SAND2006-5405C

Parallel Discrete Ordinates Methods in the CEPTRE Project

Shawn D. Pautz
Radiation Transport Department
Sandia National Laboratories

PHYSOR 2006
Vancouver, BC, Canada
September 10-14, 2006

SAND 2006-????
Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

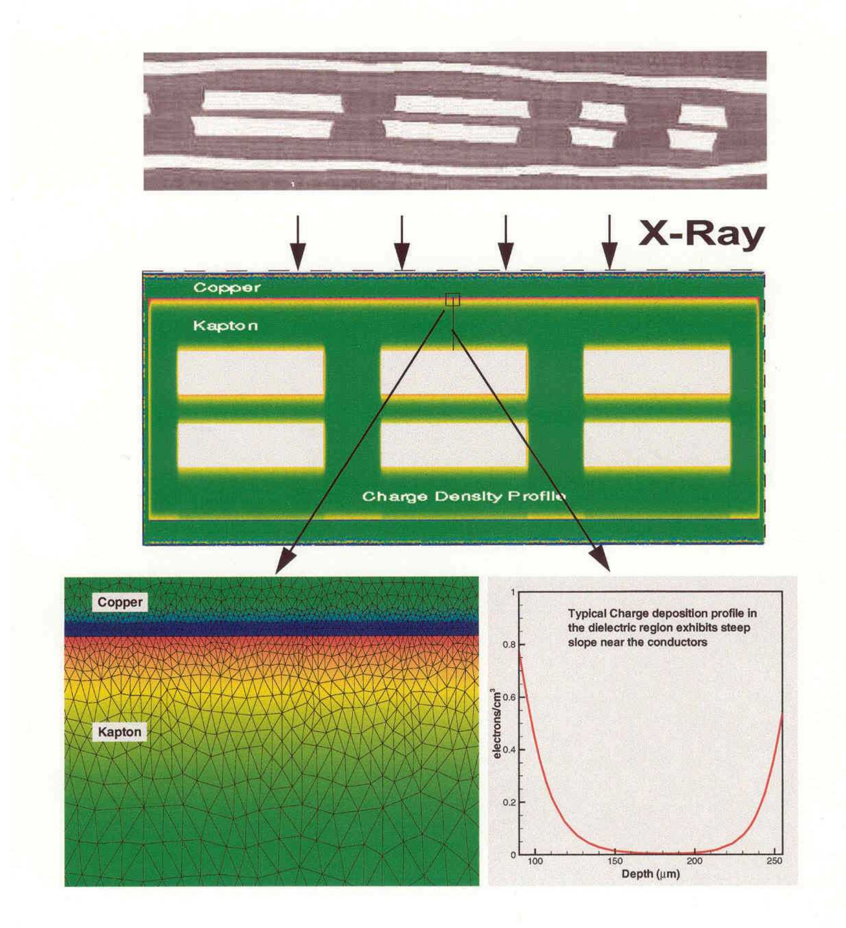
Sandia National Laboratories

Outline

- Overview of CEPTRE
- First- and Second-Order Methods
- Algorithmic Details
- Comparison of First- and Second-Order Behaviors
- Results
- Summary

Cable SGEMP Simulation Needs

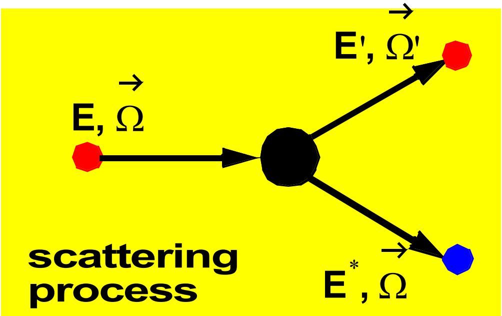
- Requires accurate resolution of dose-enhancement and charge profiles near conductor/dielectric interfaces
  - Results in extremely small mesh cells near the material interfaces
  - Use of higher-order finite elements
  - Ill-conditioned matrix for photon-transport



CEPTRE Code

(**C**oupled **E**lectron **P**hoton **T**ransport for **R**adiation **E**ffects)

- Time-independent, deterministic, coupled electron-photon transport code on unstructured mesh
- 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* approximation in direction
  - *Finite-Element* approximation in space



Sandia National Laboratories

Forms and Solution 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:

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

Conventional Source Iteration

Outer Iteration over Energy Groups

Inner Iteration over Directions

Direct or Iterative Solutions of Space

CEPTRE

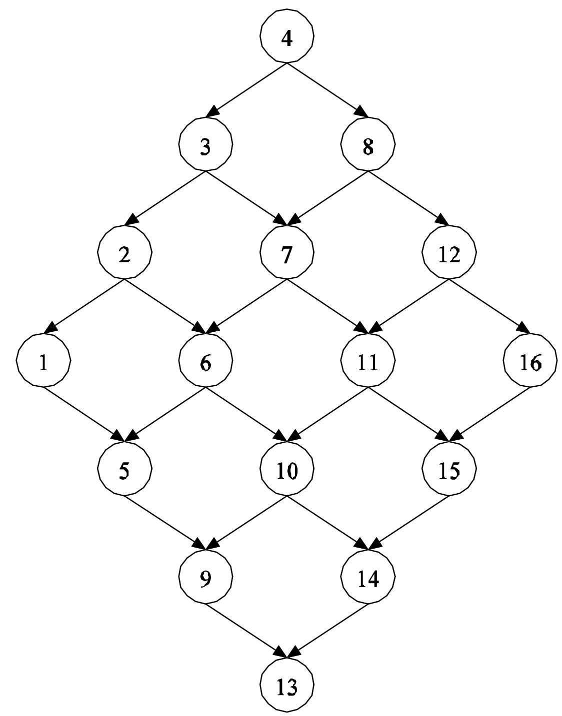
Outer Iteration over Energy Groups

Simultaneous Space-Direction Solutions (Iterative)

