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Multi-Level Acceleration of Scattering-Source Iterations with Application to Electron Transport

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Motivation

- Traditional source iteration (SI) can converge slowly for certain transport problems, e.g. electron transport
- Preconditioning/acceleration strategies have been developed over the past few decades
  - Diffusion Synthetic Acceleration (DSA)
  - Transport Synthetic Acceleration (TSA)
  - Krylov methods
- Effectiveness of theses methods are highly problem dependent
  - Scattering ratio and degree of scattering anisotropy
  - Material discontinuities, e.g. highly scattering regions and streaming/void regions
  - Different physics for different particle types and energy ranges
- Finding an effective general preconditioner difficult
- Multiple levels of preconditioning can be more effective

Overview

- Description of the capabilities of the SCEPTRE radiation transport code
- Transport Synthetic Acceleration (TSA) applied to transport sweeps
  - Overview of the method
  - Implementation into the SCEPTRE code
  - Application of the method to a practical photon/electron transport problem
- Krylov/GMRES (Generalized Minimum RESidual) alternative to transport sweeps
  - Overview of the method
  - TSA-precondioned Krylov algorithm
- Application of TSA and Krylov algorithms to a model 3-region cylinder test problem
  - Electron transport in uniform lead
  - Electron transport in non-uniform material (lead/void/lead)
  - Artificial cross sections: pure-scattering
    - *Compare* P_3 *and* P_7 *scattering*

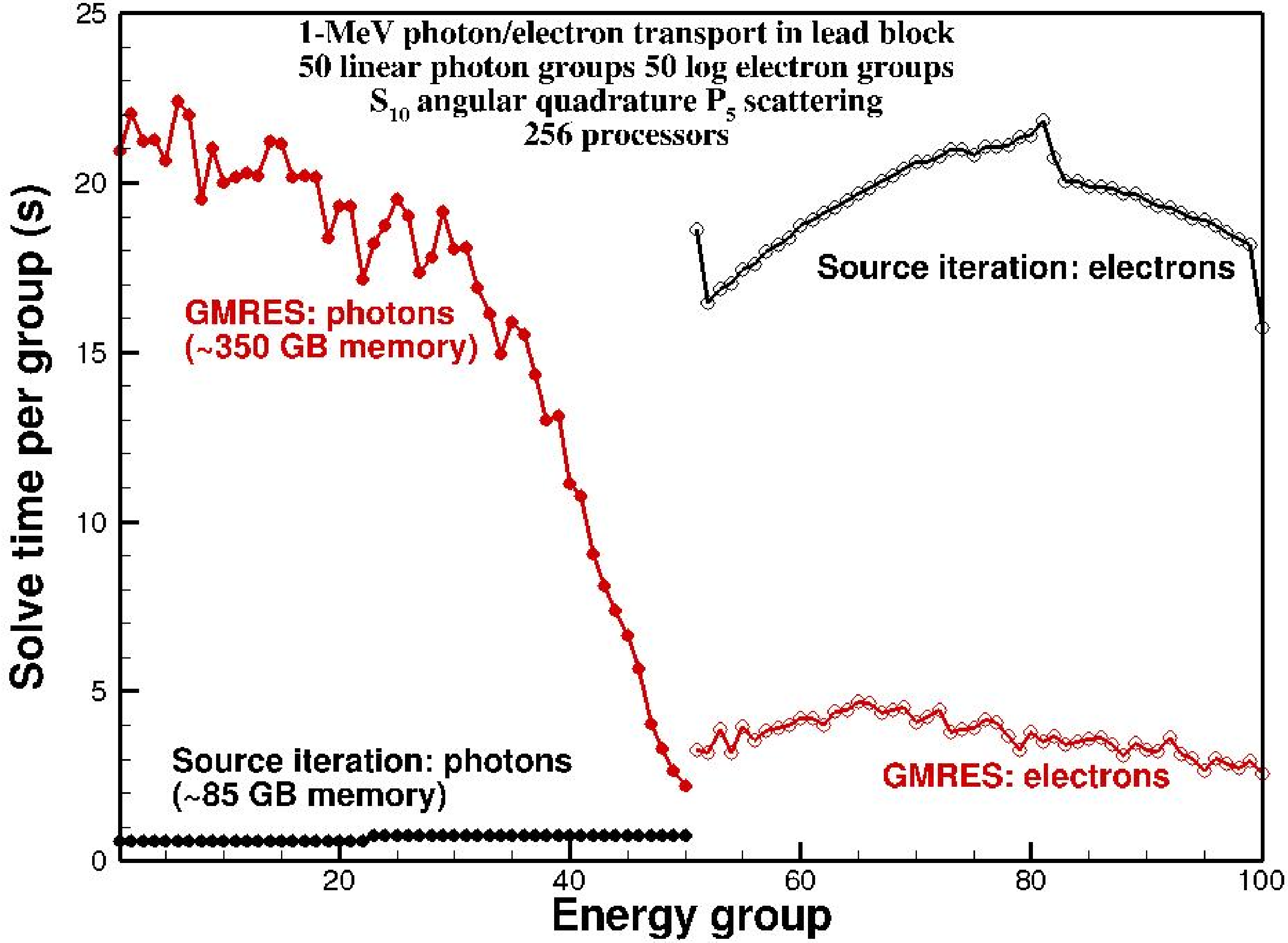
SCEPTRE radiation transport code

- **S**andia **C**omputational **E**ngine for **P**article **T**ransport for **R**adiation **E**ffects
- Unstructured-mesh spatial finite elements
  - Discontinuous finite elements (DFE)
  - Continuous finite elements (CFE)
- Discrete ordinates (S_N) or spherical harmonics (P_N) angular treatment
- Multigroup energy treatment
- Primary application: coupled photon/electron/positron transport
- Different solver type may be used for each energy group
  - User defines arbitrary number of different solvers
  - Individual solvers assigned to each energy group
  - Different solvers tend to be more efficient for specific particle types, material media, energy range …

Solvers available in SCEPTRE

- Sweep-based source iteration (SI)
  - 1st-order form of the transport equation
  - Discontinuous finite elements (DFE) in space
- Krylov-based, full-matrix-system solution
  - No within-group SI (solve space-angle dependence simultaneously using Trilinos solvers)
  - Generalized Minimum RESidual (GMRES)
    - *1st-order transport equation*
    - *DFE spatial differencing*
    - *Asymmetric*
    - P_N *or* S_N
  - Conjugate Gradients (CG)
    - *Self-adjoint angular flux (SAAF) form of the transport equation*
    - *Least-squares (LS) approximation*
    - *Continuous finite elements (CFE) in space*
    - *Symmetric Positive Definite (SPD)*
    - P_N *or* S_N
- Krylov/GMRES matrix-free
  - 1st-order transport equation
  - DFE spatial differencing
  - Sweeping algorithm used to construct Krylov subspace

