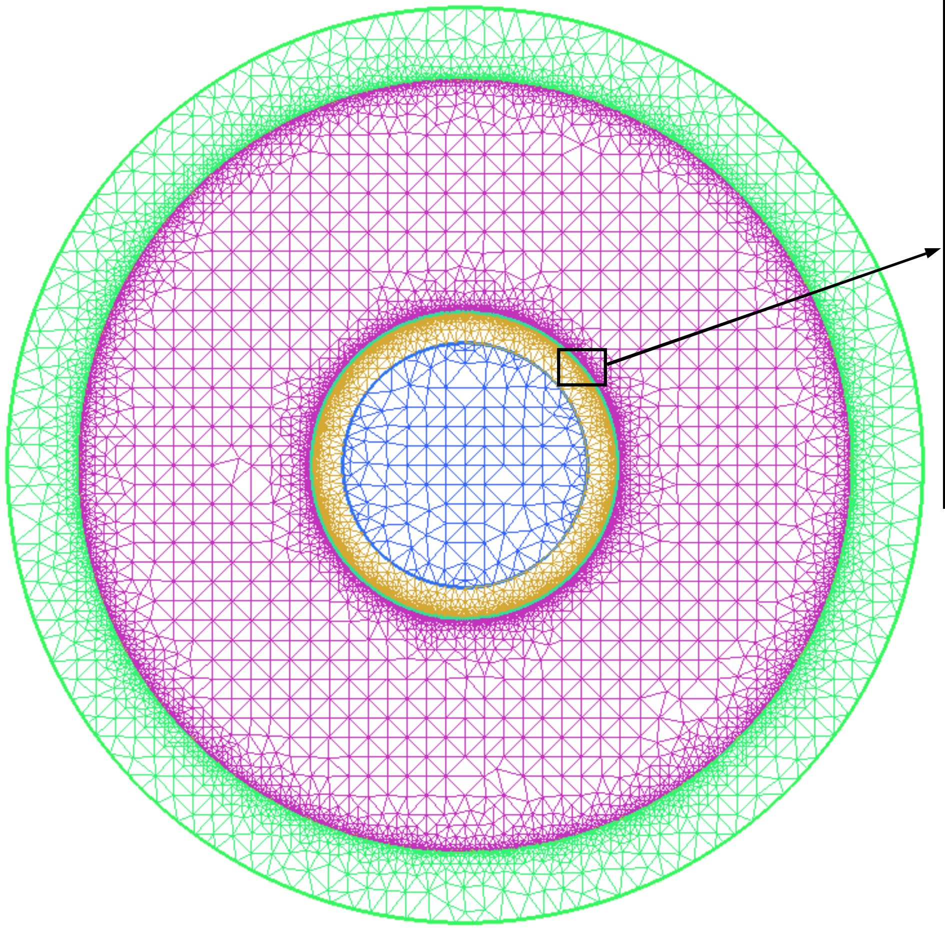
Better geometry representation with unstructured finite elements

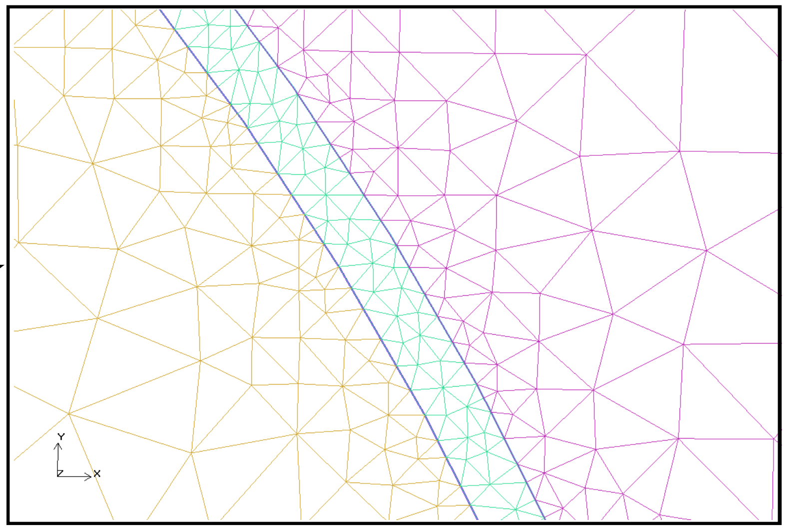




Extremely fine spatial mesh required near material interfaces for SGEMP analysis

Coaxial cable

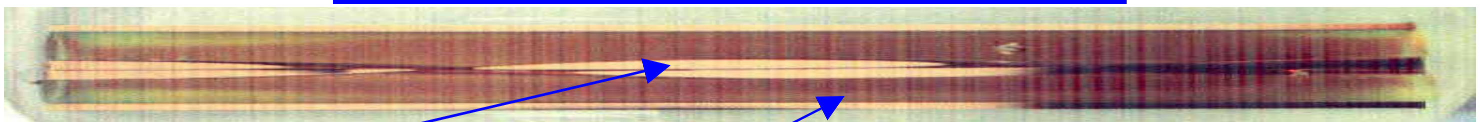




Resolving steep gradients in electron distribution near conductor/dielectric interfaces key to accurate solution

Cable SGEMP Analysis of a Twisted Shielded Pair (TSP) Coaxial Cable

cross sectional view of a TSP cable

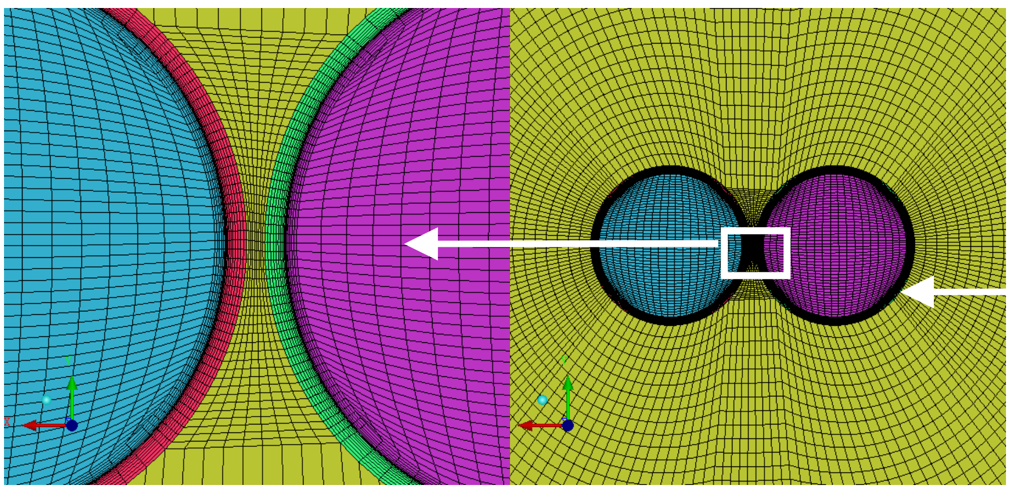


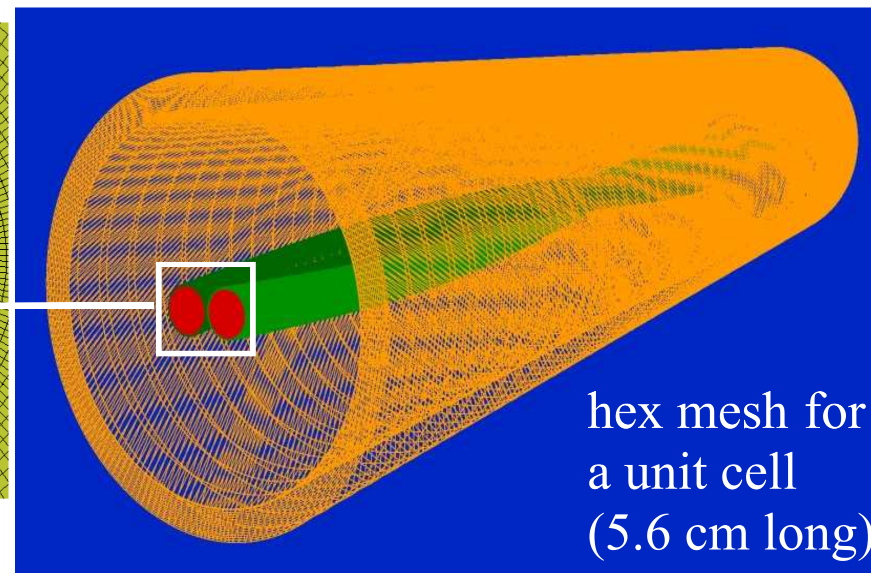
copper conductors

Dielectric (scotch cast)

aluminum or copper shield

hex mesh cross sections





μm-size elements near the center conductors

Discrete equations may be solved in different ways

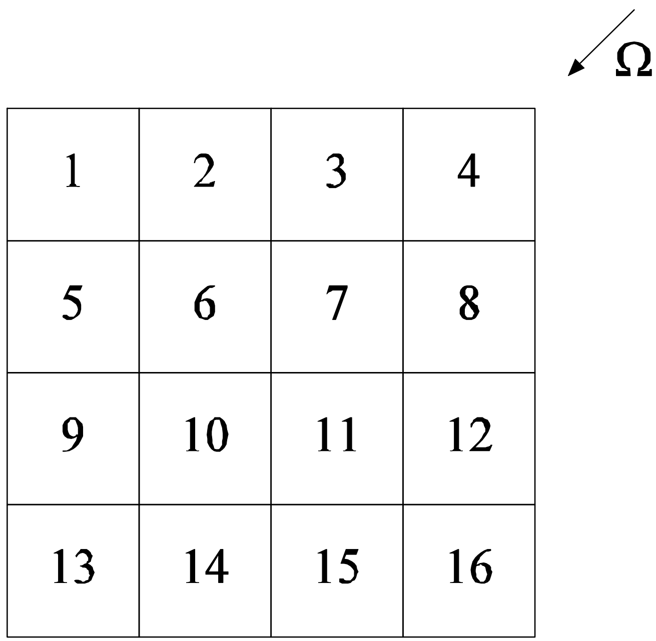
Conventional Source Iteration

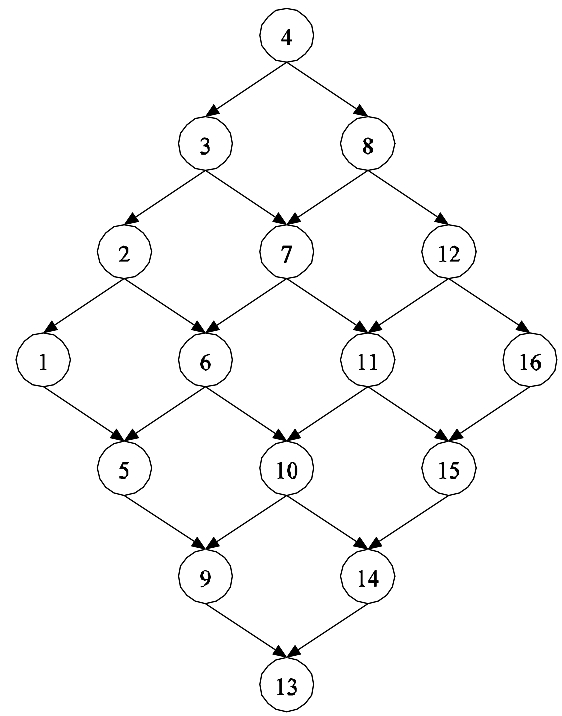
First-order forms: scattering sources are fixed during an iteration (directions decoupled)

