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Least Squares Finite Elements Algorithms in the SCEPTRE Radiation Transport Code

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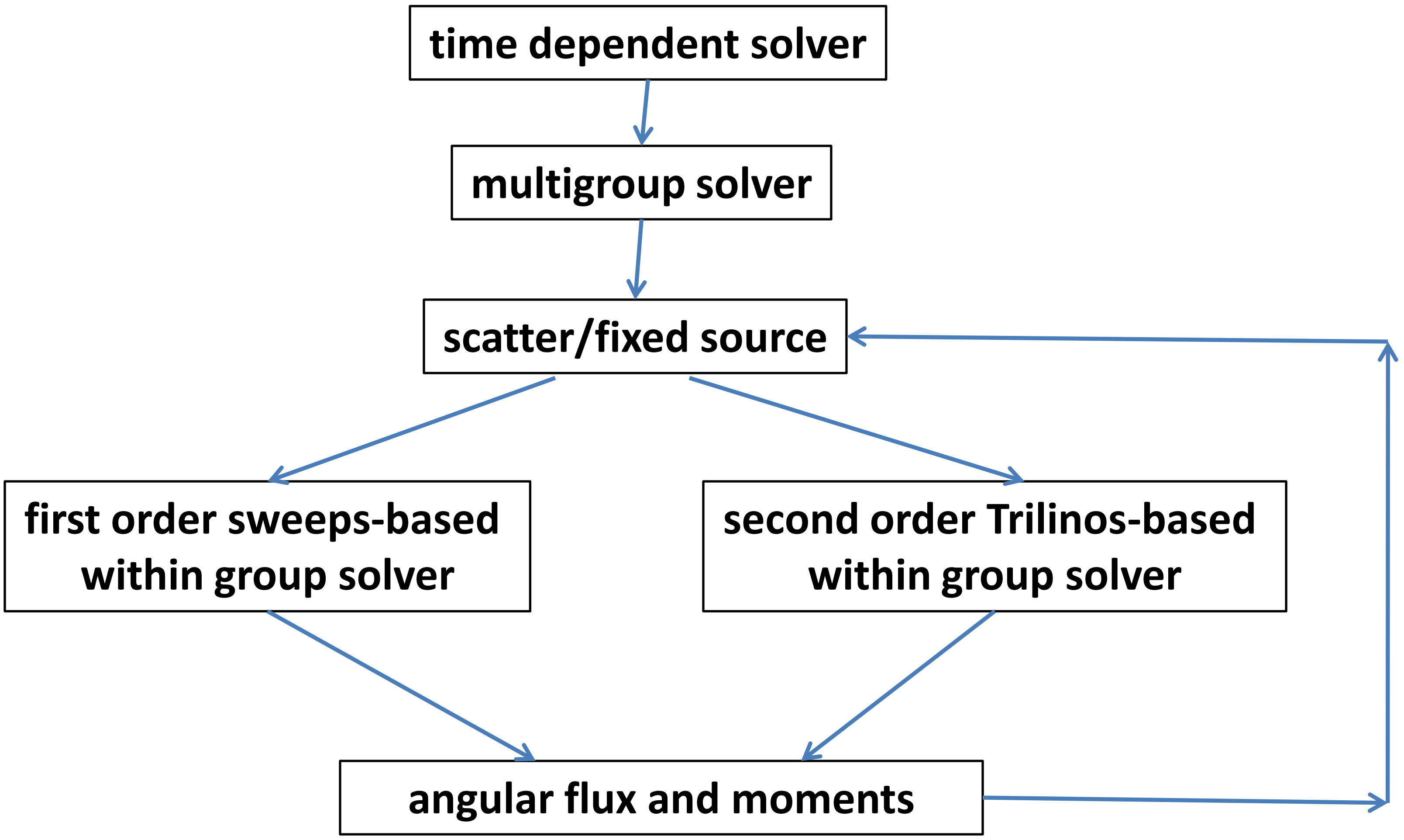
Overview of Talk

- **Overview of SCEPTRE code**
- **Motivation for this work**
- **Development of the S_N and P_N least-squares algorithms**
- **Test problem**
- **Convergence analyses**