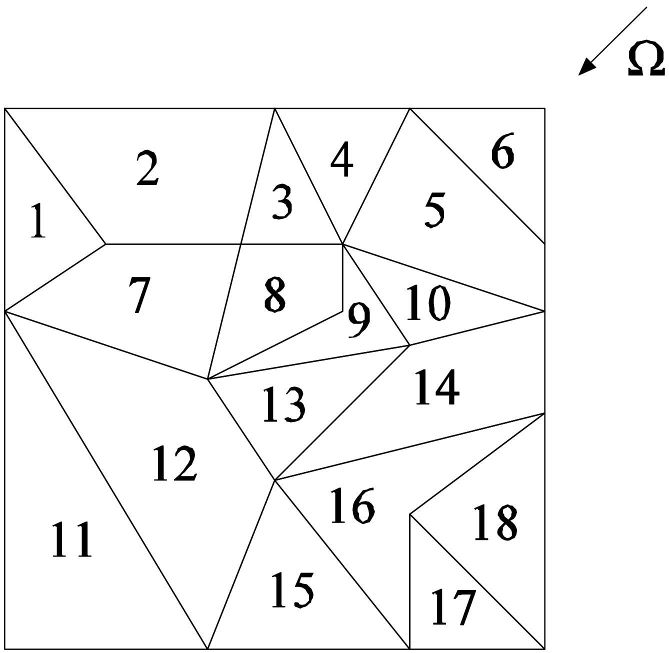
Sweeps of Structured Meshes

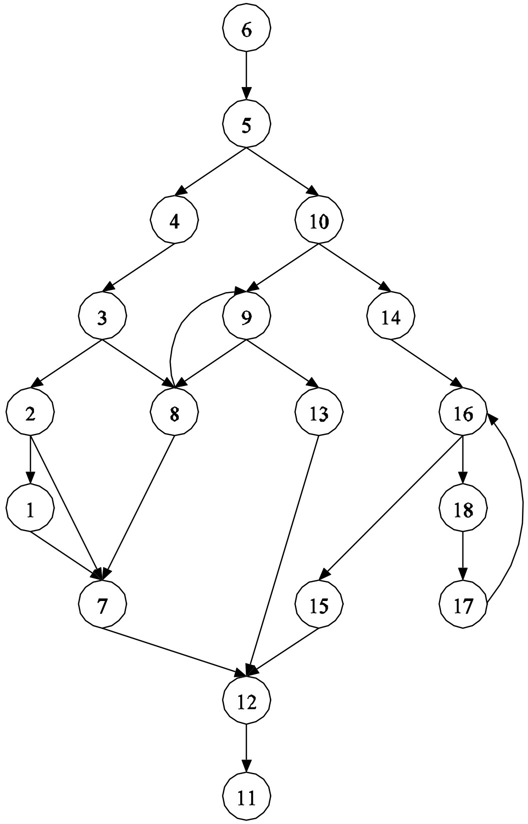
Ω

1	2	3	4
5	6	7	8
9	10	11	12
13	14	15	16



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

Second-order forms

Even-parity equation:

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

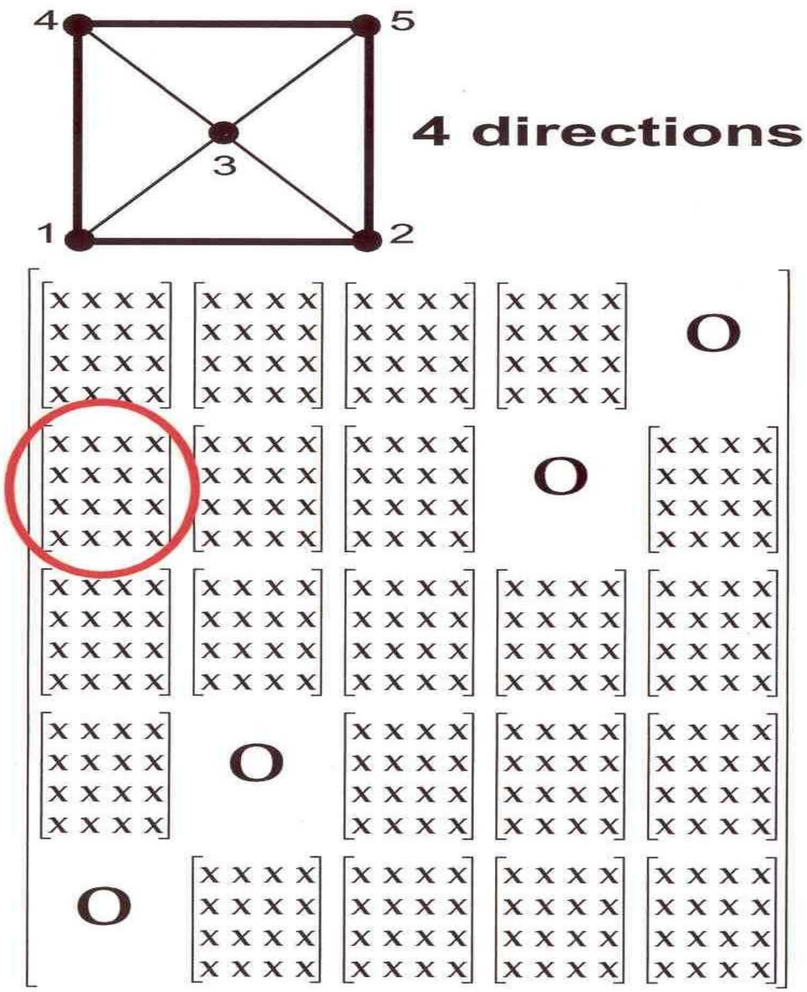
Odd-parity equation:

