SCEPTRE Convergence with Pn & Sn Order

August 11, 2010/10:50

Jeffrey Chenhall
Undergraduate Summer Intern

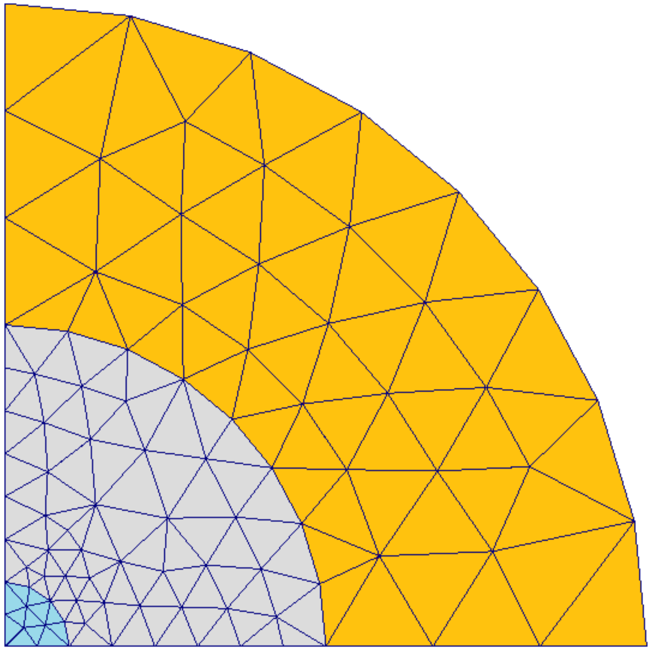
SAND2010-5282P

SCEPTRE

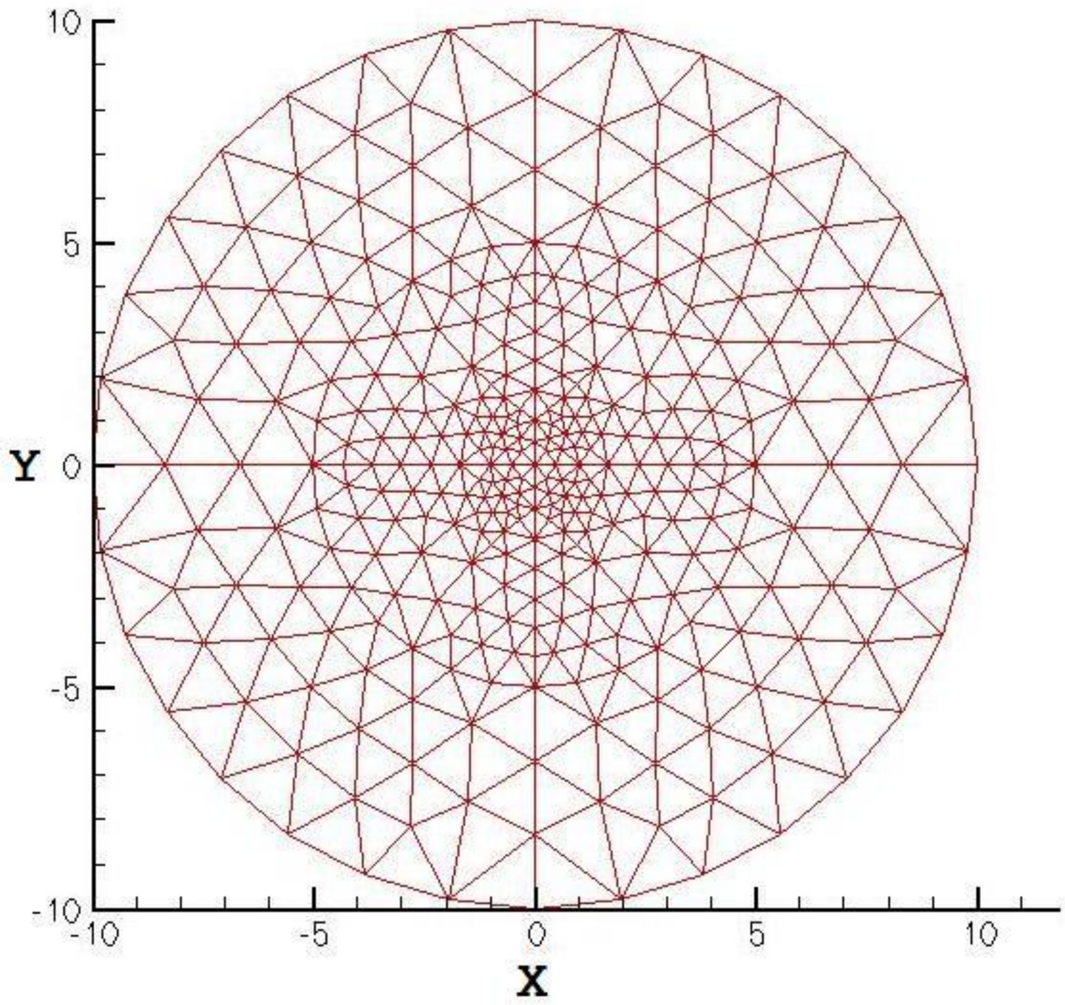
- SCEPTRE (Sandia's Computational Engine for Particle Transport for Radiation Effects)
  - A Deterministic code for solving the Boltzmann transport equation.
  - Contains first and second order solver methods
- I focused on convergence of the solution with respect to discrete ordinate (Sn) and spherical harmonic (Pn) order