CEPTRE

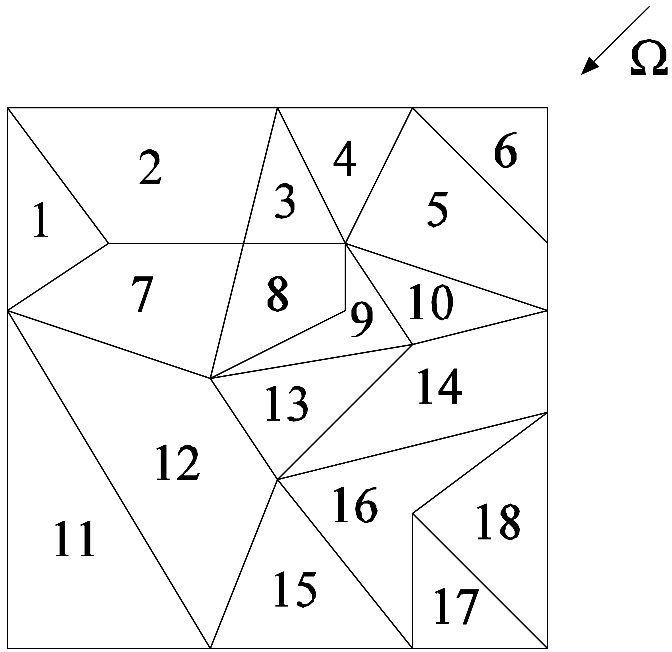
Second-order forms: all terms simultaneously solved (huge matrix)

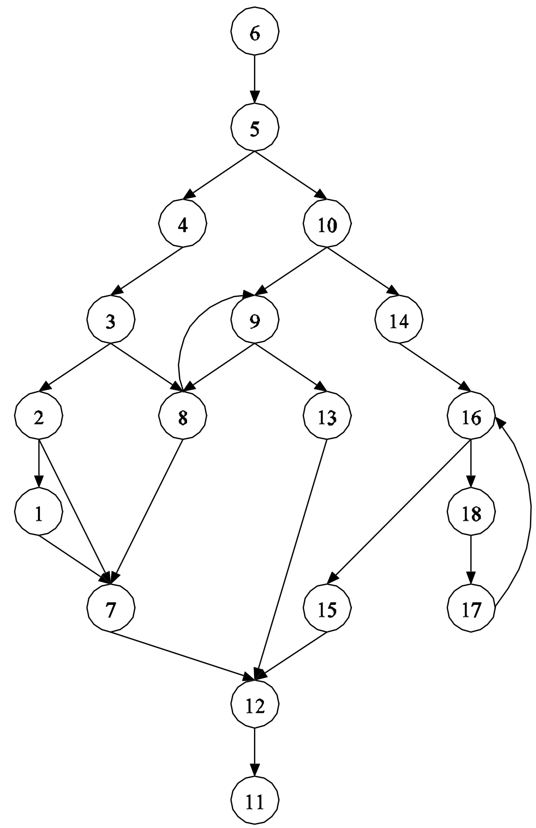
Sweeps of Structured Meshes





Sweeps of Unstructured Meshes





Parallel Sweeps of Unstructured Meshes

- Mesh decomposition
- Eliminate cycles in sweep graph
- Sweep ordering
- Communication pattern
- Violations of sweep graph
- Iterative preconditioners

The main problem for parallel sweeps is the struggle for concurrency!

Second-order forms

Even-parity equation:

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

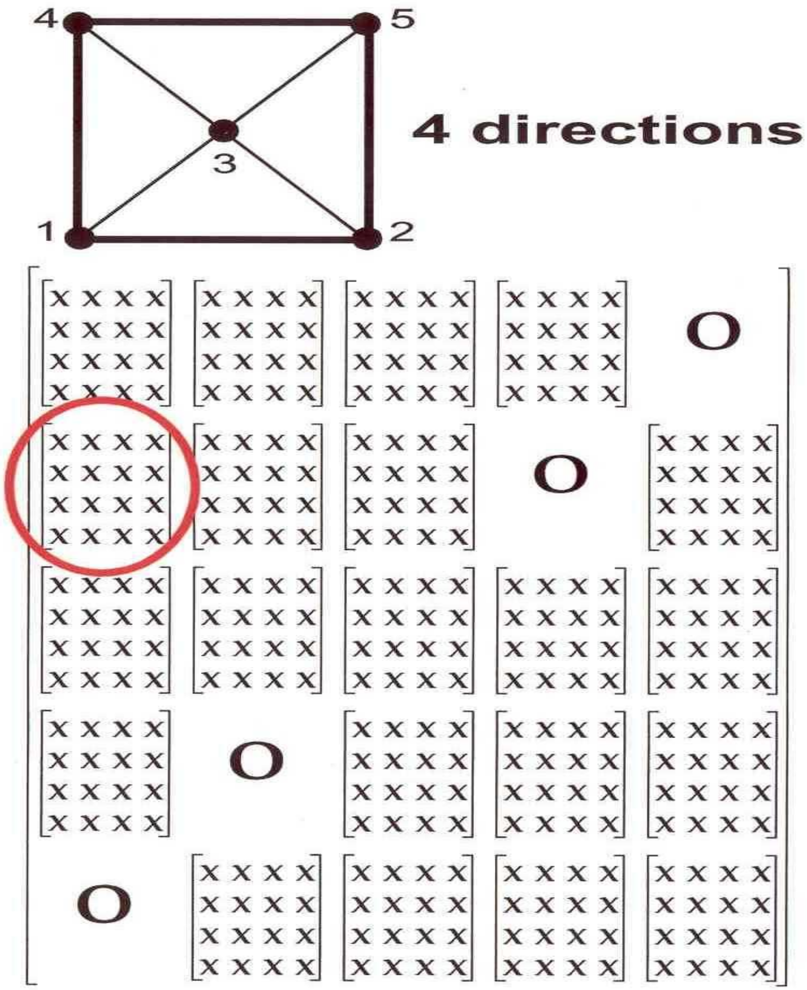
Odd-parity equation:

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

Self-adjoint angular flux (SAAF) equation:

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

Second-order matrix



- Sparse block matrix
- Symmetric Positive Definite System
- Number of block rows:
  - N_{nodes}
- Block size
  - $N_{directions}xN_{directions}$
- Blocks are full due to coupling from scattering
- Tailor-made for VBR data format
- Storage $\sim(N_{directions})^2 x N_{nodes}$
- Run time $\sim(N_{directions})^2 x (N_{nodes})^{1.5}$

First- and second-order forms exhibit different runtime behaviors

Computing Conditions	1st order		2nd order	
	Time/Source Iteration	**# Iterations**	**Time/CG Iteration**	**# Iterations**
Baseline	$N_D N_E P^{-(d-1)/d}$	$[\ln(1/c_n)]^{-1}$	$N_D^2 N_E P^{-1}$	$\langle \sigma_a h \rangle^{-1}$
Large N_D	$N_D N_E P^{-1}$	$[\ln(1/c_n)]^{-1}$	$N_D^2 N_E P^{-1}$	$\langle \sigma_a h \rangle^{-1}$
KBA Decomposition	$N_D N_E P^{-1}$	$[\ln(1/c_n)]^{-1}$	$N_D^2 N_E P^{-1}$	$\langle \sigma_a h \rangle^{-1}$
Diagonal Preconditioner	N/A	N/A	$(c_1 N_D + c_2 N_D^2) N_E P^{-1}$	$\langle \sigma_a h \rangle^{-1}$
Extended Transport Correction Preconditioner	$N_D^2 N_E P^{-(d-1)/d}$	$[\ln(1/c_{n,eff})]^{-1}$	N/A	N/A