Comparison of solver time: source iteration (SI) vs. full-matrix Trilinos/GMRES iteration



Transport-synthetic acceleration (TSA) for source iteration (SI)

$$\mathcal{T}\psi(\mathbf{r},\mathbf{\Omega}) = \mathcal{S}\psi(\mathbf{r},\mathbf{\Omega}) + Q(\mathbf{r},\mathbf{\Omega})$$

Streaming plus collision operator $\mathcal{T}\circ = \mathbf{\Omega}\cdot\nabla\circ + \sigma_t\circ$

Scattering operator $\mathcal{S}\circ = \int d\mathbf{\Omega}'\sigma_s(\mathbf{\Omega}' \rightarrow \mathbf{\Omega})\circ$

Source iteration with TSA:

1. Fine-level sweep $\mathcal{T}\psi^{(k+1/2)} = \mathcal{S}\psi^{(k)} + Q$
2. Error term $\varepsilon^{(k+1/2)} = \psi - \psi^{(k+1/2)}$
3. Residual $r^{(k+1/2)} = \mathcal{S}(\psi^{k+1/2} - \psi^{k})$
4. Coarse-level solve $(\mathcal{T}_c - \mathcal{S}_c)\varepsilon_c^{(k+1/2)} = \mathcal{R}r^{(k+1/2)}$
5. Apply correction term $\psi^{(k+1)} = \psi^{(k+1/2)} + \mathcal{P}\varepsilon_c^{(k+1/2)}$

Restriction operator

Prolongation operator

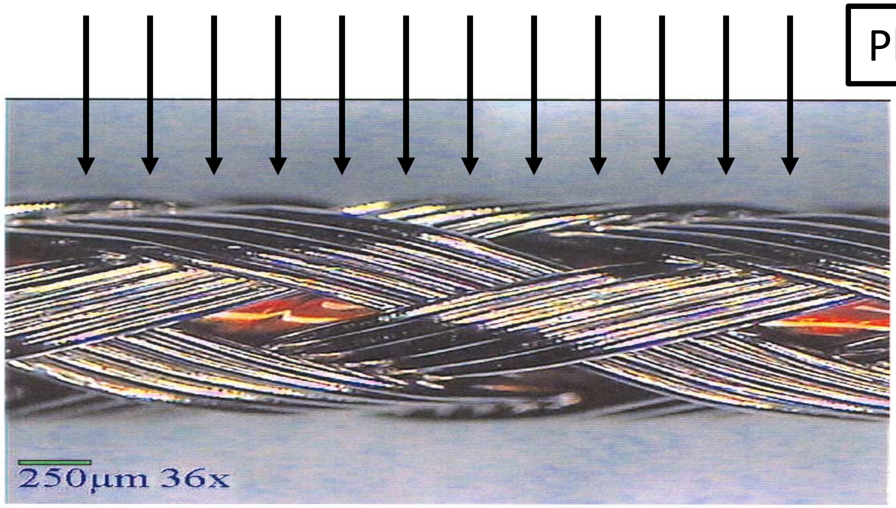
Coarse-level solve (Krylov full matrix)

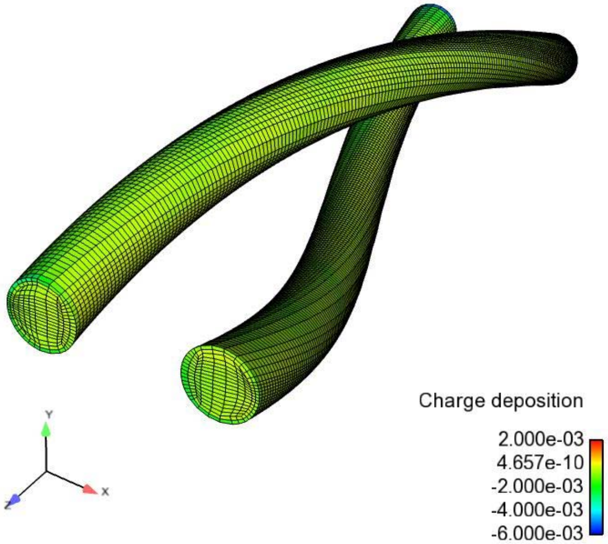
$$(\mathcal{T}_c - \mathcal{S}_c)\varepsilon_c^{(k+1/2)} = r_c^{(k+1/2)}$$

- GMRES (P_N or S_N)
  - 1st-order transport equation
  - DFE spatial differencing
  - Asymmetric
  - More expensive per iteration
  - More effective at accelerating SI
- CG (P_N or S_N)
  - Self-adjoint angular flux (SAAF) form of the transport equation
  - Least-squares (LS) approximation
  - Continuous-finite elements (CFE)
  - Symmetric Positive Definite (SPD)
  - Less expensive per iteration
  - Less effective at accelerating SI
- Off-the-shelf preconditioners from Trilinos applied to coarse-level solves
  - Incomplete-factorization (IF)
  - Multi-level (ML)
- Relative effectiveness of different TSA coarse-level solvers problem dependent
- Reasonable memory requirement for coarse-level solves

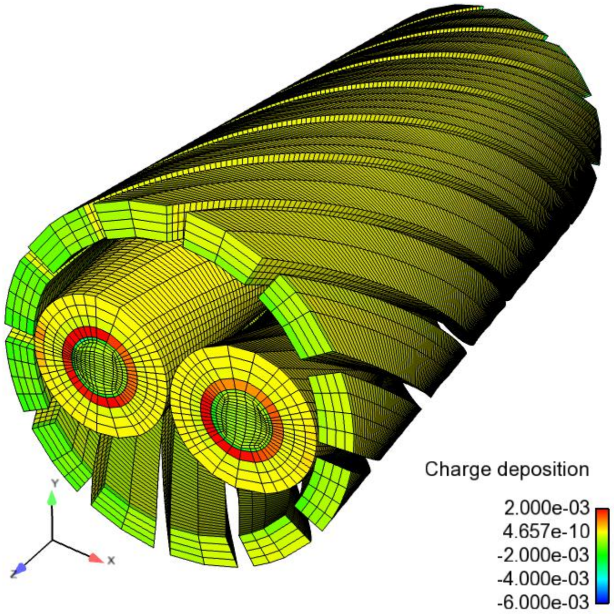
First test problem: photon/electron transport on twisted-pair braided shielded cable