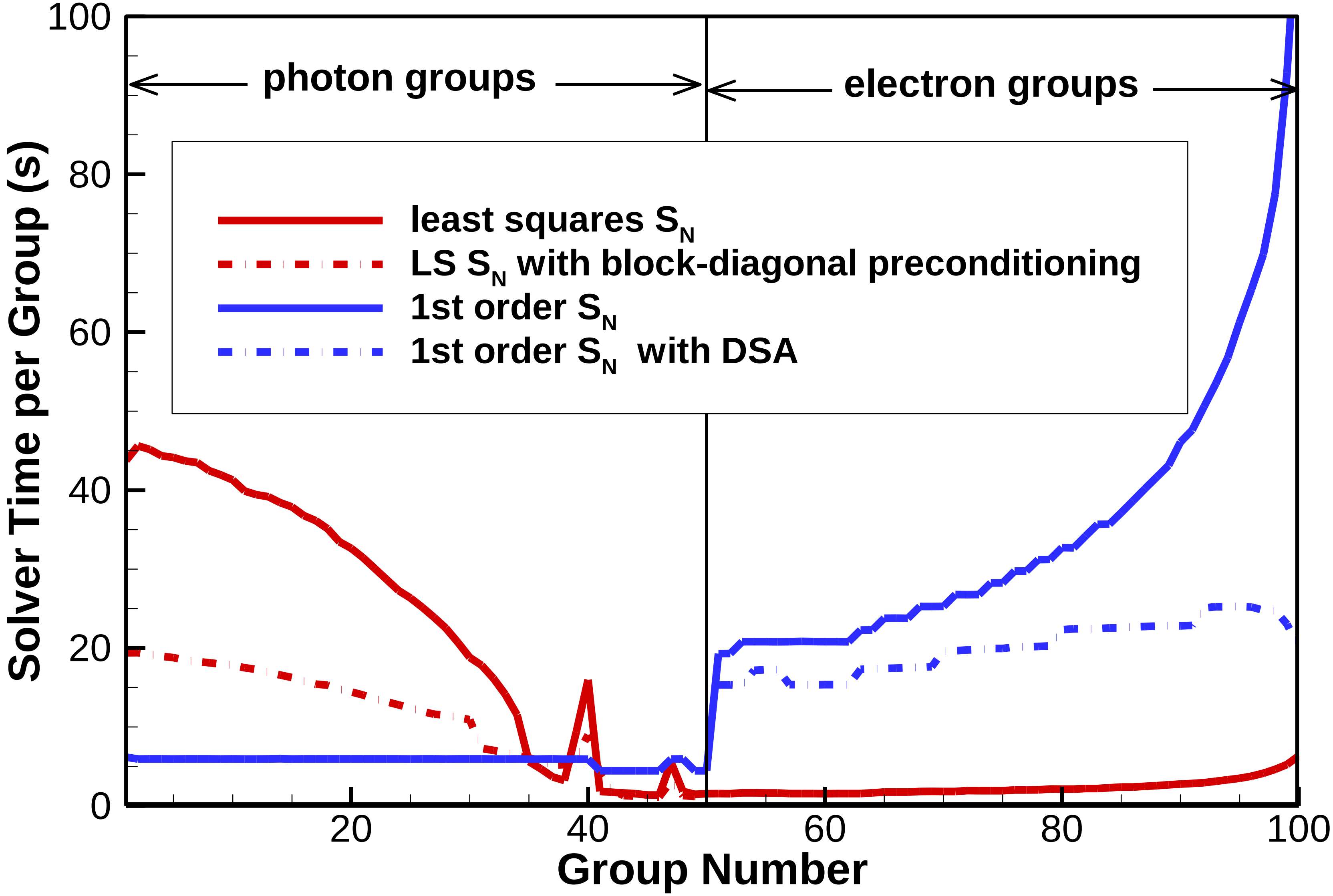
SCEPTRE Code Overview



Why Hybrid Algorithm?

- **SCEPTRE applications involve coupled photon/electron transport**
  - Vast range of cross-section magnitudes and scattering ratios
  - First-order sweeps based algorithm efficient for streaming dominated transport
  - Second-order Trilinos based algorithm efficient for scattering dominated transport
- **Ability to leverage Trilinos tools**
  - Parallel linear algebra tools
  - Built-in preconditioners
  - Multicore capability

Timing Comparison by Solver and Particle Type



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Derivation of Least Squares Algorithm (1)

First-order transport equation: $\boldsymbol{\Omega} \bullet \nabla \psi + \mathcal{G}\psi = Q$

Removal/scattering operator:

$$\mathcal{G}\psi = \sigma_t \psi - \int \sigma_s(\mathbf{r}, \boldsymbol{\Omega}' \bullet \boldsymbol{\Omega}) \psi(\mathbf{r}, \boldsymbol{\Omega}') d\boldsymbol{\Omega}'$$

Expand angular flux in a set of interpolation functions:

$$\psi(\mathbf{r}, \boldsymbol{\Omega}) \simeq \sum_{n'} \widetilde{\psi}_{n'} u_{n'}(\mathbf{r}, \boldsymbol{\Omega})$$

Form weighting functions from 1st-order transport operator and interpolation functions:

$$w_n(\mathbf{r}, \boldsymbol{\Omega}) = \boldsymbol{\Omega} \bullet \nabla u_n + \mathcal{G} u_n(\mathbf{r}, \boldsymbol{\Omega})$$

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Derivation of Least Squares Algorithm (2)

- Substitute angular flux expansion into 1st-order transport equation
- Multiply by weighting functions
- Integrate over space and angle
- Assemble linear system (symmetric positive definite)
- Solve for angular flux coefficients

$$\sum_{n'} \tilde{\psi}_{n'} [\langle \mathbf{\Omega} \cdot \nabla u_n \mathbf{\Omega} \cdot \nabla u_{n'} \rangle + \langle \mathbf{\Omega} \cdot \nabla u_n \mathcal{G} u_{n'} \rangle$$

$$+ \langle \mathcal{G} u_n \mathbf{\Omega} \cdot \nabla u_{n'} \rangle + \langle \mathcal{G} u_n \mathcal{G} u_{n'} \rangle]$$

$$= \langle \mathbf{\Omega} \cdot \nabla u_n Q \rangle + \langle \mathcal{G} u_n Q \rangle, \text{ for all } n$$