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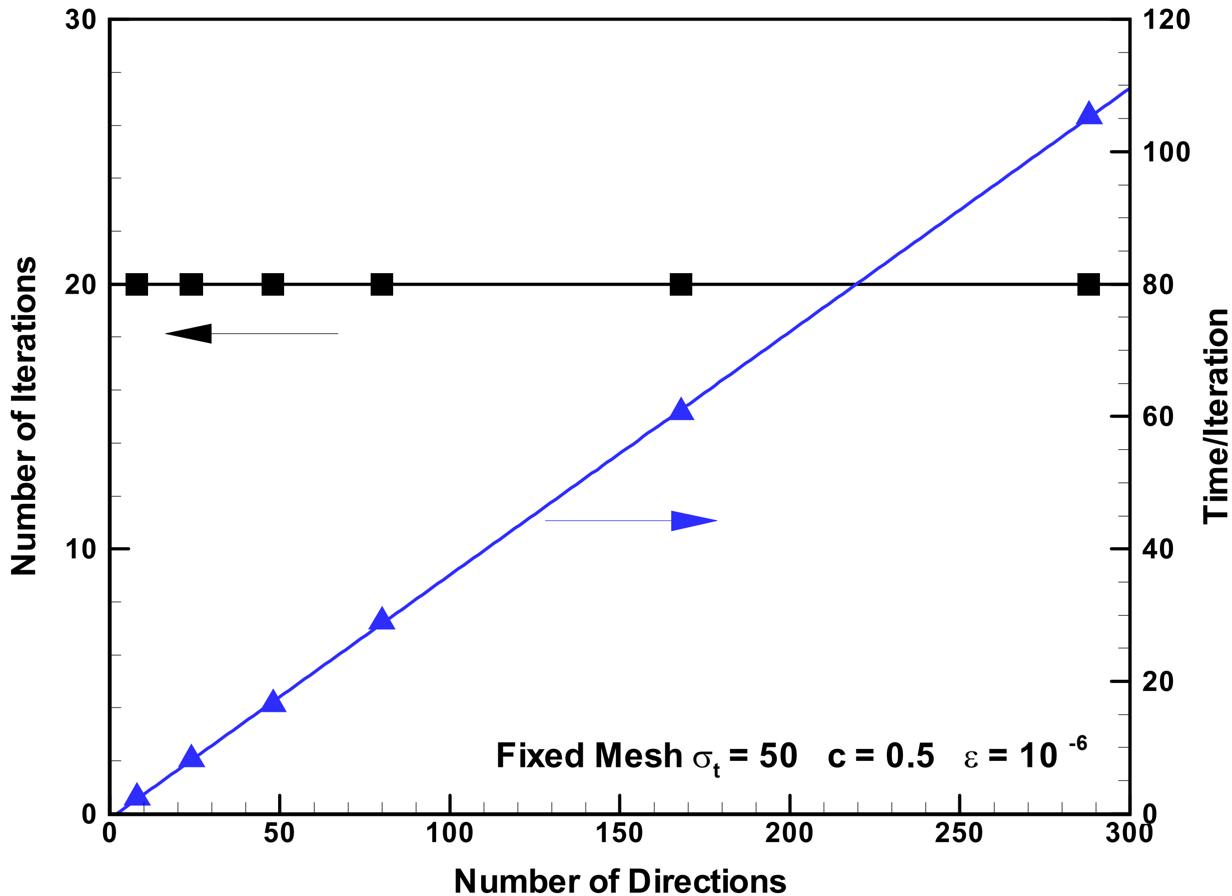
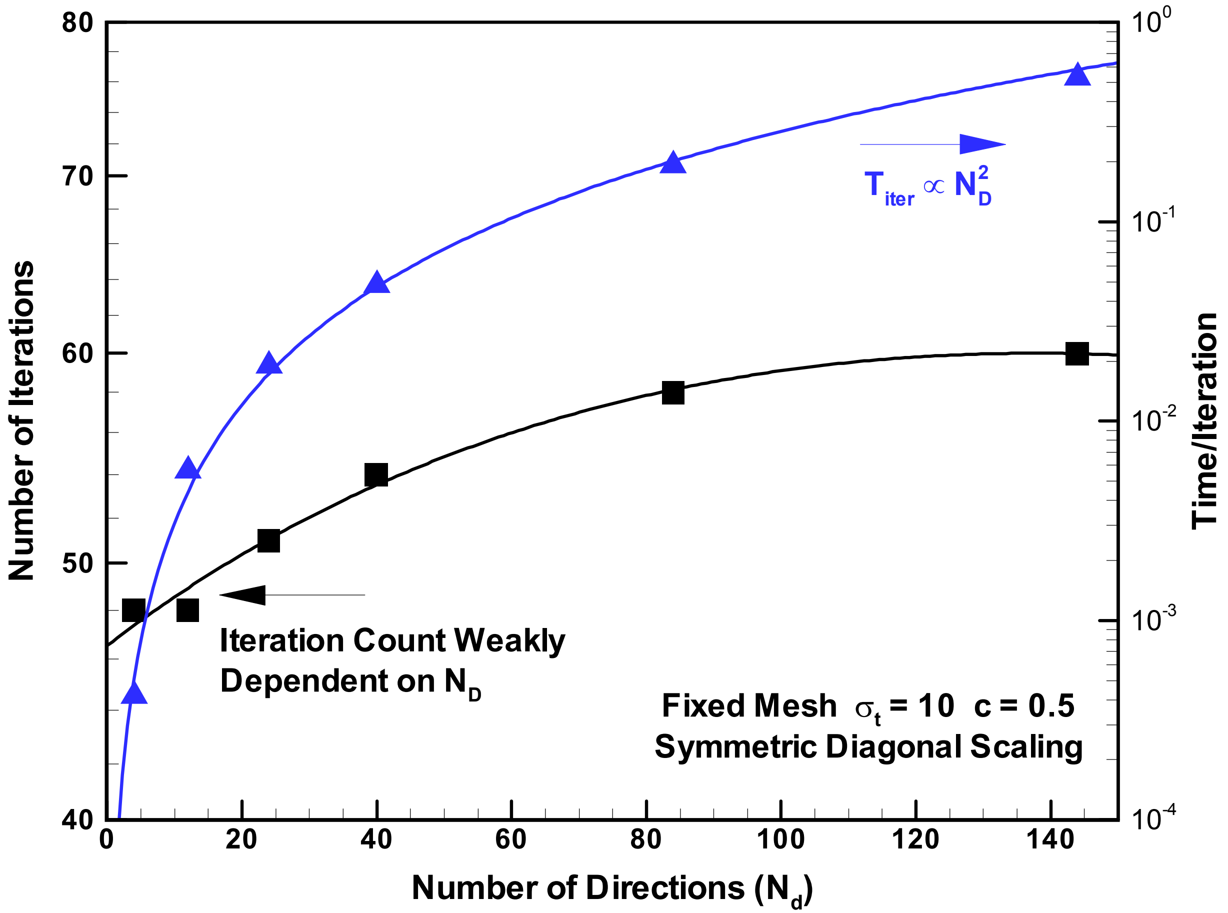
Scaling with number of angles, first-order



Scaling with number of angles, second-order



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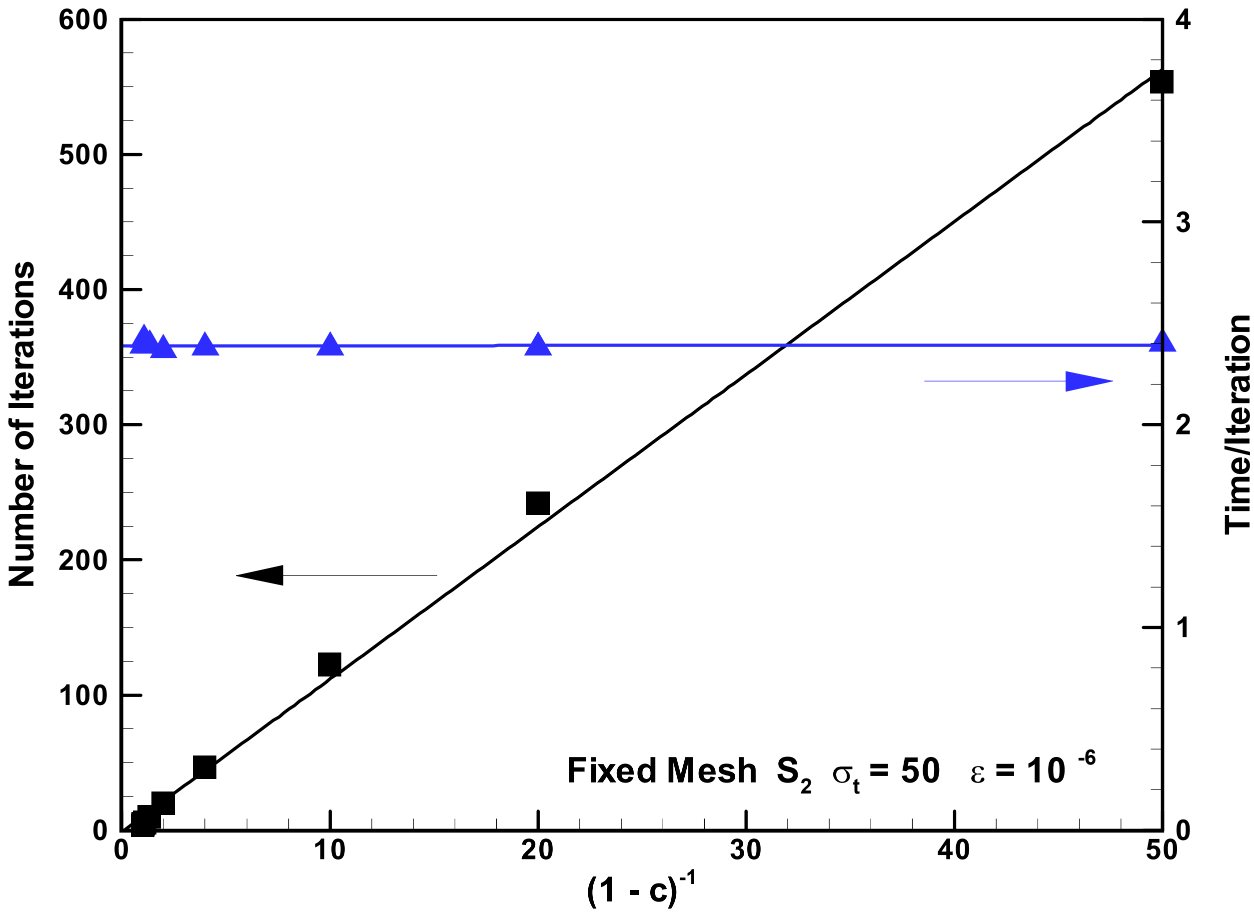
Scaling with scattering ratio, first-order