The Meshes

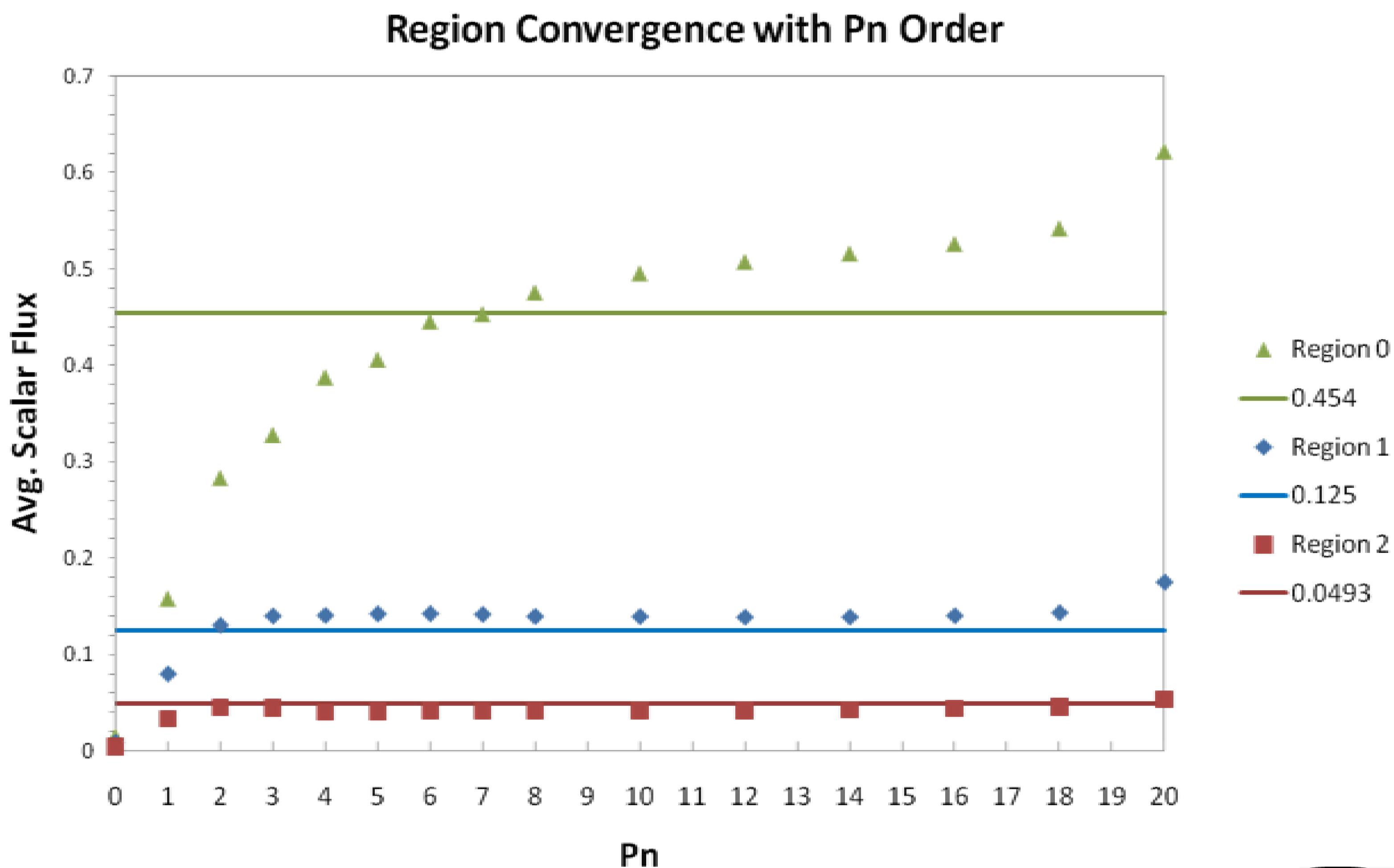
- Used full and quarter meshes
  - Four levels of refinement used (r = 2)
- Meshes Contained Three regions
  - Source (blue)
  - Void (grey)
  - Reflector (orange)