Comparison of Least Squares Algorithm with Self-Adjoint Angular Flux Algorithm

- **Least squares form has no dependence on the inverse of the removal/scattering operator**
- **Internal voids can be handled without modification**

term	self adjoint	least squares
streaming	$\langle \mathbf{\Omega} \cdot \nabla u_n \mathcal{G}^{-1} \mathbf{\Omega} \cdot \nabla u_{n'} \rangle$	$\langle \mathbf{\Omega} \cdot \nabla u_n \mathbf{\Omega} \cdot \nabla u_{n'} \rangle$
cross terms	-	$\langle \mathbf{\Omega} \cdot \nabla u_n \mathcal{G} u_{n'} \rangle + \langle \mathcal{G} u_n \mathbf{\Omega} \cdot \nabla u_{n'} \rangle$
removal	$\langle u_n \mathcal{G} u_{n'} \rangle$	$\langle \mathcal{G} u_n \mathcal{G} u_{n'} \rangle$
boundary	$\oint \mathbf{\Omega} \cdot \mathbf{n} u_n u_{n'} \mathbf{ds}$	-
source	$\langle \mathbf{\Omega} \cdot \nabla u_n \mathcal{G}^{-1} Q \rangle + \langle u_n Q \rangle$	$\langle \mathbf{\Omega} \cdot \nabla u_n Q \rangle + \langle \mathcal{G} u_n Q \rangle$

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Imposition of Boundary Conditions

- **For S_N apply vacuum boundary conditions as Dirichlet BC**
  - Replace rows corresponding to incoming directions on external boundary with boundary conditions
  - Perform row and column rearrangements to maintain symmetry
- **For P_N apply the divergence theorem to the cross terms to expose boundary terms**
  - Split boundary integrals between incoming and outgoing directions
  - For outgoing directions add contribution to the system matrix
  - For incoming directions add contribution to the source vector

$$\langle \mathbf{\Omega} \cdot \nabla u_n \mathcal{G} u_{n'} \rangle = -\langle u_n \mathbf{\Omega} \cdot \nabla \mathcal{G} u_{n'} \rangle + \oint (\mathbf{\Omega} \cdot \mathbf{n}) u_n \mathcal{G} u_{n'} \mathbf{ds}$$

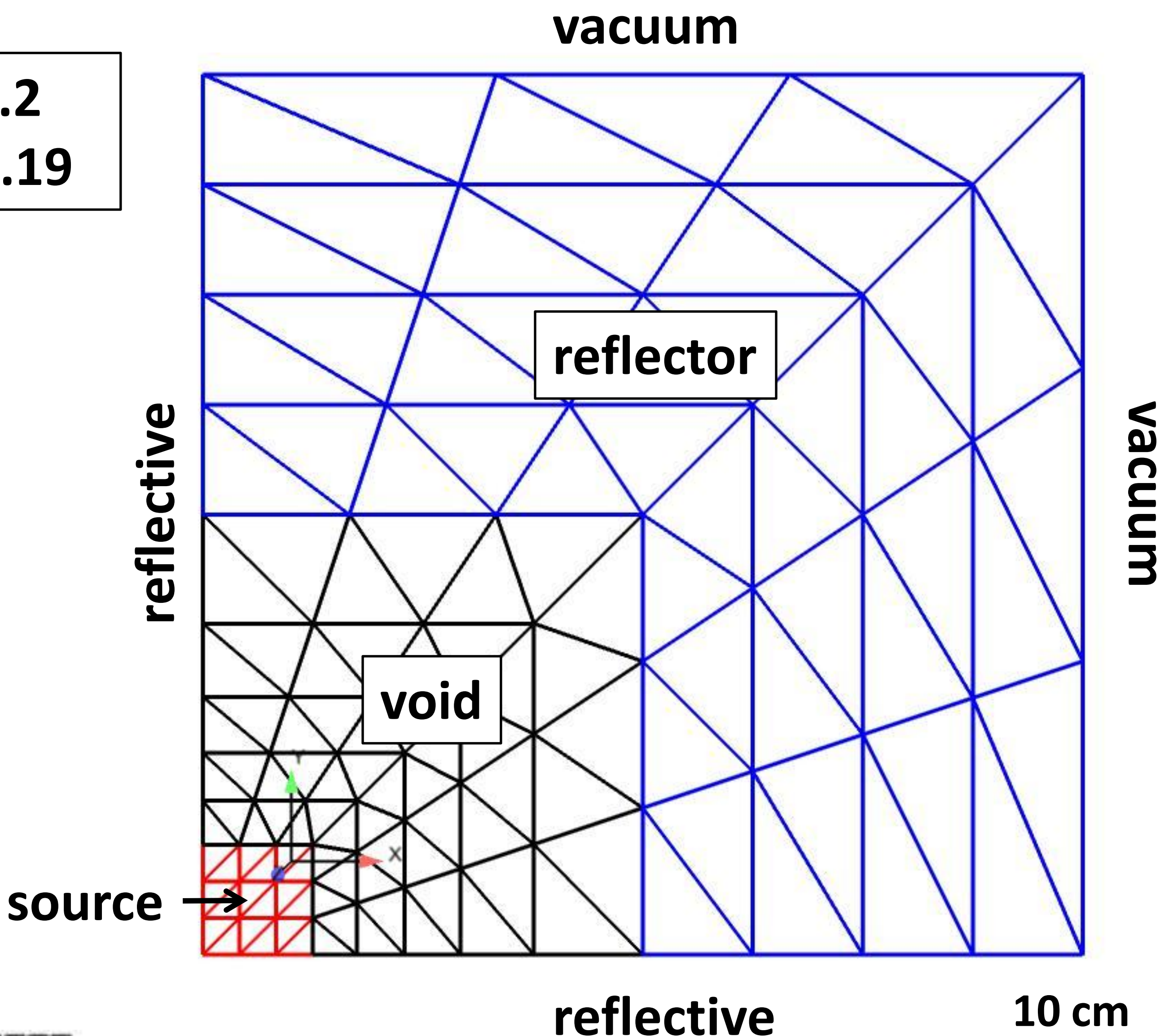
$$\langle \mathcal{G} u_n \mathbf{\Omega} \cdot \nabla u_{n'} \rangle = -\langle \mathbf{\Omega} \cdot \nabla \mathcal{G} u_n u_{n'} \rangle + \oint (\mathbf{\Omega} \cdot \mathbf{n}) \mathcal{G} u_n u_{n'} \mathbf{ds}$$