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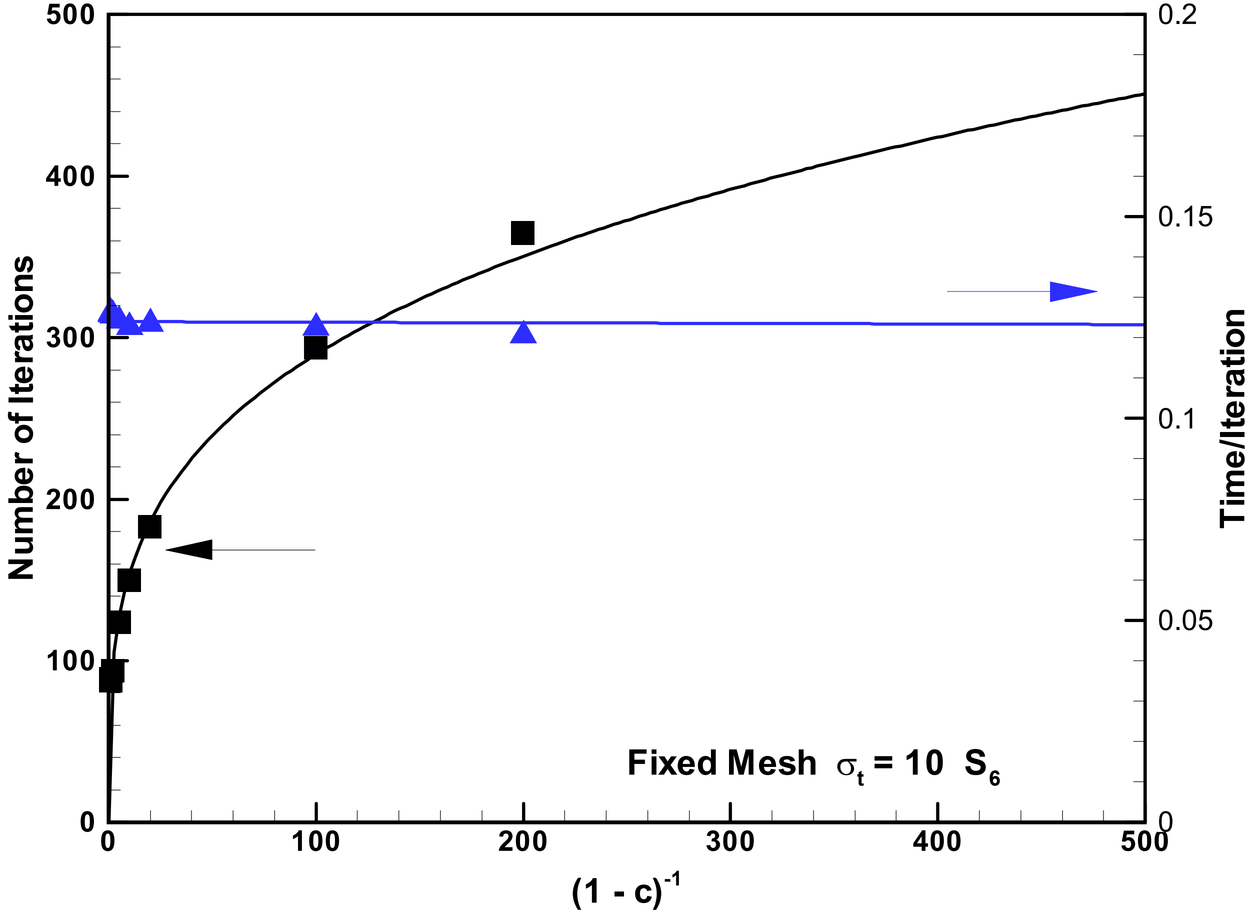
Scaling with scattering ratio, second-order



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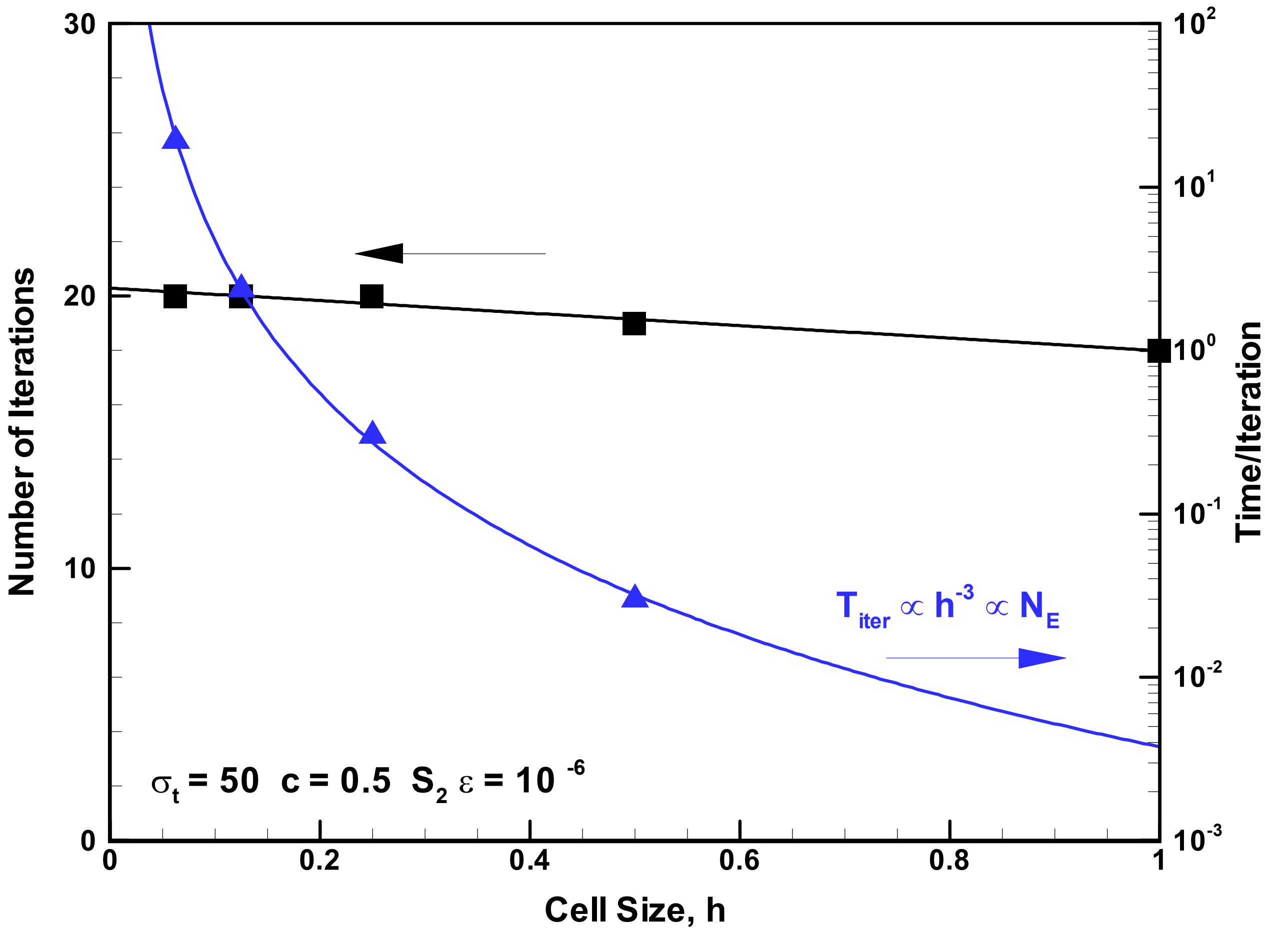
Scaling with cell thickness, first-order (3D)



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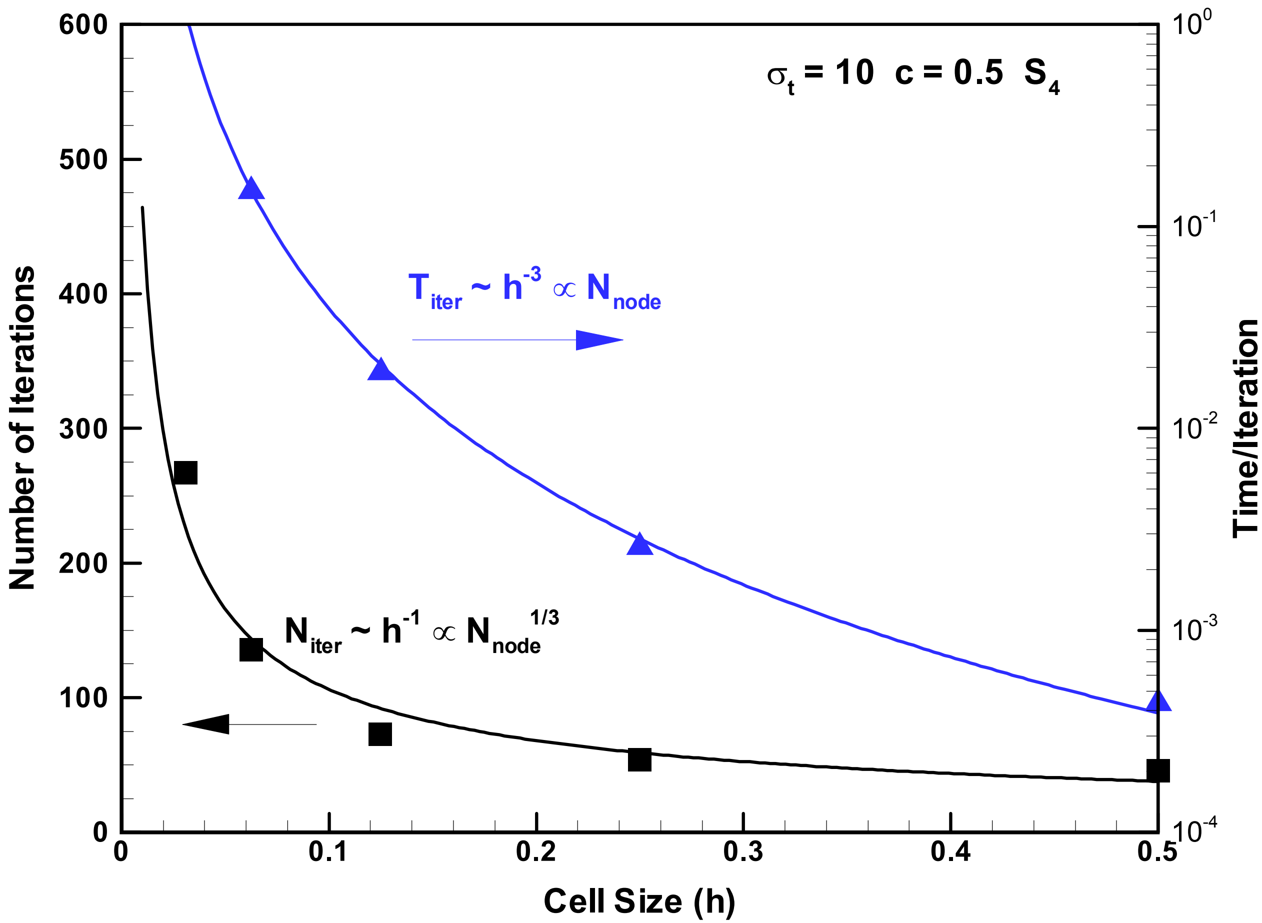
Scaling with cell thickness, second-order (3D)