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

Self-adjoint angular flux (SAAF) equation:

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

Second-order matrix

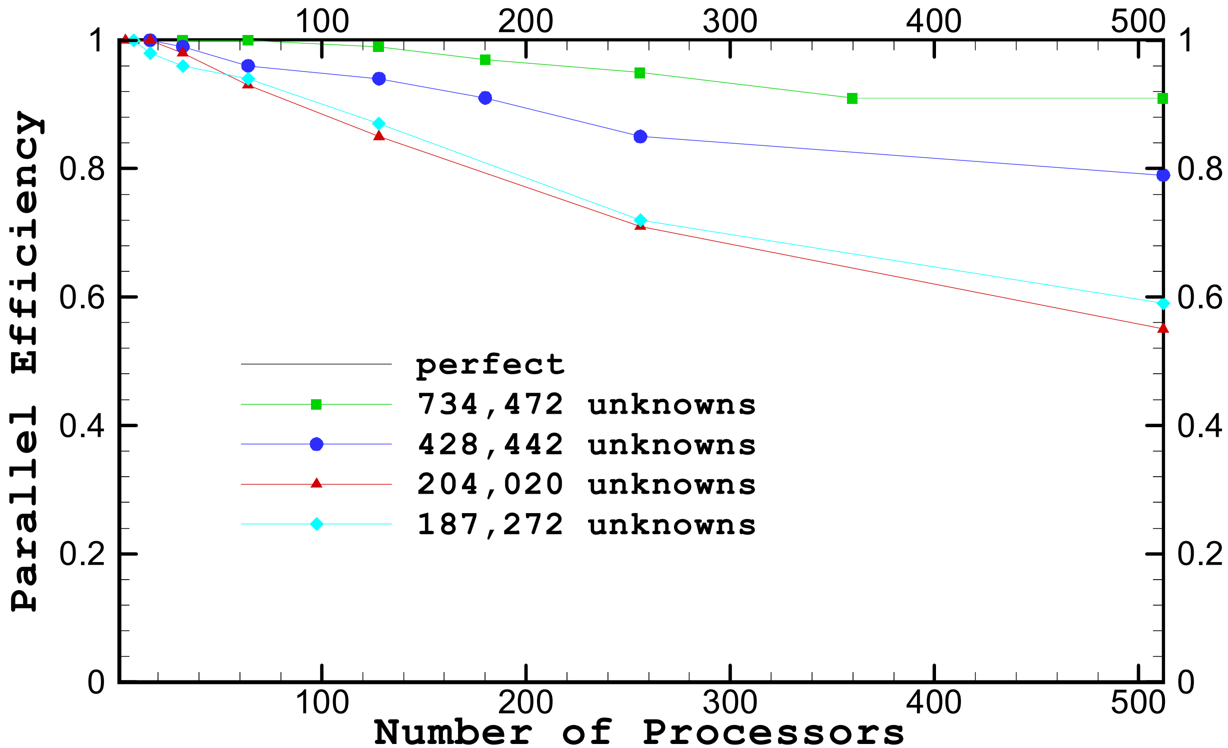


- Sparse block matrix
- Symmetric Positive Definite System
- Number of block rows:
  - N_{nodes}
- Block size
  - $N_{directions} x N_{directions}$
- Blocks are full due to coupling from scattering
- Tailor-made for VBR data format
- Storage $\sim (N_{directions})^2 x N_{nodes}$
- Run time $\sim (N_{directions})^2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