Comparison of S_N and P_N Least Squares Formulations

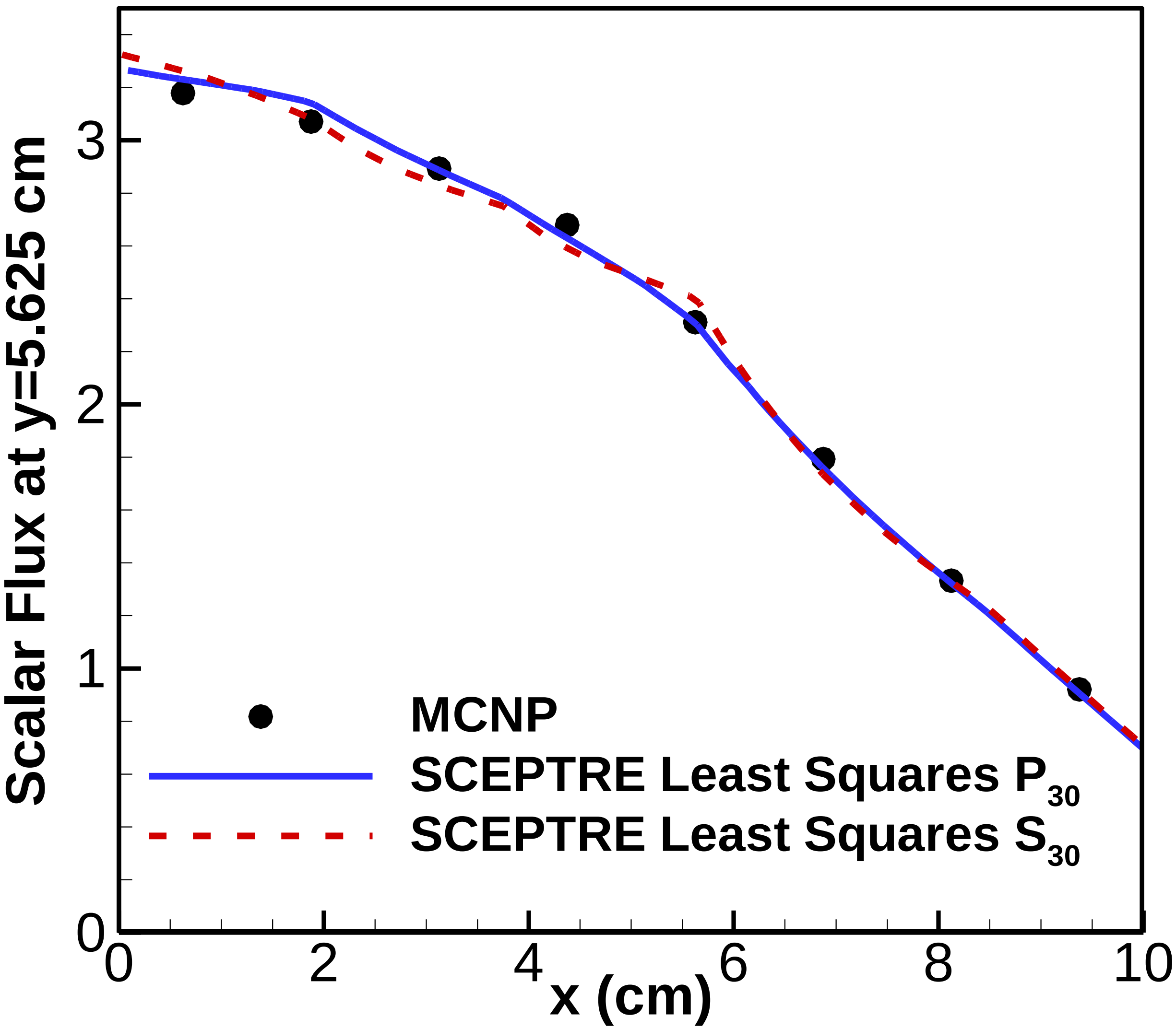
term	least squares S_N	least squares P_N
streaming	$\langle \mathbf{\Omega} \cdot \nabla u_n \mathbf{\Omega} \cdot \nabla u_{n'} \rangle$	$\langle \mathbf{\Omega} \cdot \nabla u_n \mathbf{\Omega} \cdot \nabla u_{n'} \rangle$
cross terms	$\langle \mathbf{\Omega} \cdot \nabla u_n \mathcal{G} u_{n'} \rangle + \langle \mathcal{G} u_n \mathbf{\Omega} \cdot \nabla u_{n'} \rangle$	$-\langle u_n \mathbf{\Omega} \cdot \nabla \mathcal{G} u_{n'} \rangle - \langle \mathbf{\Omega} \cdot \nabla \mathcal{G} u_n u_{n'} \rangle$
removal	$\langle \mathcal{G} u_n \mathcal{G} u_{n'} \rangle$	$\langle \mathcal{G} u_n \mathcal{G} u_{n'} \rangle$
boundary	-	$\oint \mathbf{\Omega} \cdot \mathbf{n} (u_n \mathcal{G} u_{n'} + \mathcal{G} u_n u_{n'}) \mathbf{ds}$
source	$\langle \mathbf{\Omega} \cdot \nabla u_n Q \rangle + \langle \mathcal{G} u_n Q \rangle$	$\langle \mathbf{\Omega} \cdot \nabla u_n Q \rangle + \langle \mathcal{G} u_n Q \rangle$