Planar photon source

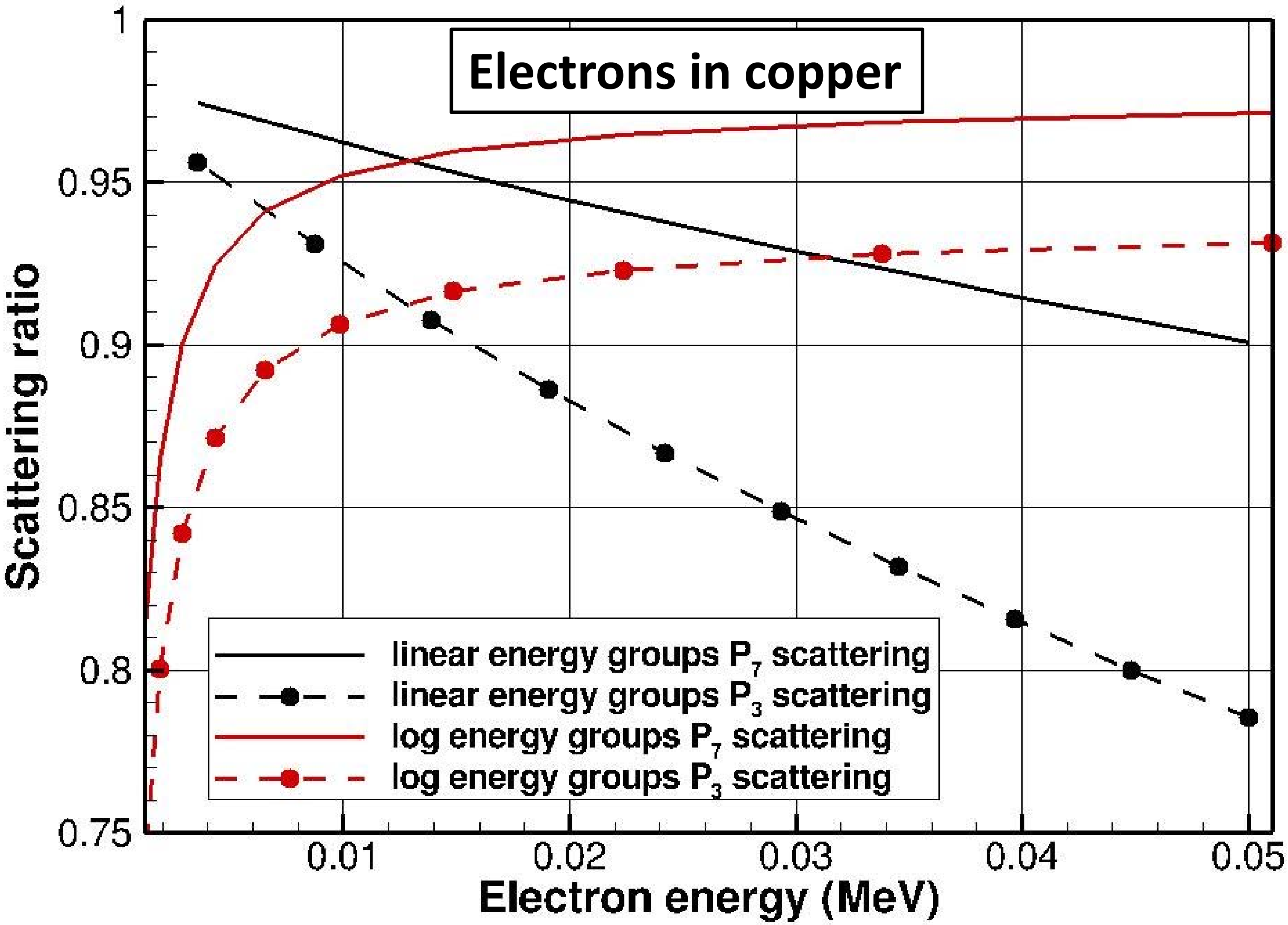




Twisted-pair with shield removed

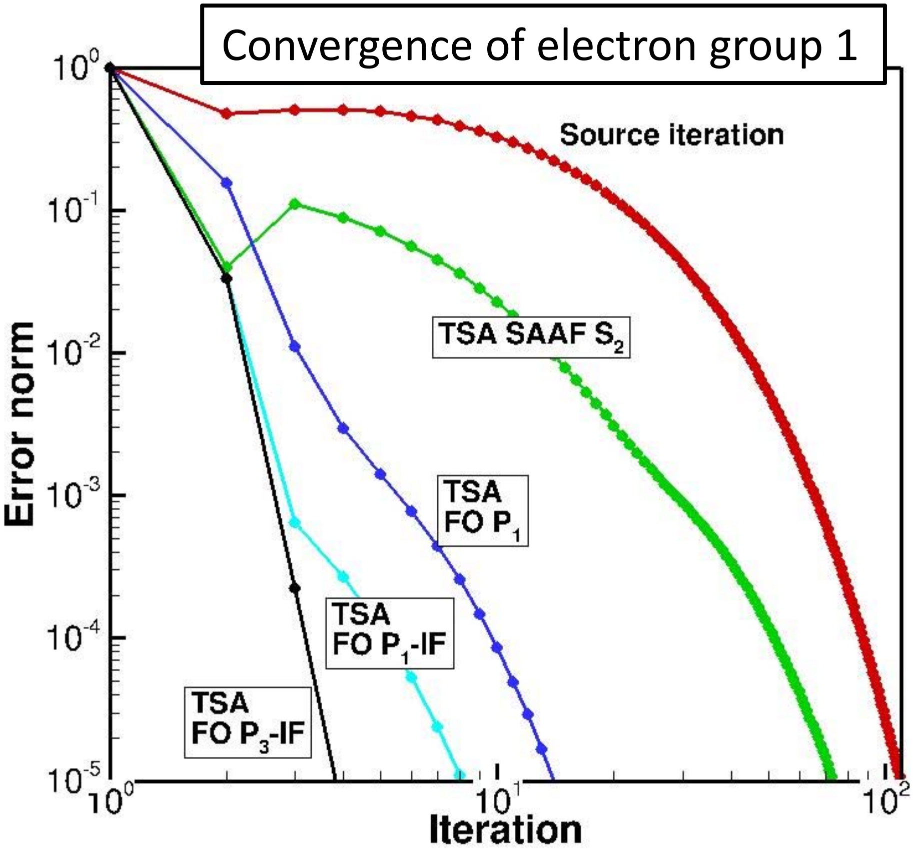


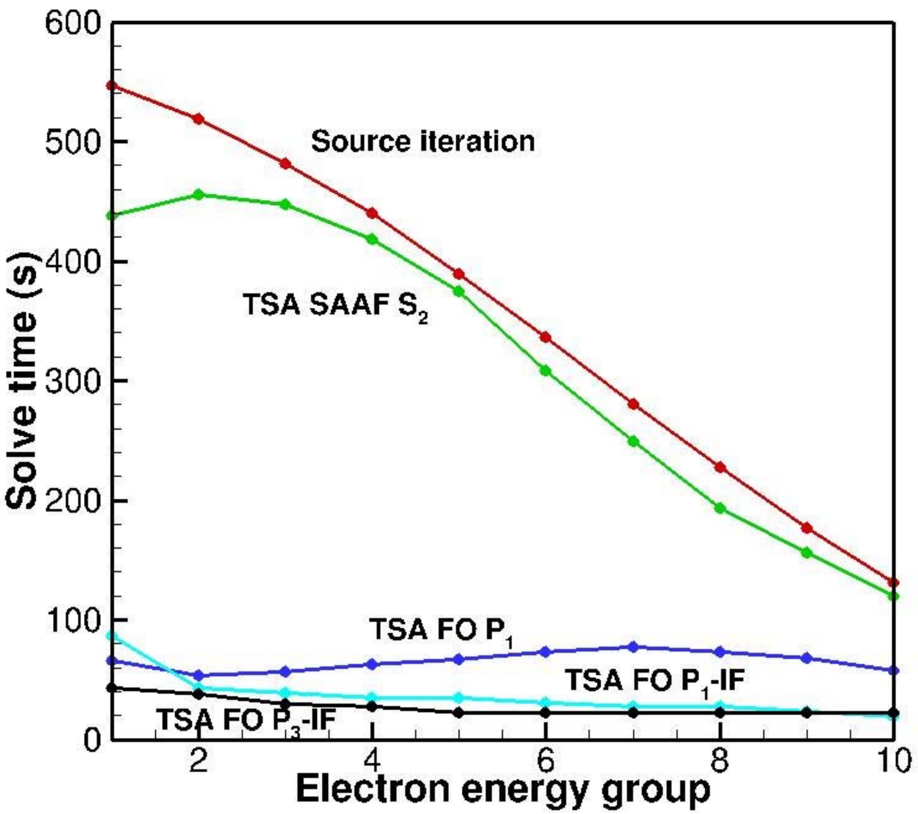
Scattering ratio depends on energy group structure and Legendre expansion order



Effectiveness of TSA methods in accelerating convergence and reducing solve time

- Source iteration with Trilinos-based TSA
- S_8 quadrature, P_3 scattering, 10 linear photon and 10 log electron energy groups
- Timing results with 256 Intel Sandy Bridge 2.6 GHz cores


Convergence of electron group 1



Effectiveness of TSA depends upon which coarse-level solver is used

TSA method	Coarse-level parameters			Total solve time for electron groups (s)	Speed up
	Preconditioner	Convergence tolerance	Max iterations		
None	-	-	-	3530	1
FO P_1	None	0.01	100	653	5.4
FO P_1	Incomplete factorization	0.01	10	365	9.7
FO P_3	Incomplete factorization	0.01	10	272	13.
SAAF S_2	none	10^{-4}	1000	3160	1.1

GMRES iteration applied to within-group iteration

- **Generalized Minimum Residual Method (Saad, 1986) to solve a linear system of equations based on the Krylov subspace**

  Linear System $Ax = b$

  Krylov Subspace $\mathcal{K}_m = span[r_0, Ar_0, A^2 r_0, \cdots, A^{m-1} r_0]$

  Projection $x_m = x_0 + \boldsymbol{V}_m y_m$