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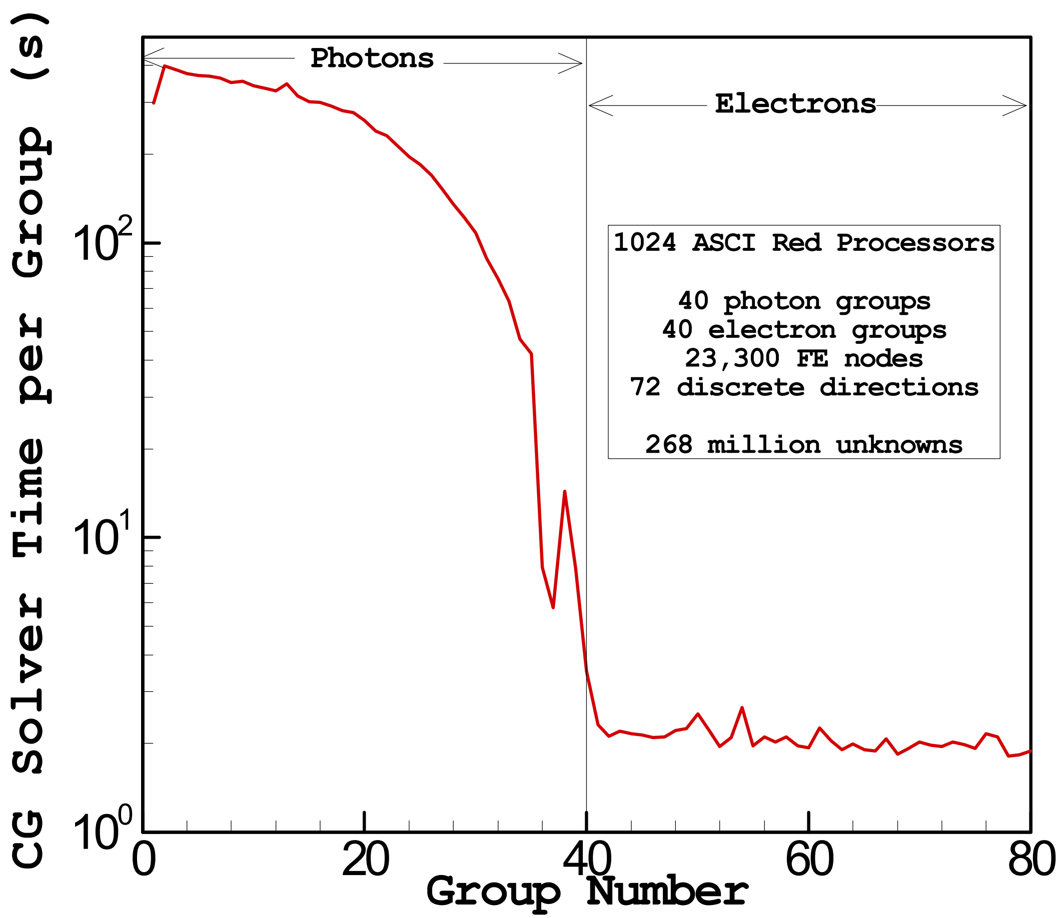
Optical thickness differences for photons/electrons affects second-order performance



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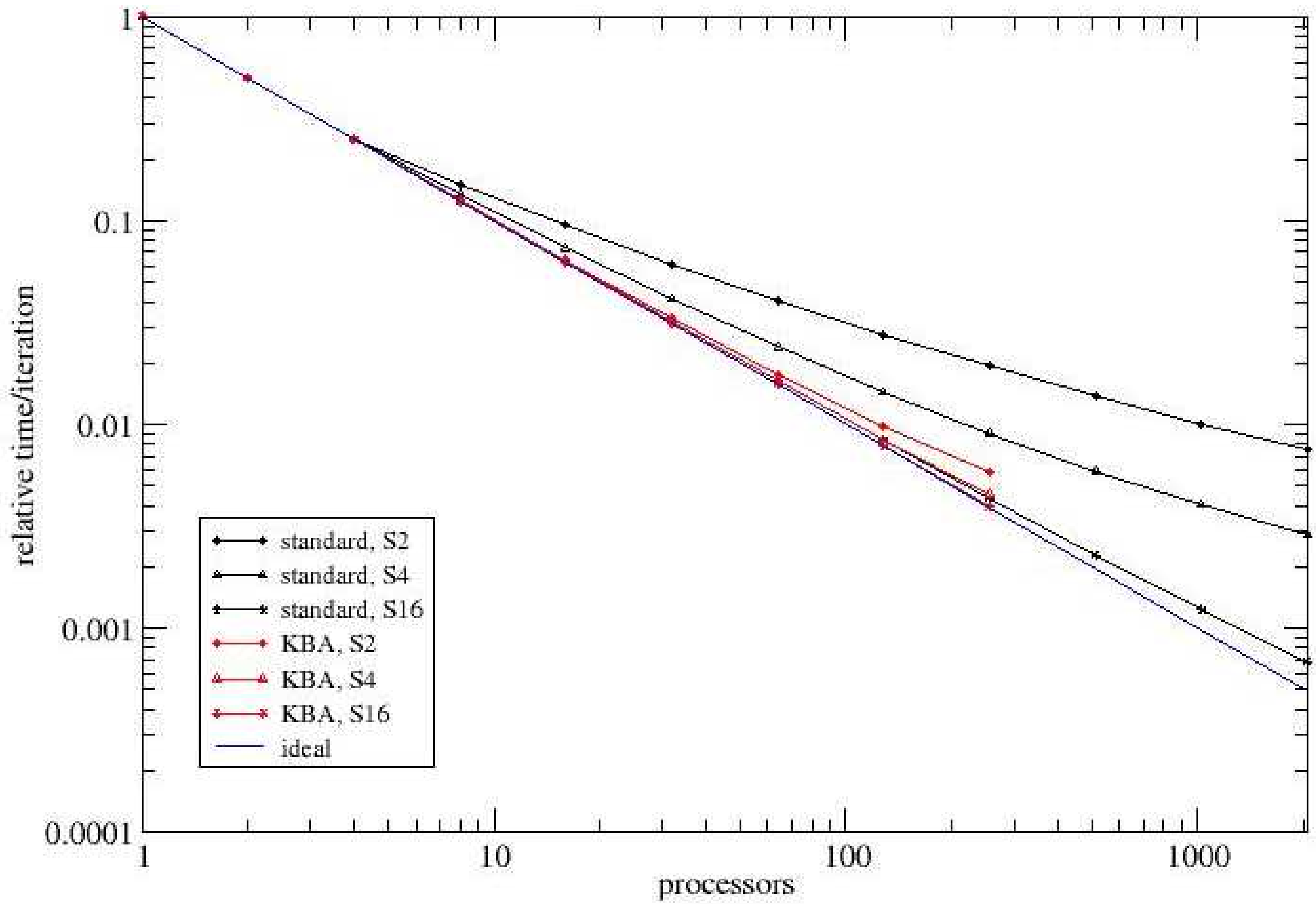
Currently implementing hybrid solver

- First-order solver performs well for optically thin problems
- Second-order solver performs well for optically thick problems
- Proposed solution: Use different solver for each energy group / particle type

First-order theoretical parallel scaling (strong)