Source Void Test Problem (Ackroyd/Watanabe)

$\sigma_t = 0.2$
$\sigma_s = 0.19$

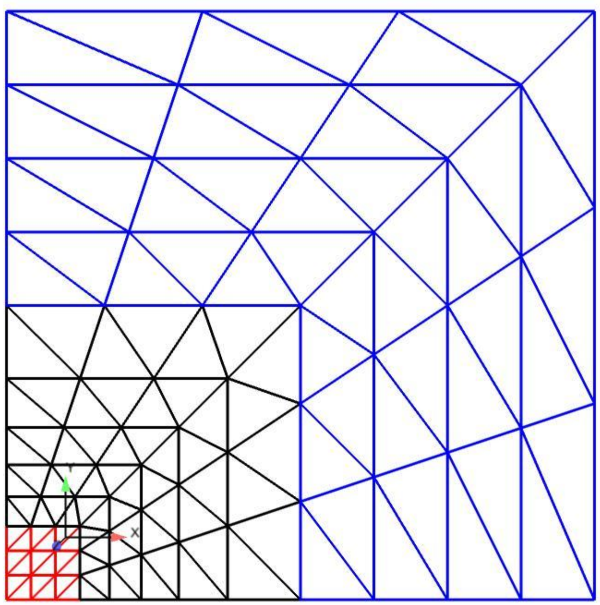


Scalar Flux Distribution Compared with Ackroyd's Reported MCNP Results

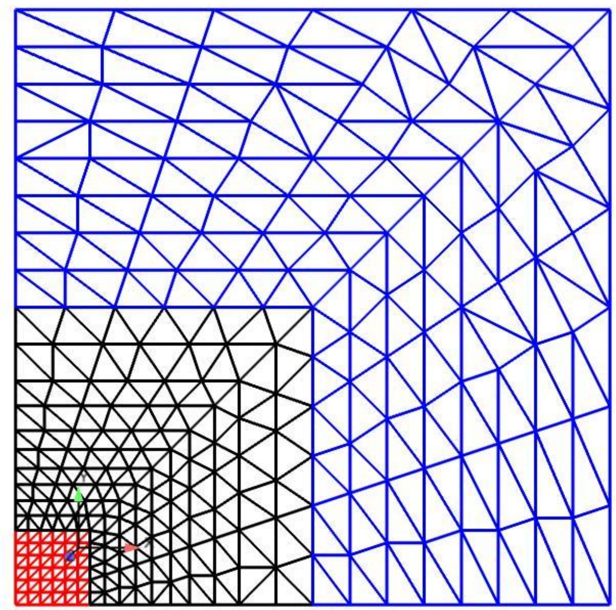


Convergence analysis

- **Start with coarse unstructured triangular mesh**
- **Successively refine by subdividing triangles into four parts**