First- and second-order forms exhibit different behaviors

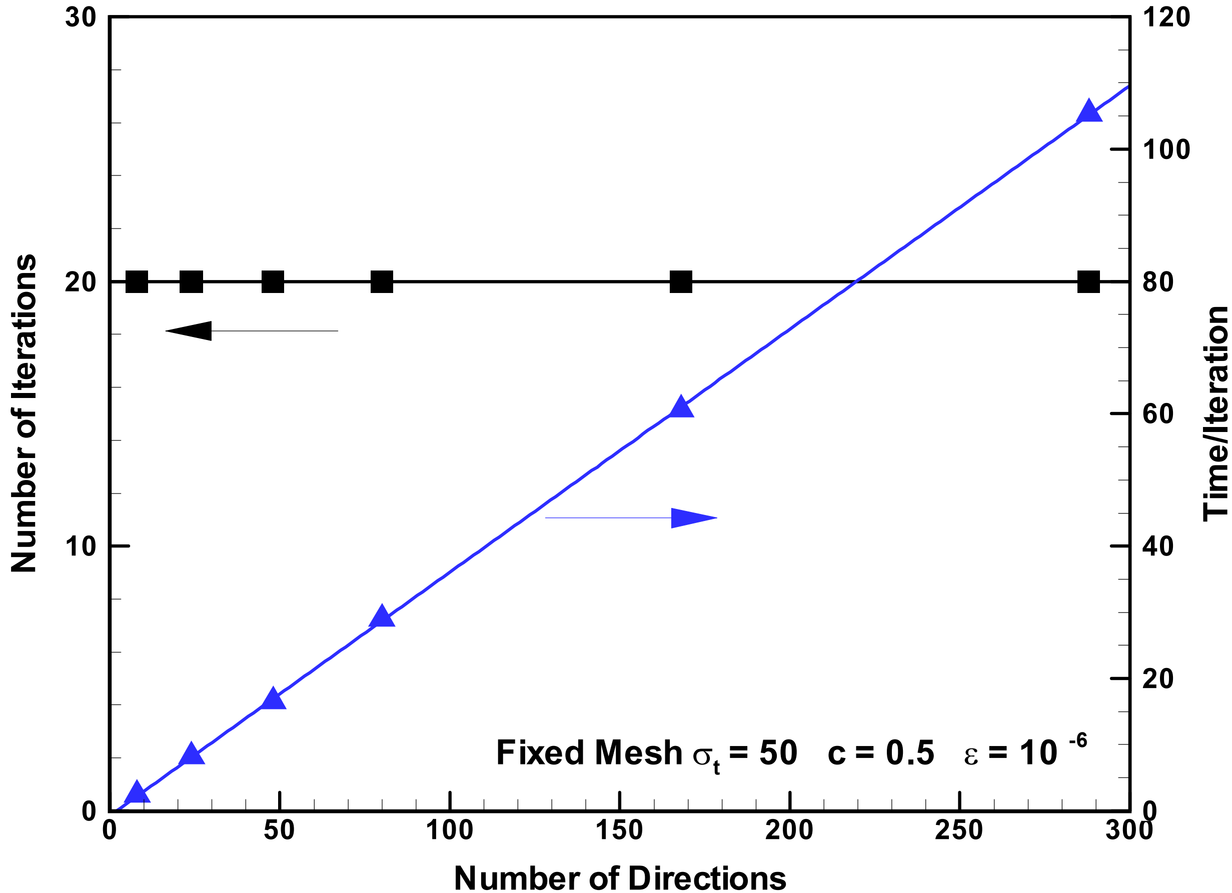
Computing Conditions	1st order		2nd order	
	Time/Source Iteration	**# Iterations**	**Time/CG Iteration**	**# Iterations**
Baseline	$N_D N_E P^{-(d-1)/d}$	$[\ln(1/c_n)]^{-1}$	$N_D^2 N_E P^{-1}$	$\langle \sigma_a h \rangle^{-1}$
Large N_D	$N_D N_E P^{-1}$	$[\ln(1/c_n)]^{-1}$	$N_D^2 N_E P^{-1}$	$\langle \sigma_a h \rangle^{-1}$
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