128x128 mesh, S16, comm ratio = 0



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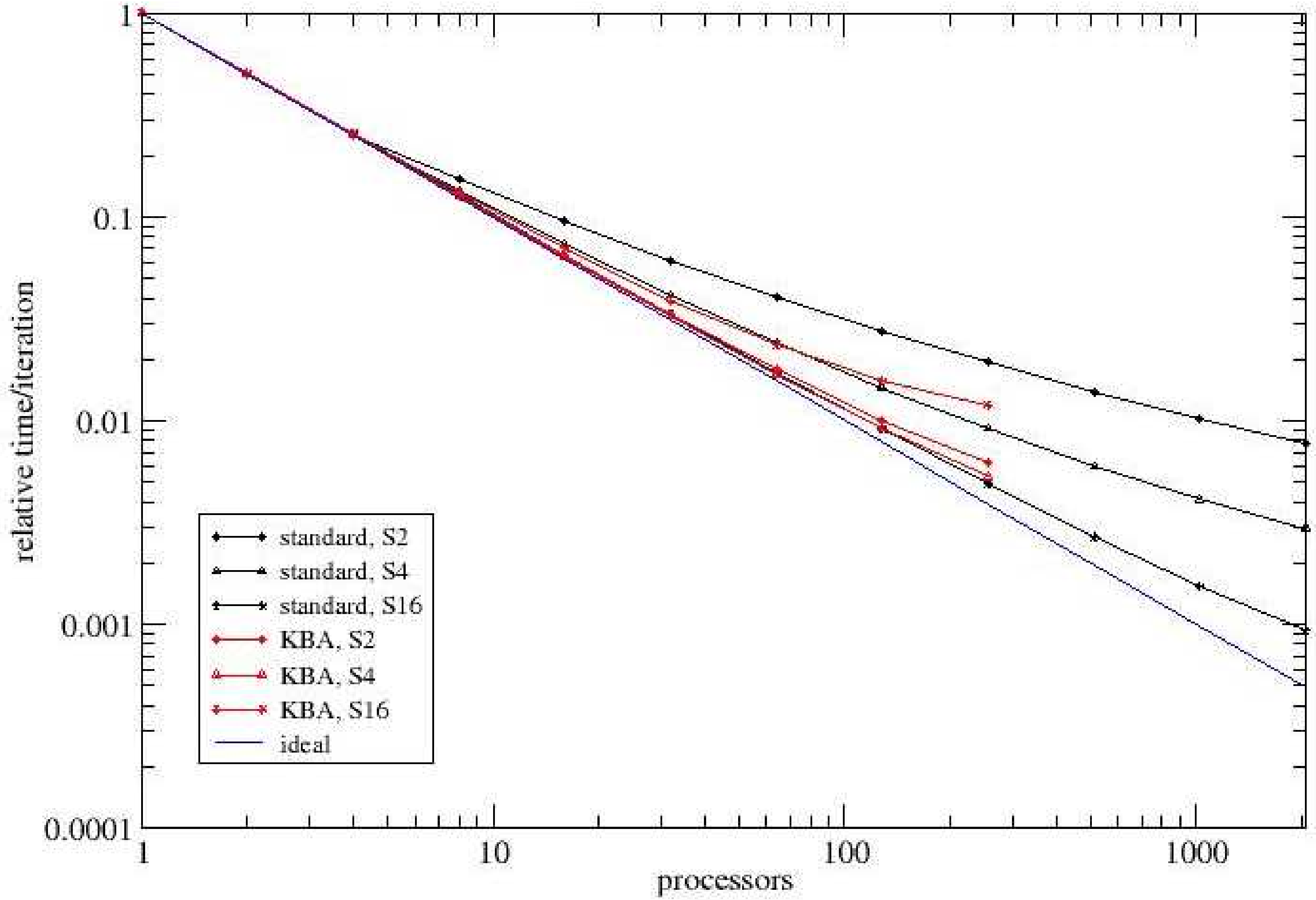
First-order theoretical parallel scaling (strong)

128x128 mesh, S16, comm ratio = 1



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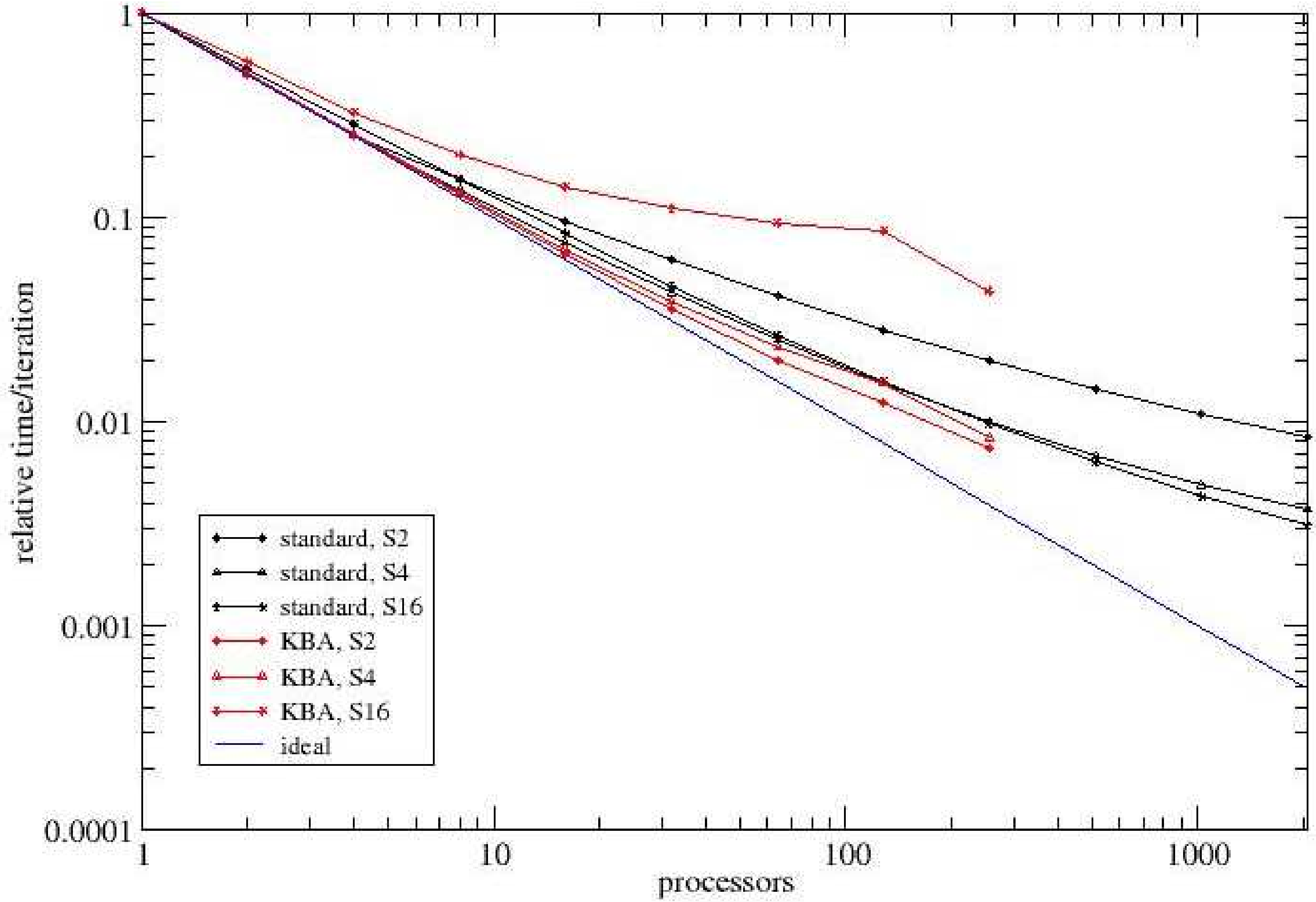
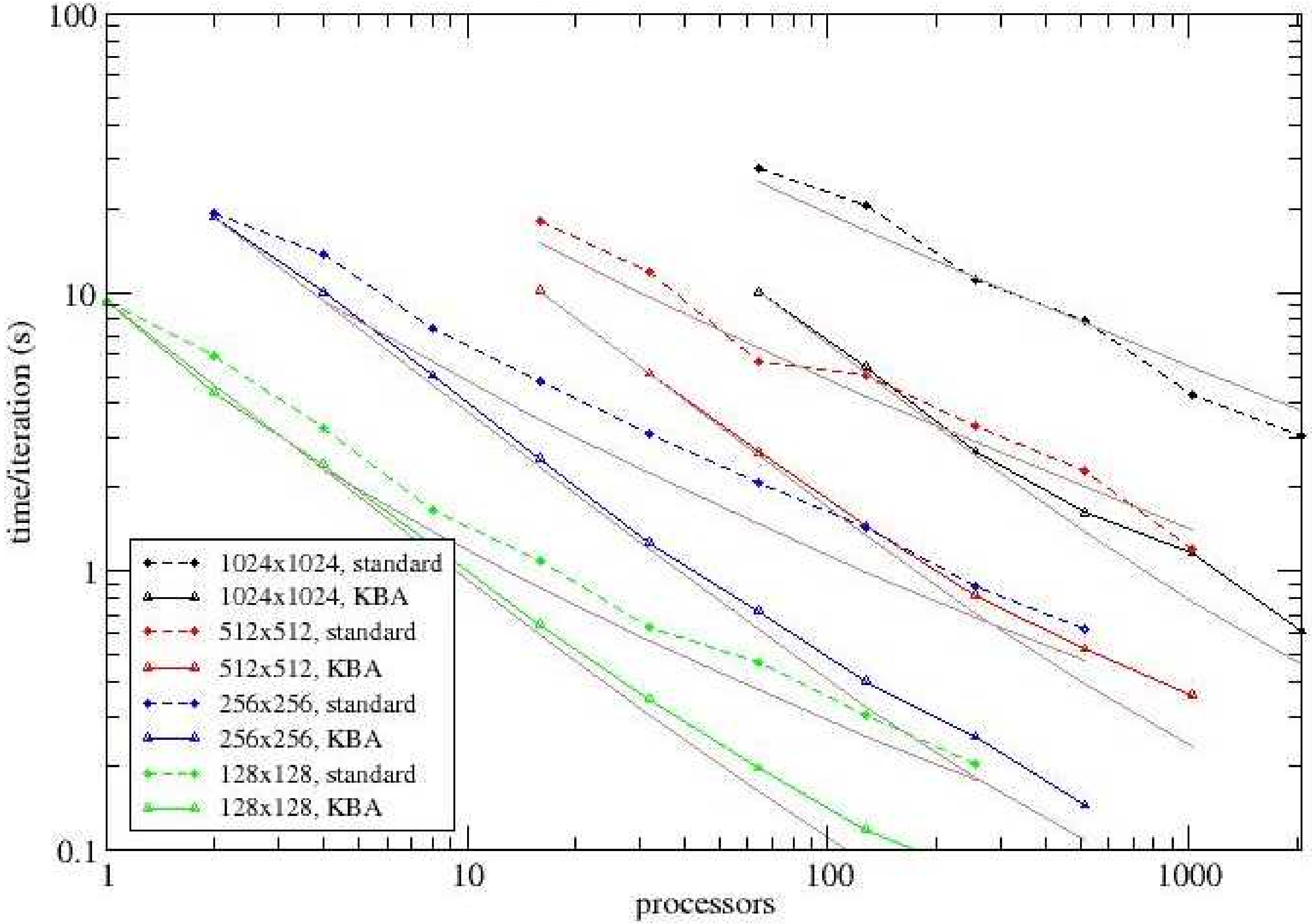
First-order theoretical parallel scaling (strong)