  $y_m = min_y ||Ax - b||_2$

- **Applied to radiation transport by Patton (1996), Warsa (2004) and others**

  Transport Equation $\mathcal{T}\psi = \mathcal{S}\psi + Q$

  $(I - \mathcal{T}^{-1}\mathcal{S})\psi = \mathcal{T}^{-1}Q$

  $\mathcal{T}^{-1}$ *is simply a transport sweep operation*

  Map to Linear System $Ax \rightarrow (I - \mathcal{T}^{-1}\mathcal{S})\psi$

  $b \rightarrow \mathcal{T}^{-1}Q$

  Av_j *operations are replaced by* $(I - \mathcal{T}^{-1}\mathcal{S})v_j$ *without forming a matrix system.*

- **Convergence depends on the distribution of eigenvalues of** $I - \mathcal{T}^{-1}\mathcal{S}$ **rather than the maximum eigenvalue, as in source iteration**

GMRES Algorithm with TSA

- **Preconditioned solver for linear system**

  Linear System $Ax = b$

  Left Preconditioning $M^{-1}Ax = M^{-1}b$

  M^{-1} *is chosen such that* $M^{-1} \approx A^{-1}$

- **TSA-based preconditioner**

  Transport Equation $(I - \mathcal{T}^{-1}\mathcal{S})\psi = \mathcal{T}^{-1}Q$

  Inverse Operator $(I - \mathcal{T}^{-1}\mathcal{S})^{-1} = I + (\mathcal{T} - \mathcal{S})^{-1}\mathcal{S}$

  TSA Preconditioner $\mathcal{M}^{-1} = I + \mathcal{P}(\mathcal{T}_c - \mathcal{S}_c)^{-1}\mathcal{R}\mathcal{S}$

  $\mathcal{T}_c$ and $\mathcal{S}_c$ are coarse level transport and scattering operators