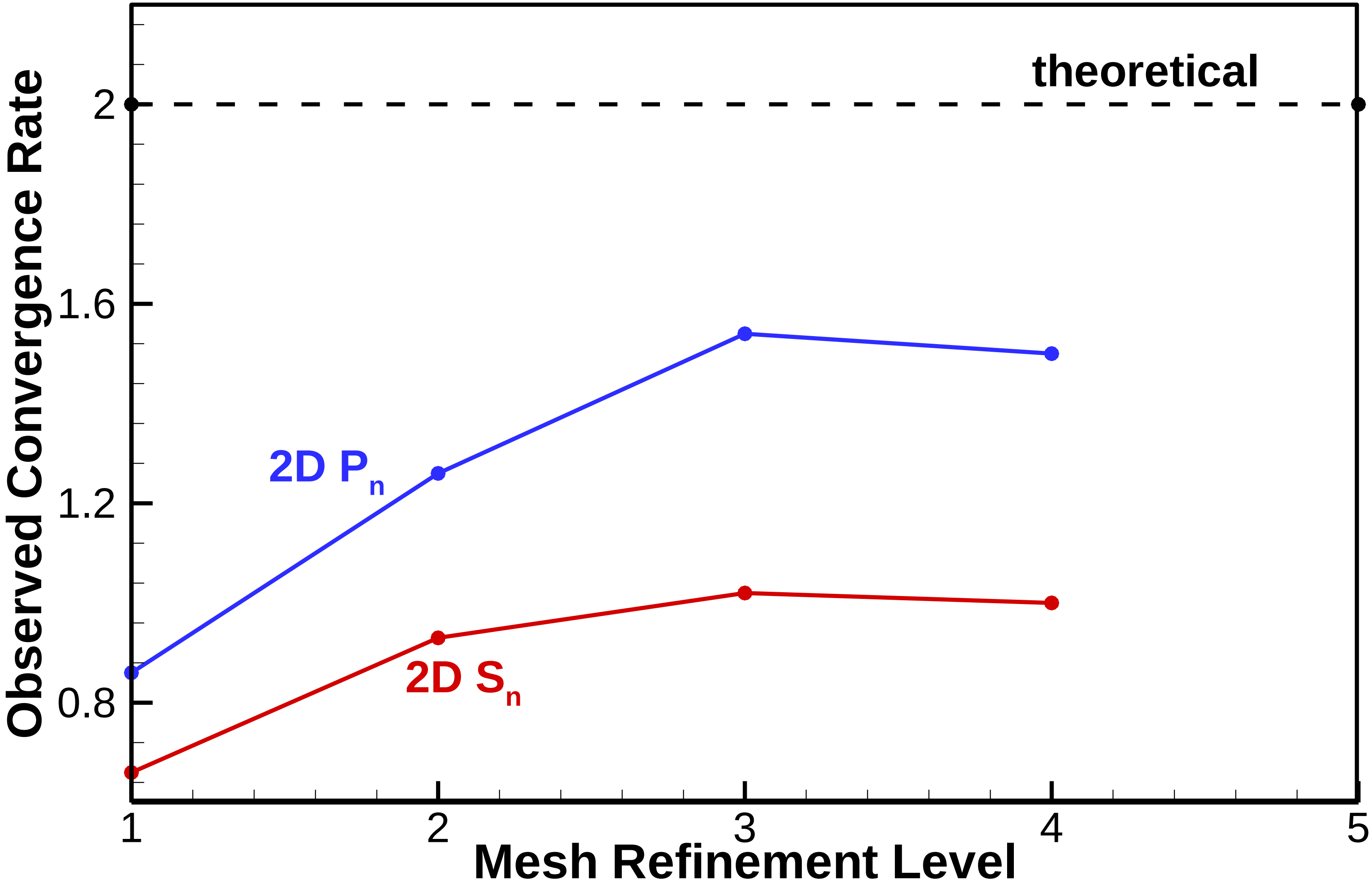


level 0

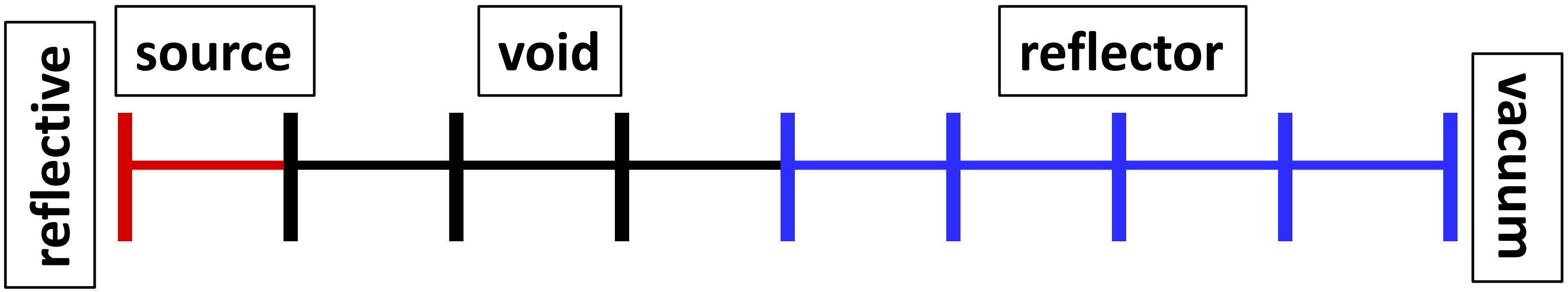


level 1

Observed Convergence Rates for Source-Void Test Problem