Parallel scaling, second-order

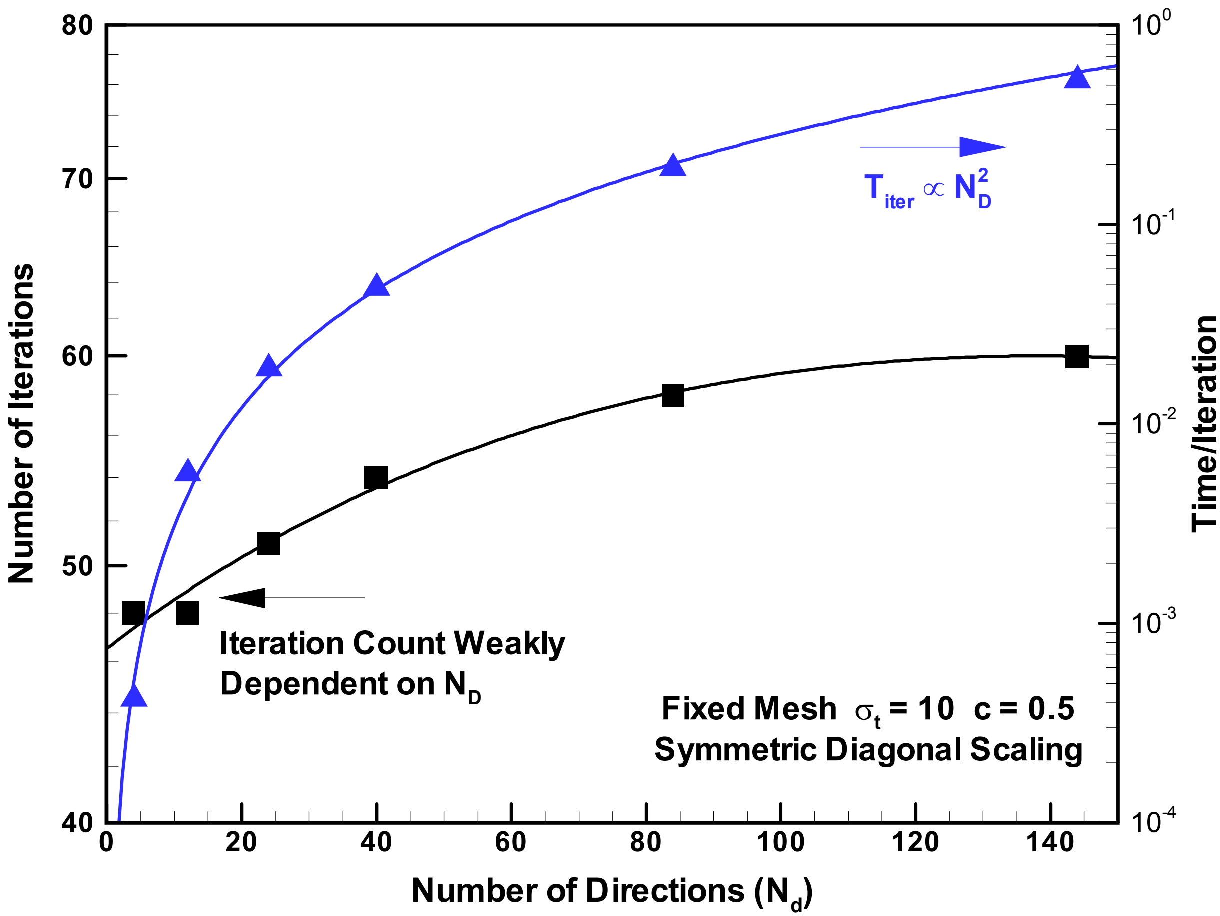


Sandia National Laboratories

Scaling with number of angles, first-order

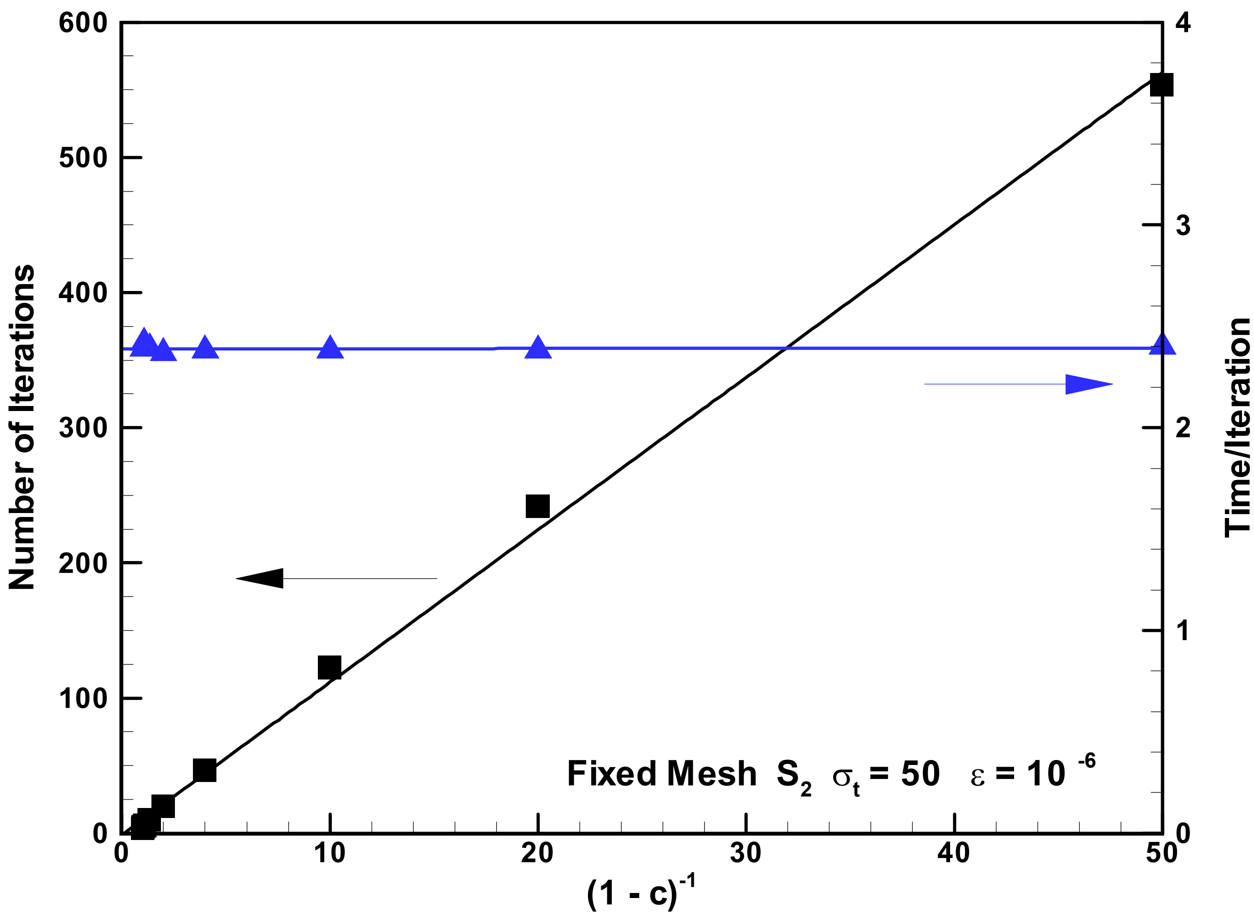