  $\mathcal{R}$ and $\mathcal{P}$ are restriction and prolongation operators

- **Each GMRES iteration involves two steps**

  a transport sweep operation $(\mathrm{I} - \mathcal{T}^{-1}\mathcal{S})v_j$

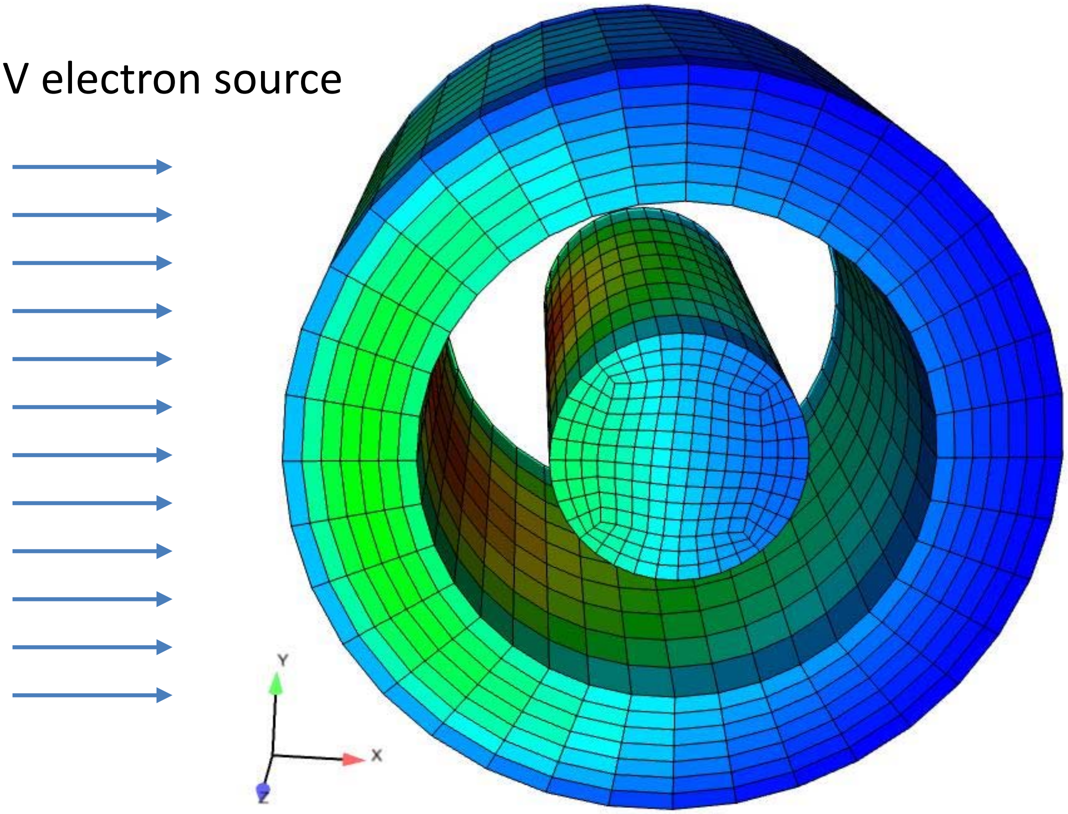
  a coarse transport solve $(\mathcal{T}_\mathrm{c} - \mathcal{S}_\mathrm{c})u_c = v_c$

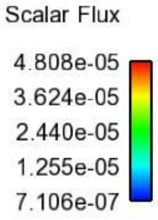
- **Coarse-level transport equation solved by GMRES iteration**

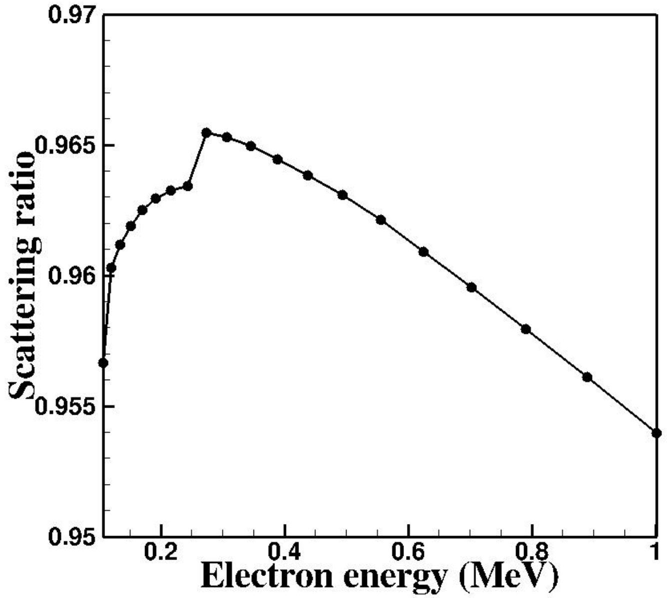
Test problem: three-region cylinder (Z=0.05 cm R=0.03 cm)

- Compare preconditioners for:
  - Material discontinuities
  - Scattering anisotropy