128x128 mesh, S16, comm ratio = 10



Sceptre first-order parallel scaling (strong)

tri3 meshes, S8/S2, Red Storm



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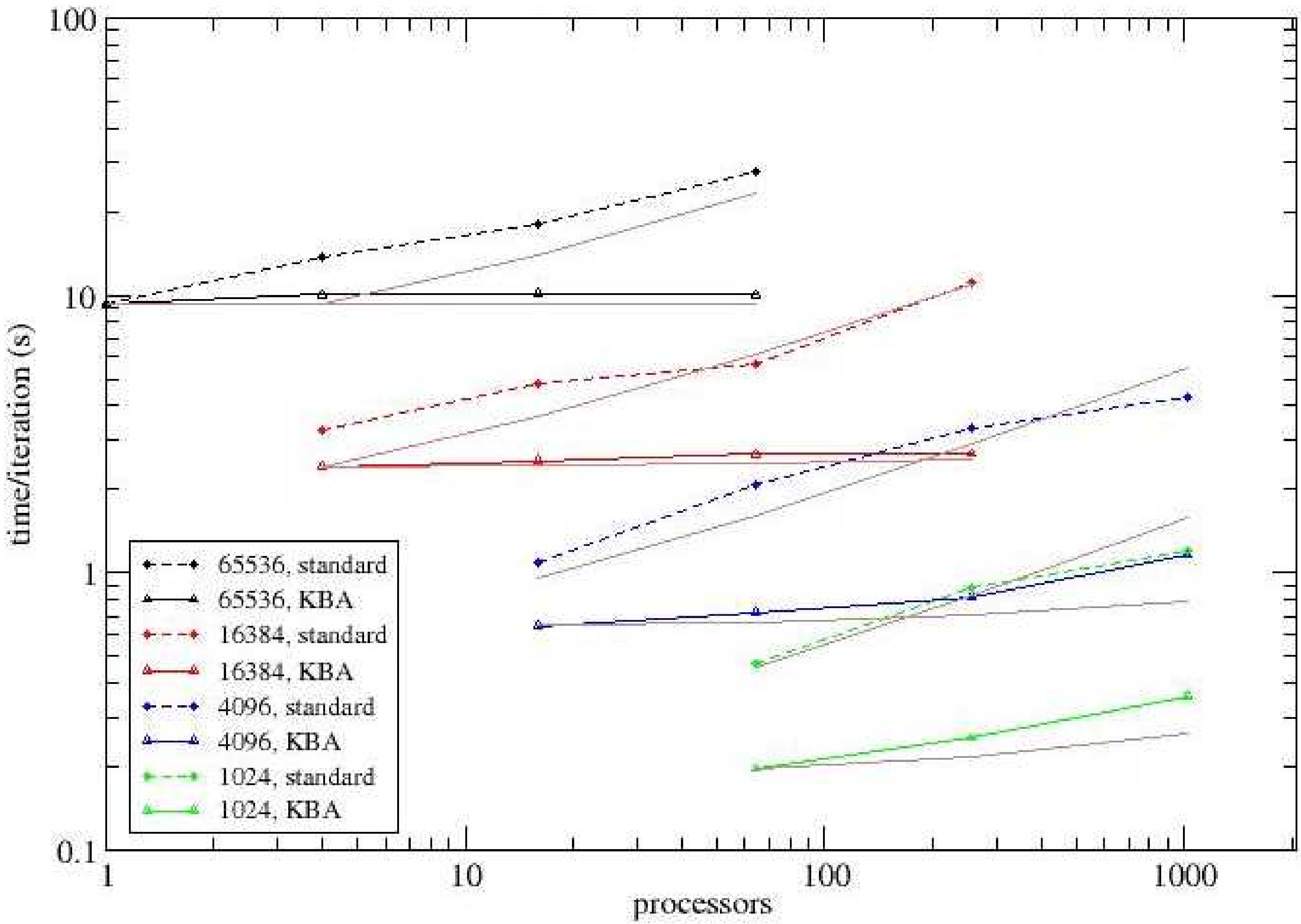
Sceptre first-order parallel scaling (weak)

tri3 meshes, S8/S2, Red Storm



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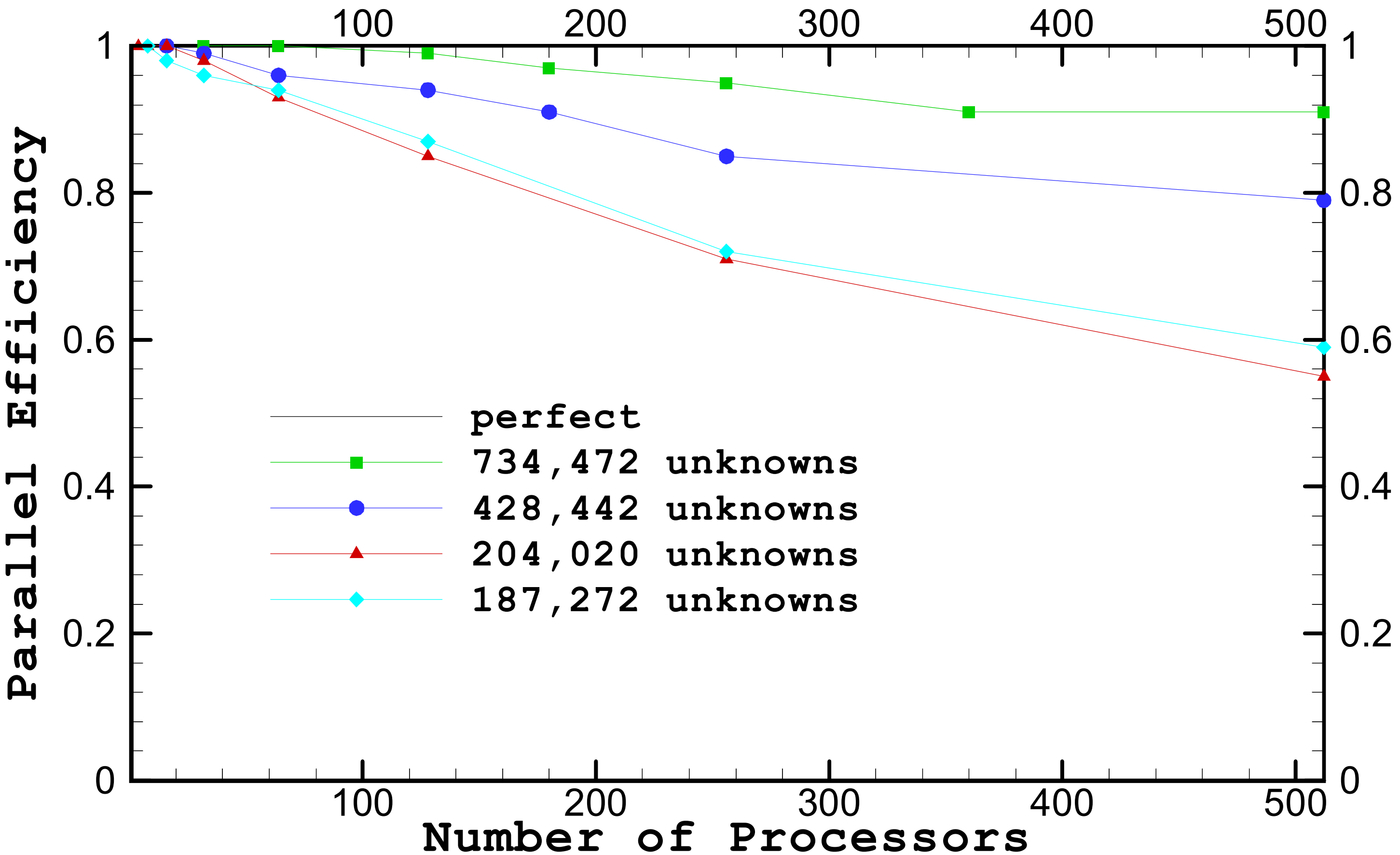
CEPTRE parallel scaling, second-order



V & V: Verification and Validation

- VERIFICATION: The process of determining that a computational software implementation correctly represents a model of a physical process (Are we solving the equations right?)
- VALIDATION: The process of determining the degree to which a computer simulation is an accurate representation of the real world for a specific application (Are we solving the right equations? Is the right physics modeled?)

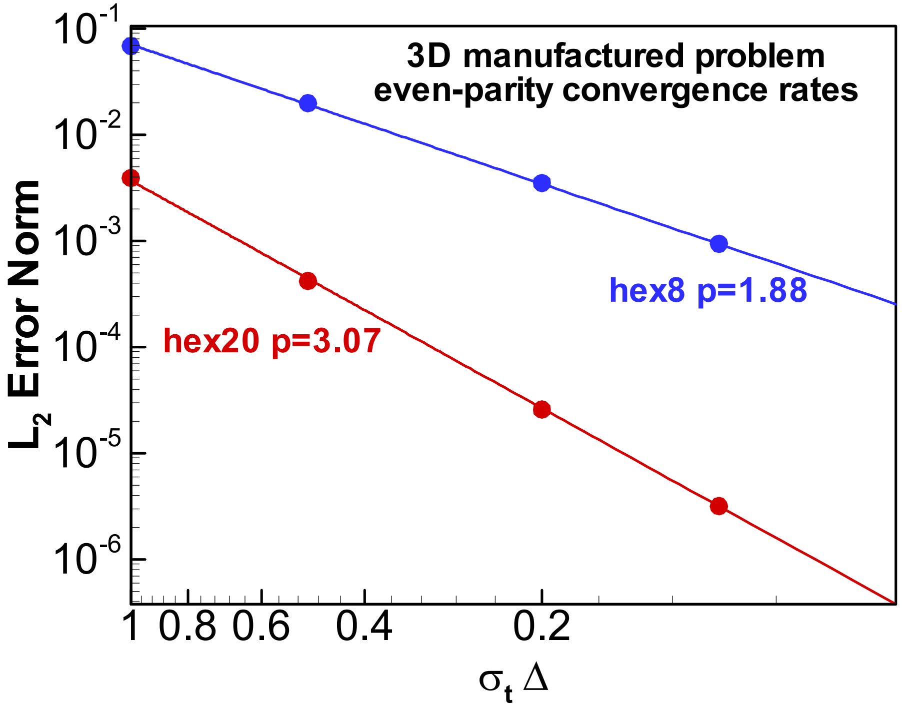
Verification: Method of Manufactured Solutions (MMS)