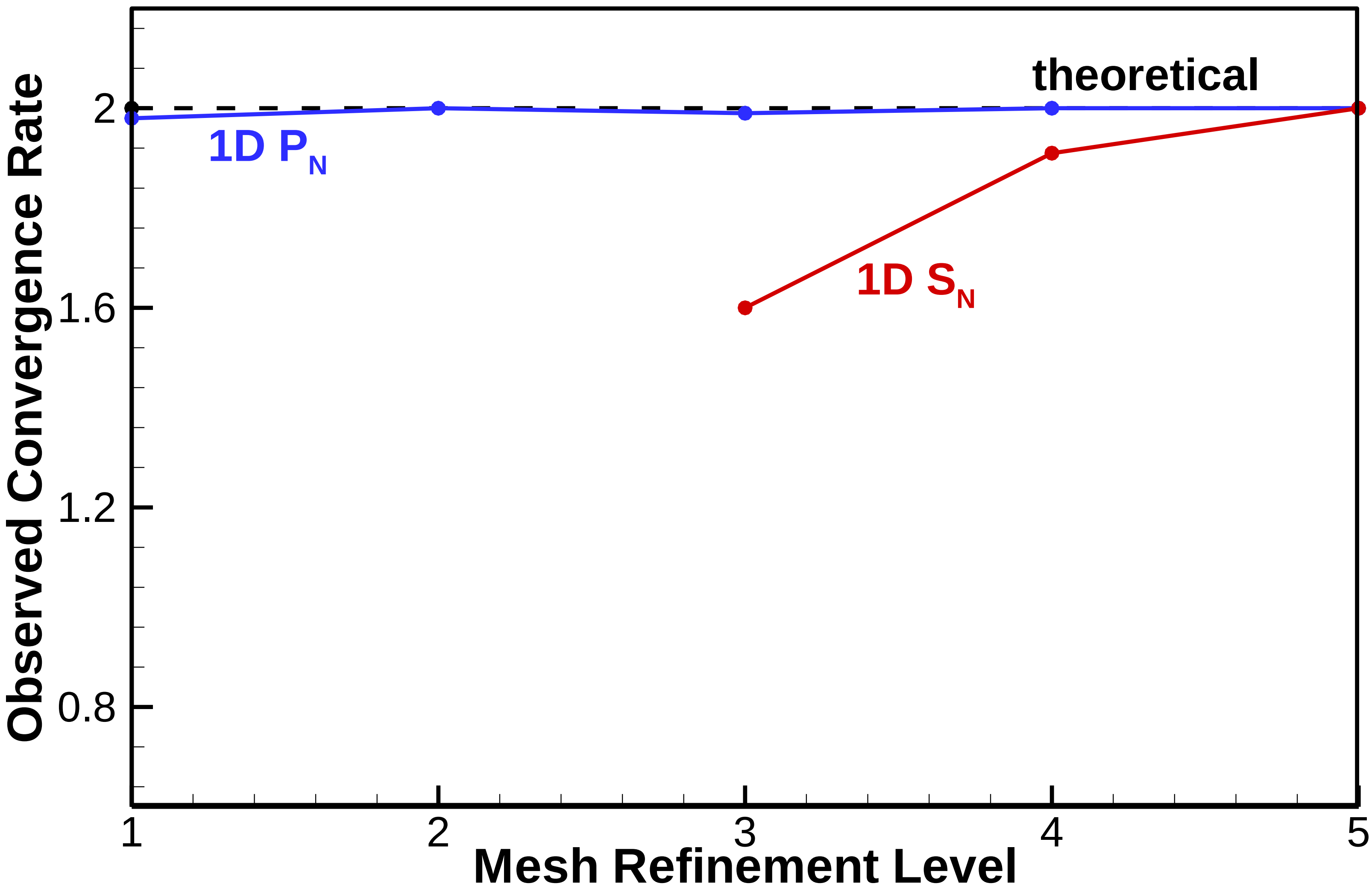


1D Mockup of Test Problem for Convergence Analysis



σ_t=0.2
σ_s=0.19

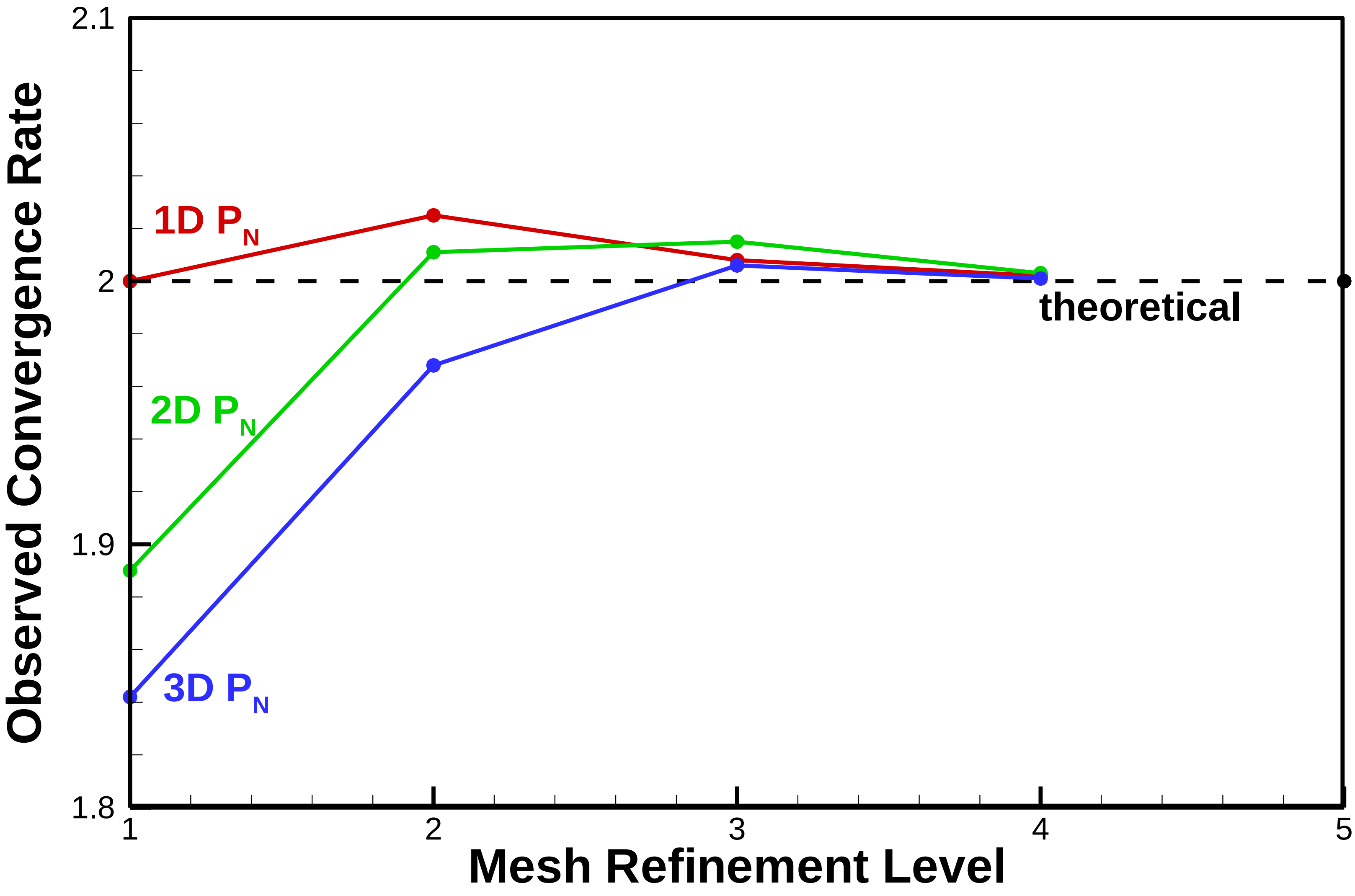
Observed Convergence Rates for 1D Mockup