1-MeV electron source

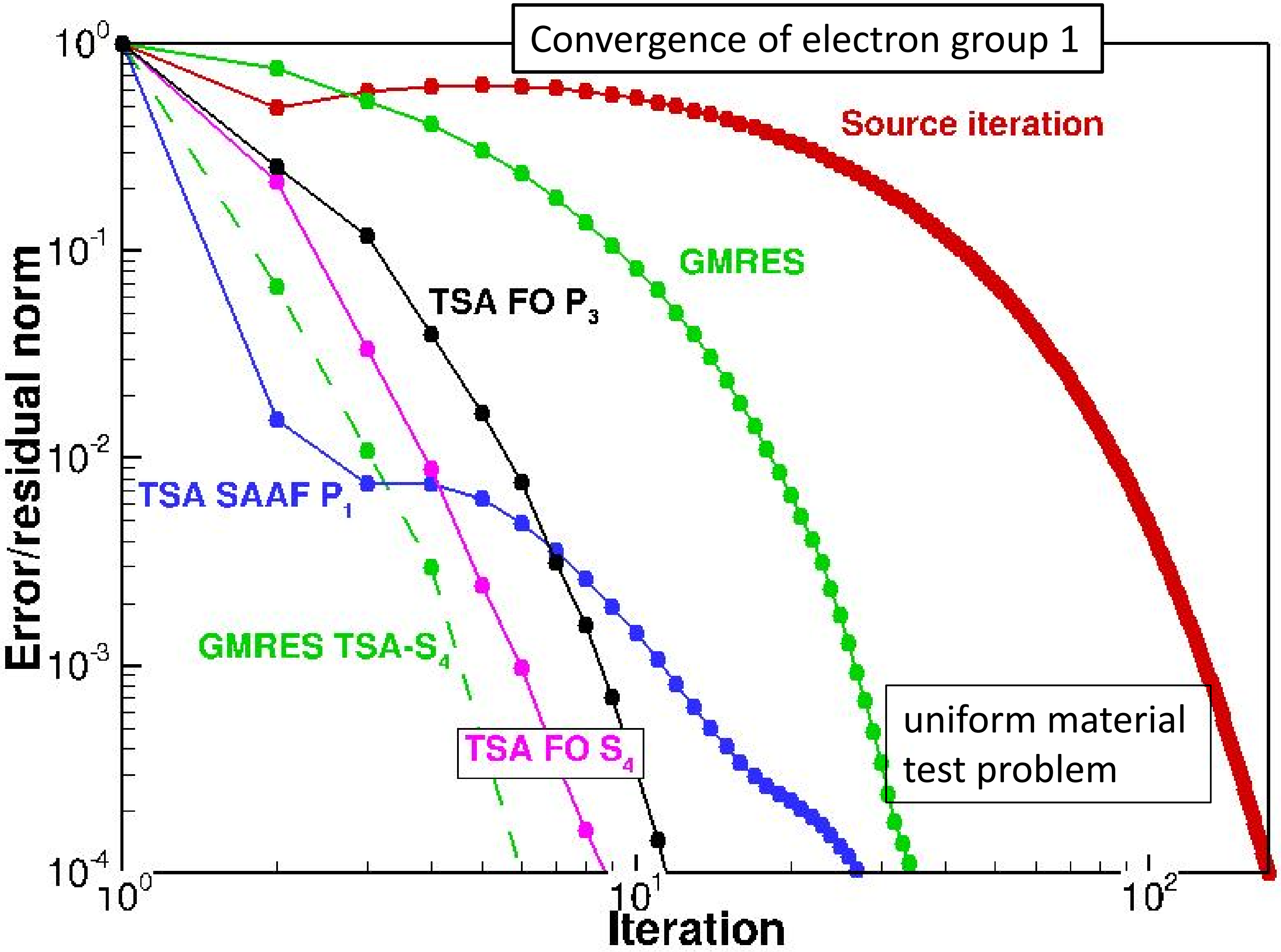






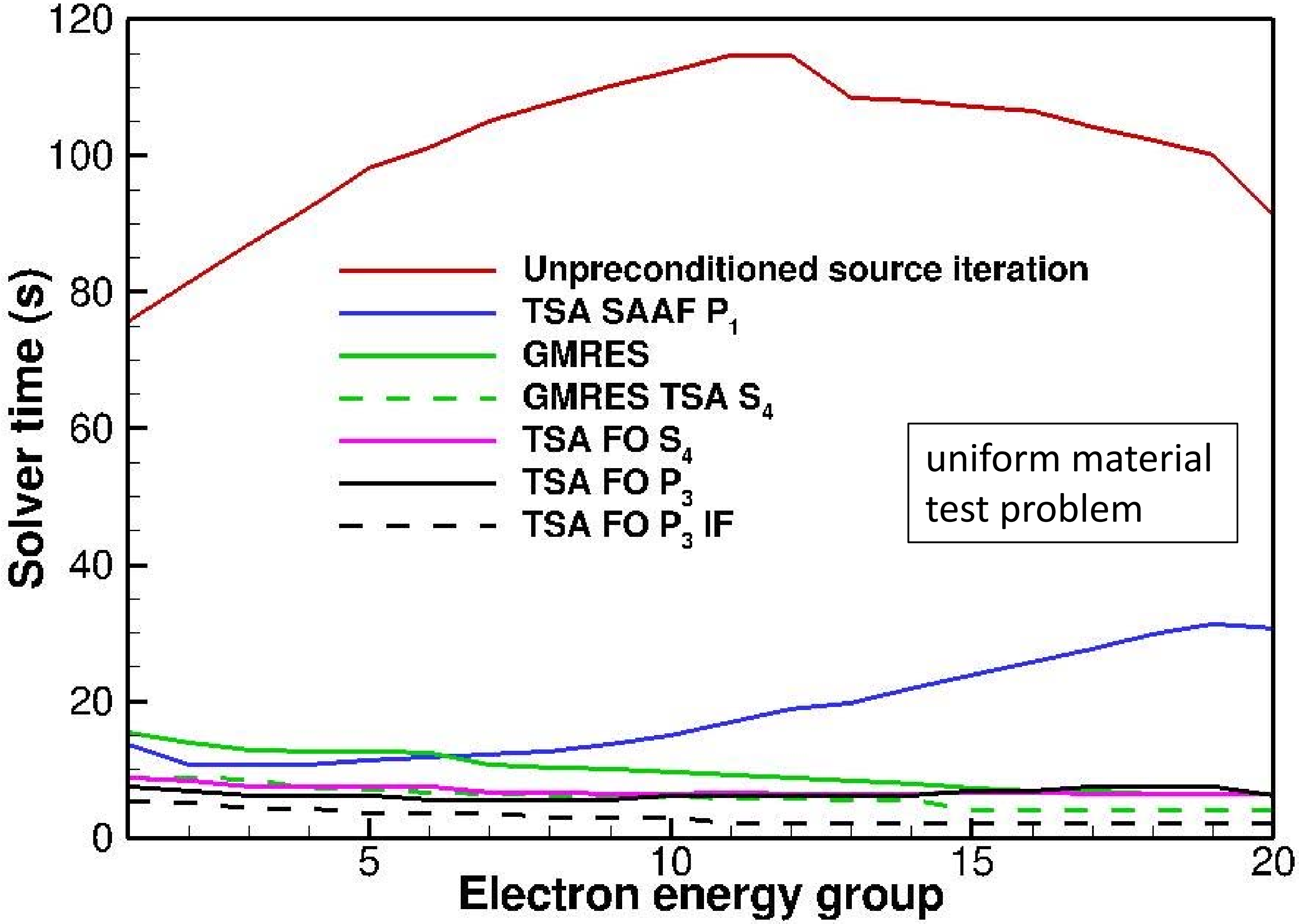
Scattering ratio:
electron transport in lead
20 log energy groups
P_5 scattering