- Need: closed-form/exact solutions useful for code verification
- Challenge: limited number of closed-form solutions to the transport equation
- MMS approach: specify ("manufacture") a solution and use transport equation to determine the source term and boundary conditions; use these as code inputs
- Unlimited number of closed-form solutions available with this approach

Instead of searching for a (possibly non-closed-form) solution to a problem, we find a problem to a solution

3D Manufactured Solution Example

- Unit cube
- Unit total cross section
- Linearly anisotropic scattering, c=1/2
- S8 quadrature
- Tet4 and Tet10 elements

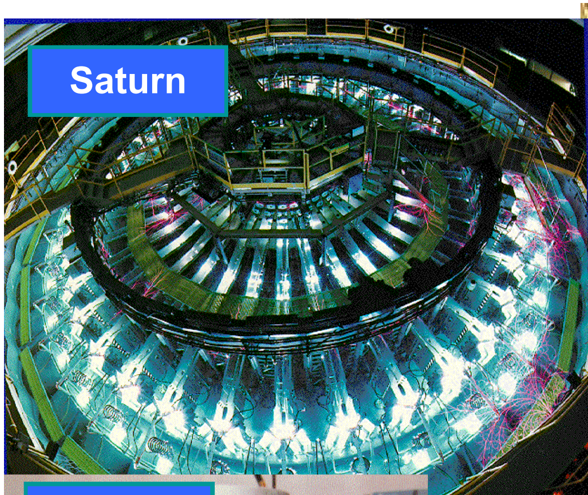


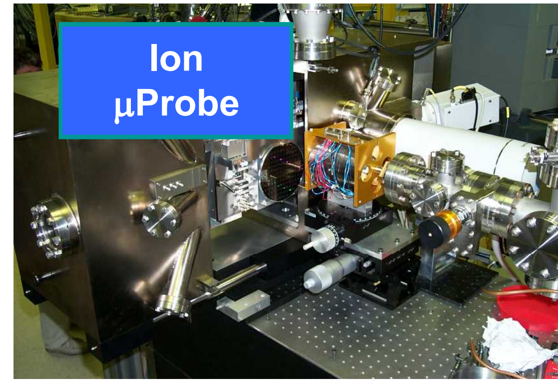
Assumed solution: $\Phi(x,y,z,\mu_z) = \mu_z^2 e^{-x} e^{-y} e^{-z}$

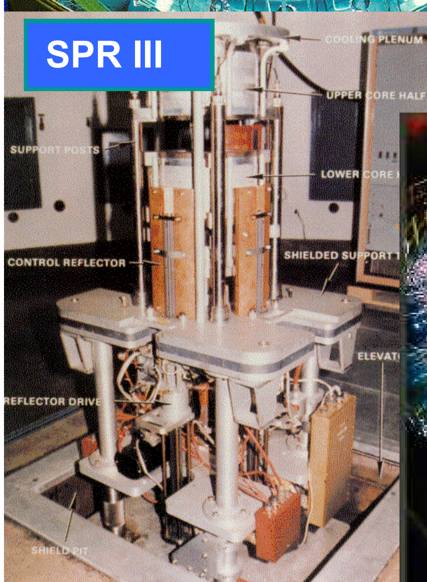
Distributed source: $Q(x,y,z,\mu_x,\mu_y,\mu_z) = \left[\mu_z^2(1-\mu_x-\mu_y-\mu_z) - \frac{1}{6}\right] e^{-x} e^{-y} e^{-z}$

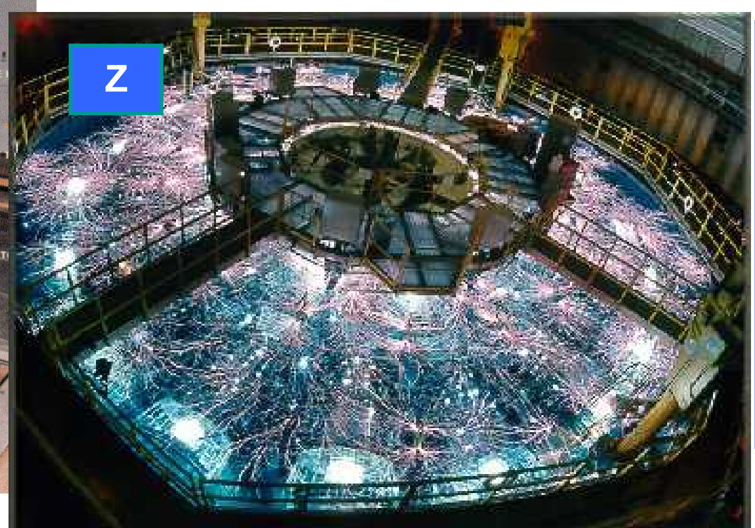
Boundary conditions: $\Phi_b(x,y,z,\mu_z) = \mu_z^2 e^{-x} e^{-y} e^{-z},\ for\ (x,y,z) \in \partial V$

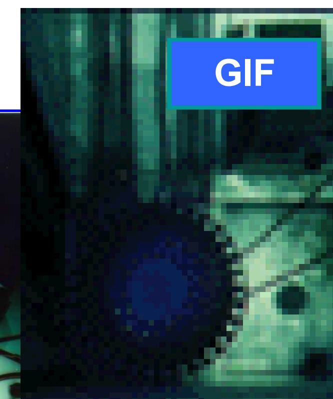
Sandia radiation facilities used for testing, research, and code validation





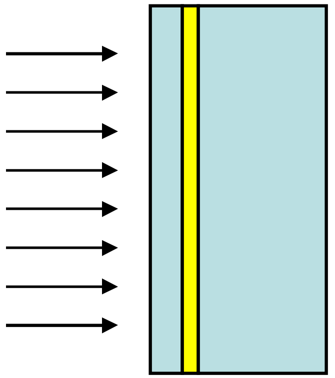


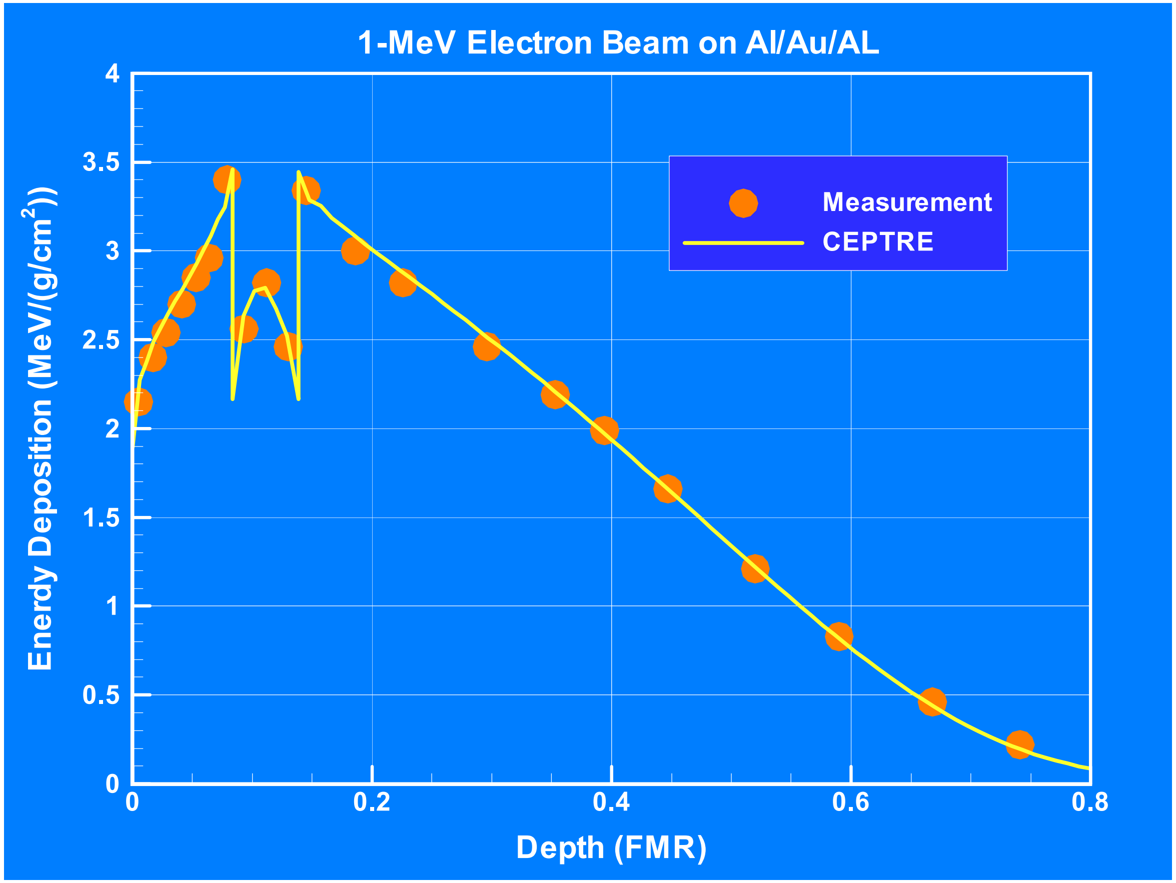




Sandia National Laboratories

CEPTRE 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)

Future Work

- Couple first-order and second-order transport solvers
- Develop multi-stage preconditioning strategy using AMG (Algebraic MultiGrid) (tools available in Trilinos)
- Coarse photon mesh/fine electron mesh
- Develop more efficient parallel strategies
- Compare continuous vs. discontinuous finite elements
- Compare higher-order interpolation functions vs. finer mesh for increasing accuracy
- Compare spherical harmonics vs. discrete ordinates

Summary

- First- and second-order forms have complementary strengths and weaknesses
- Both forms are (being) implemented in CEPTRE/SCEPTRE
- Either form may be used separately, or together as a hybrid solver
- These forms are not restricted to electron/photon problems