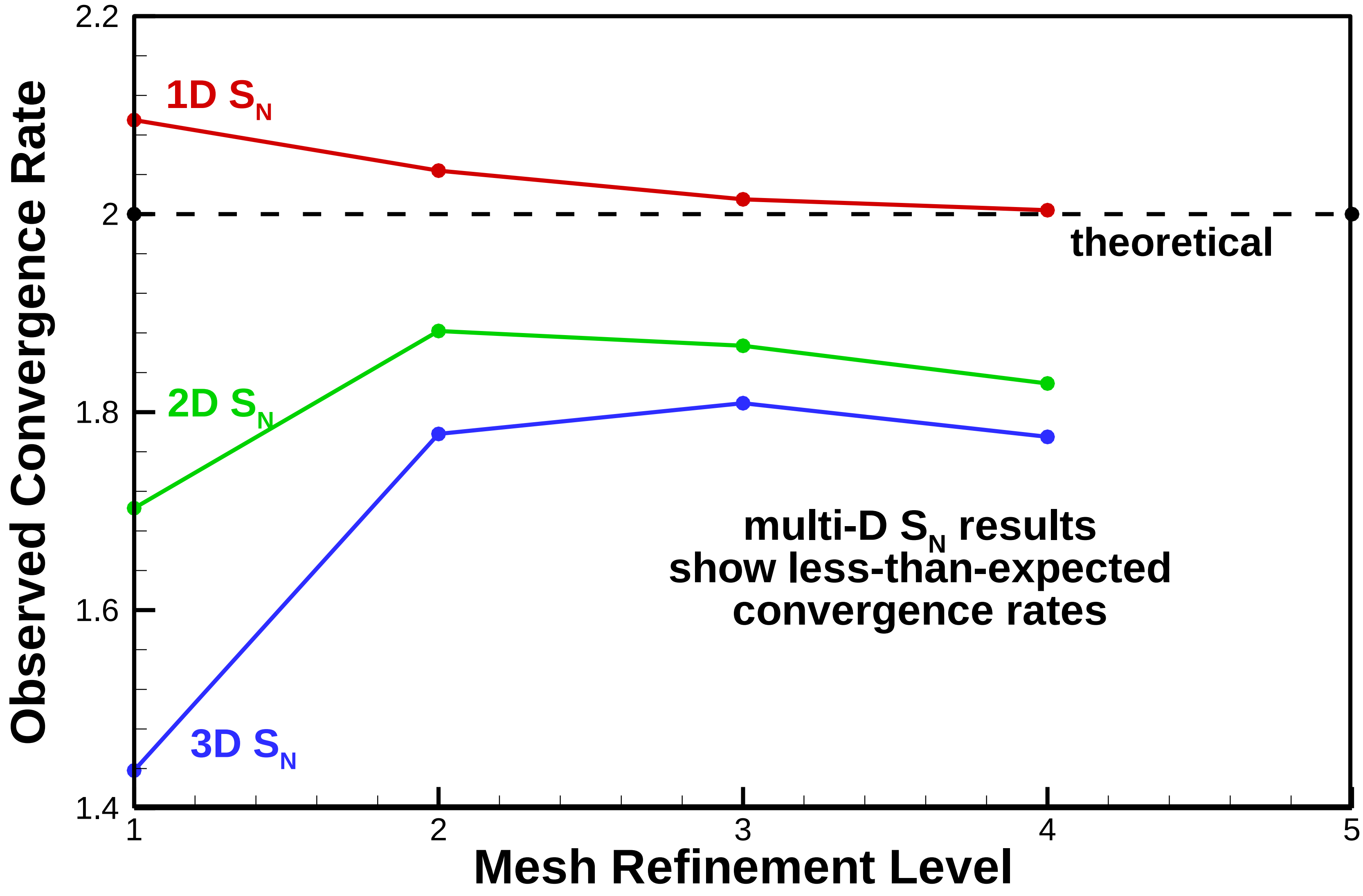
Smooth Manufactured Test Problems

- Unit slab, square or cube
- Isotropic angular flux
- Quadratic spatial dependence of angular flux
- Linear finite elements (edge, triangle or tetrahedron)
- Unit total cross section
- No scattering

Observed Convergence Rates for Smooth P_N MMS Test



Observed Convergence Rates for Smooth S_N MMS Test



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Why Does Multidimensional LS S_N Solver Exhibit Lower-Than-Expected Convergence Rate?

- **Differences compared with first-order transport solver**
  - Continuous finite elements vs. discontinuous
  - Transport operator (includes spatial cross-derivative terms)
- **Differences compared with LS P_N Solver**
  - Boundary condition treatment
  - Angular moments vs. discrete directions
- **Differences compared with 1D transport**
  - Unstructured mesh vs. structured mesh
  - Angular quadrature set
  - Transport operator (includes spatial cross-derivative terms)

Galerkin Treatment for Lebedev quadrature

- **Needed for mapping between discrete and moments space without loss of accuracy**
- **Lebedev quadrature sets have fewer directions than comparable level-symmetric sets for the same accuracy**
- **Lebedev quadrature contains directions along coordinate axes**
- **Need fewer spherical harmonics to form non-singular moment-to-discrete matrix**
- **Use Gram-Schmidt procedure to extract non-singular set of spherical harmonics**

S_N order	Number directions		Maximum complete Legendre order in Galerkin moment-to-discrete matrix	
	Level symmetric	Lebedev	Level symmetric	Lebedev
2	8	6	1	1
4	24	14	3	2
8	80	38	7	4
16	288	110	15	8

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Summary

- Least-squares S_N and P_N algorithms implemented and tested in SCEPTRE
- Coupled with first-order sweeps-based algorithm
- Expected convergence rates observed for 1D S_N and P_N LS tests
- Less-than-expected convergence rates observed for multi-D S_N LS tests
- Developed procedure for computing Galerkin scattering set for Lebedev quadrature