Comparison of convergence rates for various solvers and preconditioners


Convergence of electron group 1

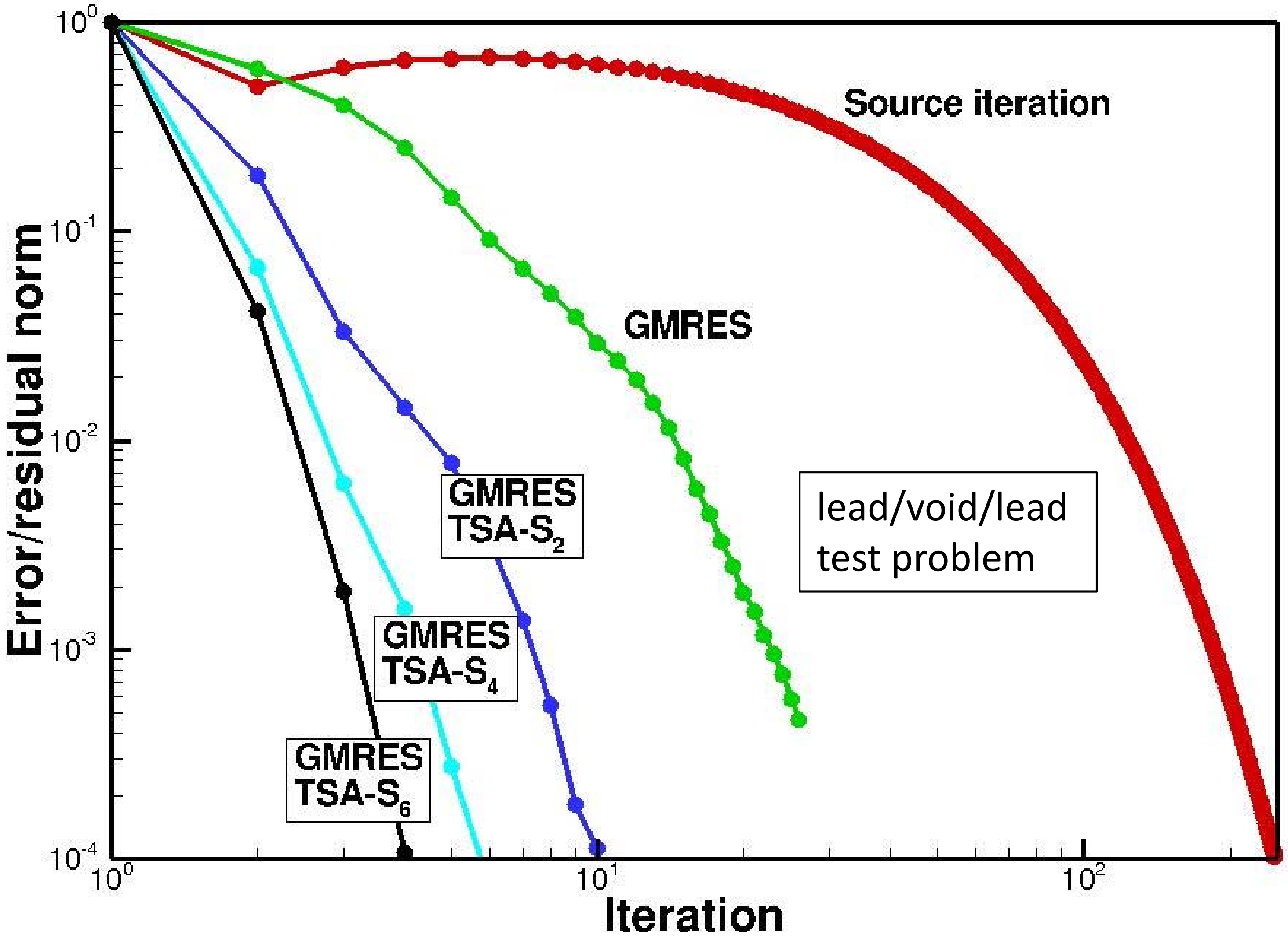
uniform material test problem

Timing results for various solvers and preconditioners



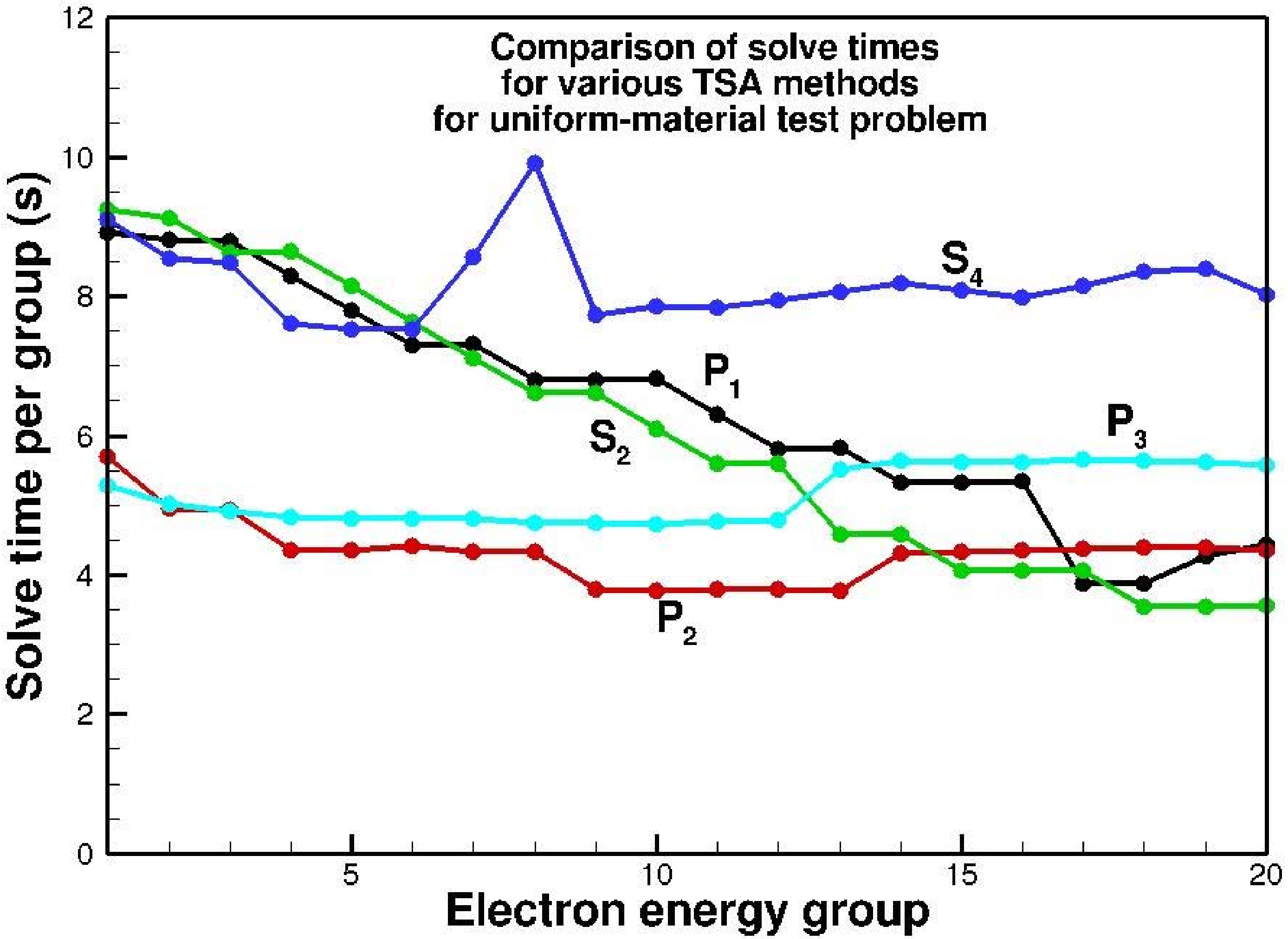
uniform material test problem

TSA preconditioning of GMRES solver accelerates convergence

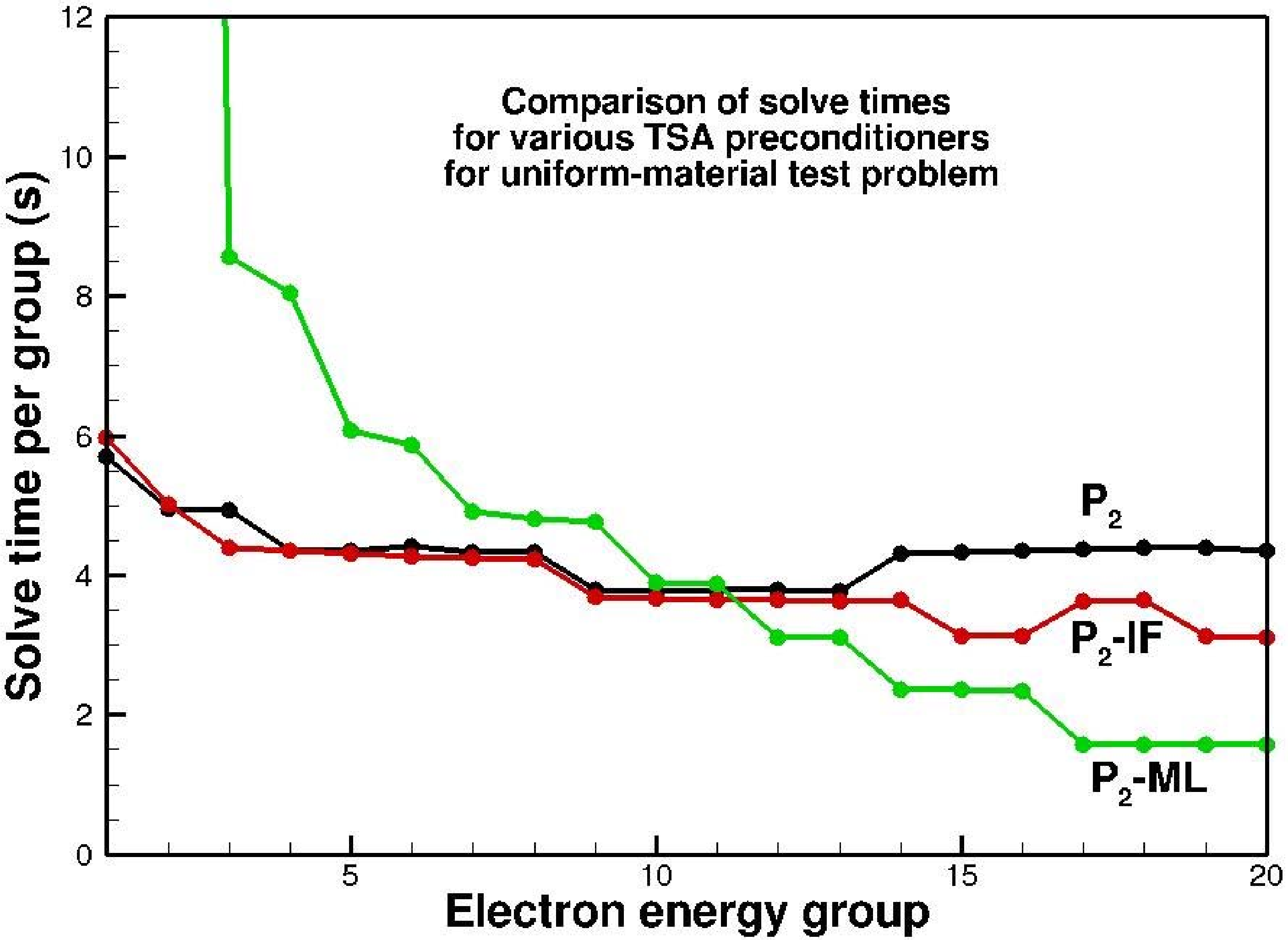


lead/void/lead test problem

Effectiveness comparison of various coarse-level solvers



Effectiveness of preconditioning applied to the coarse-level solver



Solver time comparisons: uniform vs. non-uniform

solver	**TSA method**	**Solve time**		**Speed up**	
		Uniform material	Non-uniform material	Uniform material	Non-uniform material
SI	none	2030	1940	1	1
GMRES	none	214	243	9.5	8.0
GMRES	GMRES-S_2	212	241	9.6	8.0
SI	FO-P_3	151	173	13.	11.
SI	FO-P_3 IF	83	166	25.	12.
SI	FO-P_3 ML	311	Not converged	6.5	-
SI	FO-S_2 ML	192	Not converged	11.	-

Preconditioner effectiveness vs. scattering order

$$\sigma_t = 10^4 \qquad \sigma_s = \left[10^4, 0.9\text{x}10^4, 0.8\text{x}10^4, 0.7\text{x}10^4 \ldots\right]$$

$$c = 1$$

- Three concentric cylinders
- Void region between two material regions
- S_{16} discrete ordinates
- Planar boundary source term

Acceleration method	Solver time (s)	
	P_3 scattering	P_7 scattering
none	-	-
GMRES	110	140
GMRES TSA S_4	88	102
FO TSA P_1	36	38

Summary and future work

- Two acceleration methods implemented and tested
  - TSA applied to source iteration (SI)
  - Krylov/GMRES alternative to SI
- Order of magnitude speedup demonstrated
- Preconditioning of the preconditioner
  - Off-the-shelf IF or ML applied to TSA
  - TSA applied to Krylov/GMRES
- Preconditioner effectiveness highly problem-dependent
  - Material discontinuities
  - Scattering anisotropy
  - Characteristics of the source term
  - Problem size
  - Characteristics of the coarse-level solver
  - Convergence metrics applied to the coarse-level solver
  - Tuning parameters applied to the IF and ML preconditioners