Scaling with number of angles, second-order



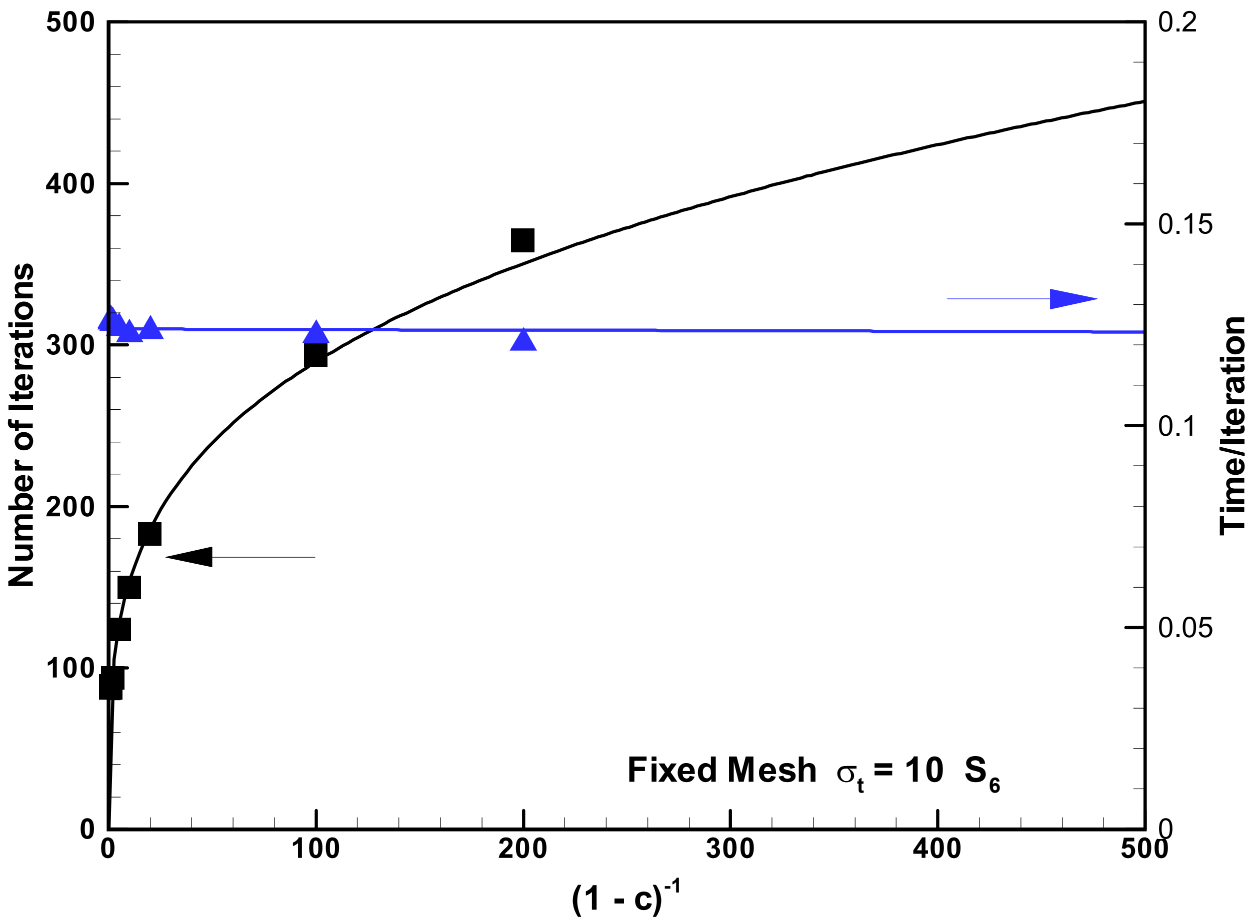
Sandia National Laboratories

Scaling with scattering ratio, first-order

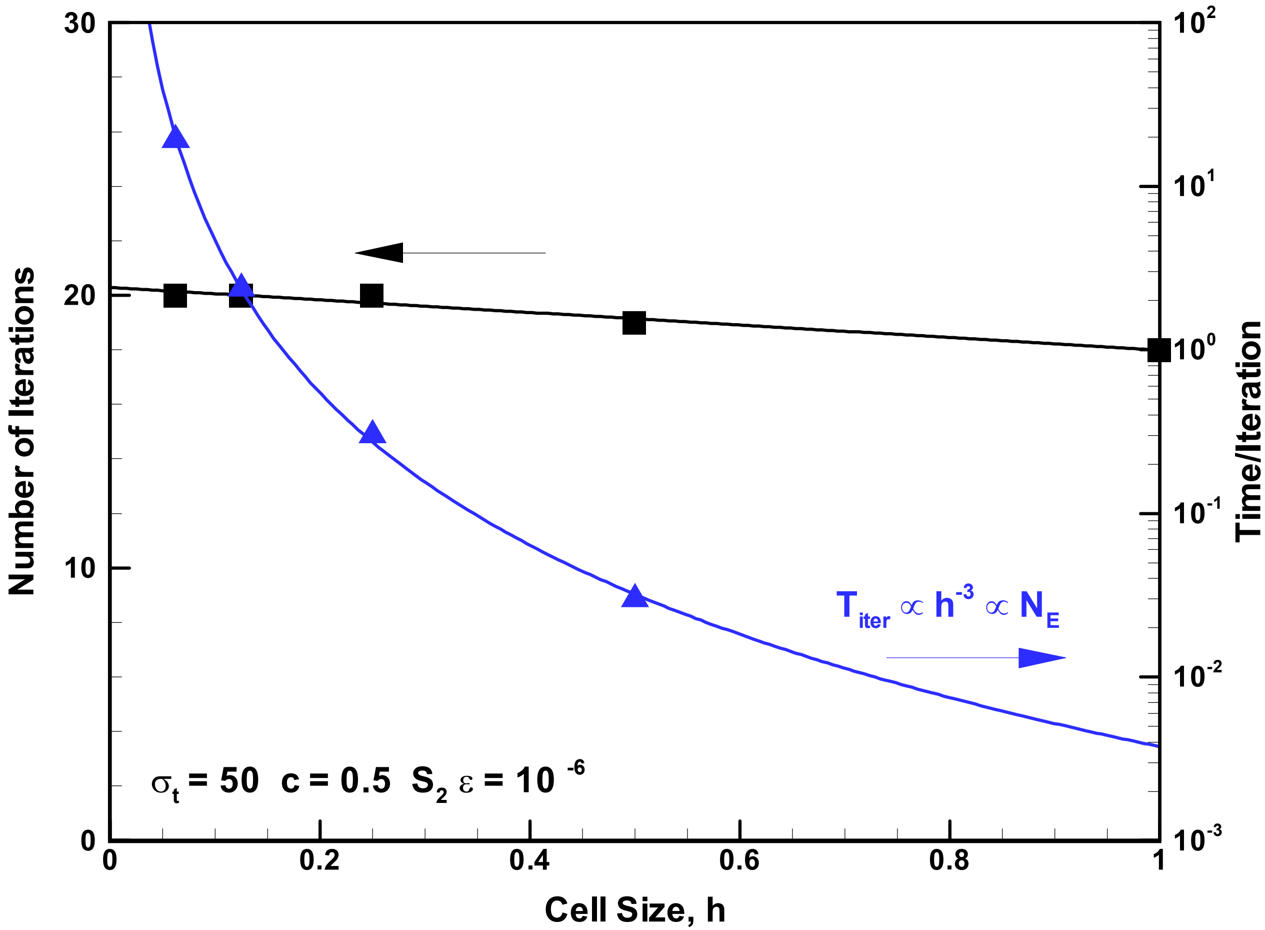


Sandia National Laboratories

Scaling with scattering ratio, second-order

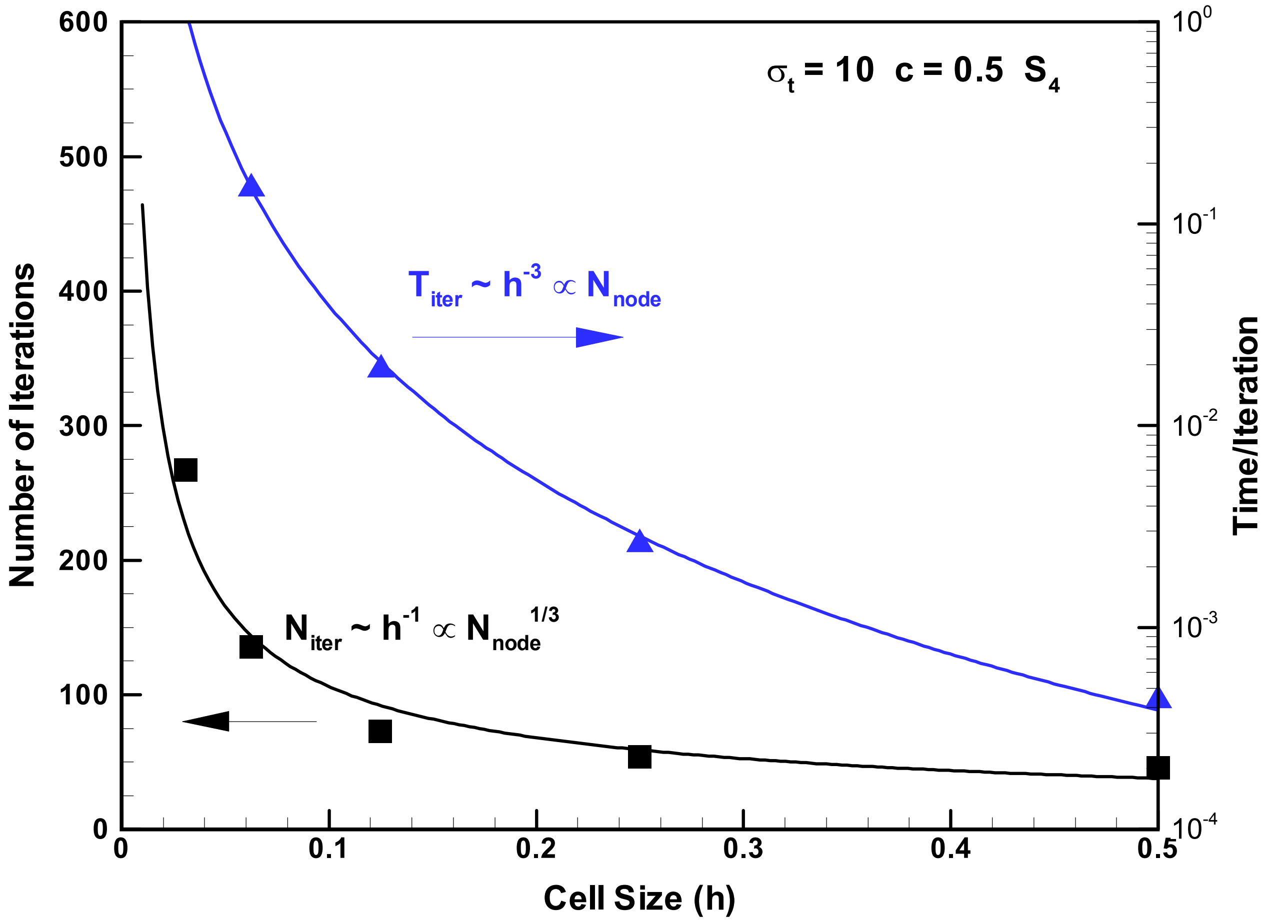


Scaling with cell thickness, first-order

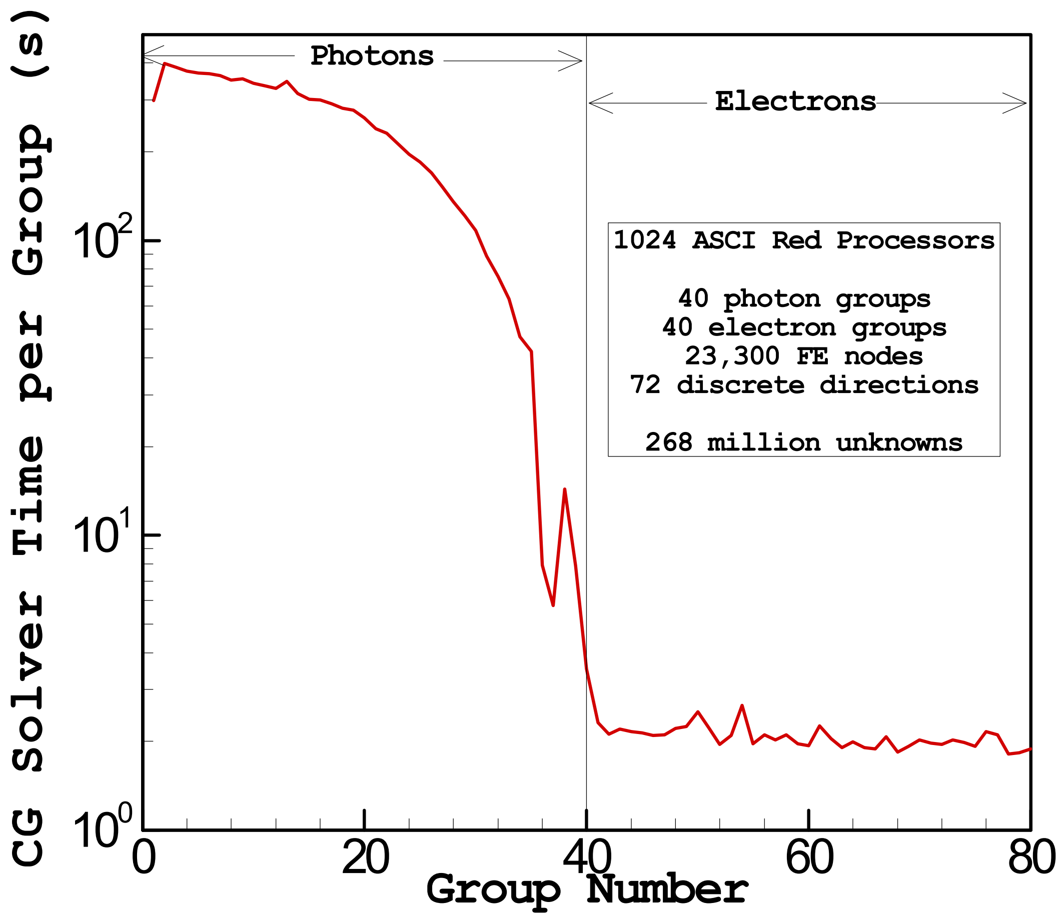


Sandia National Laboratories

Scaling with cell thickness, second-order



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



Summary

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