Full Mesh



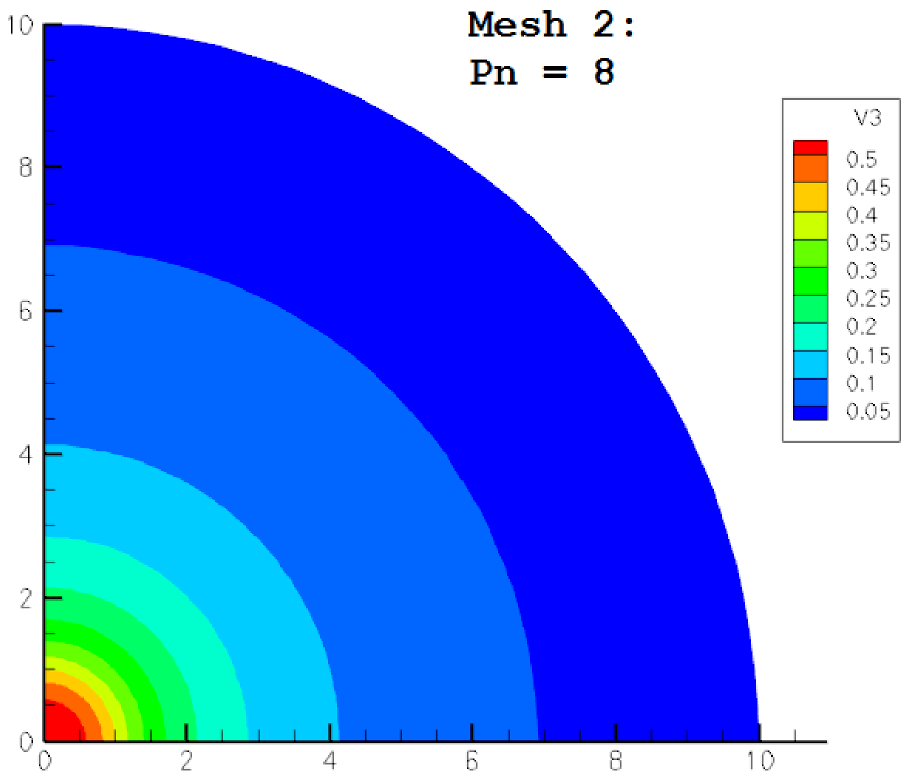
Pn Method

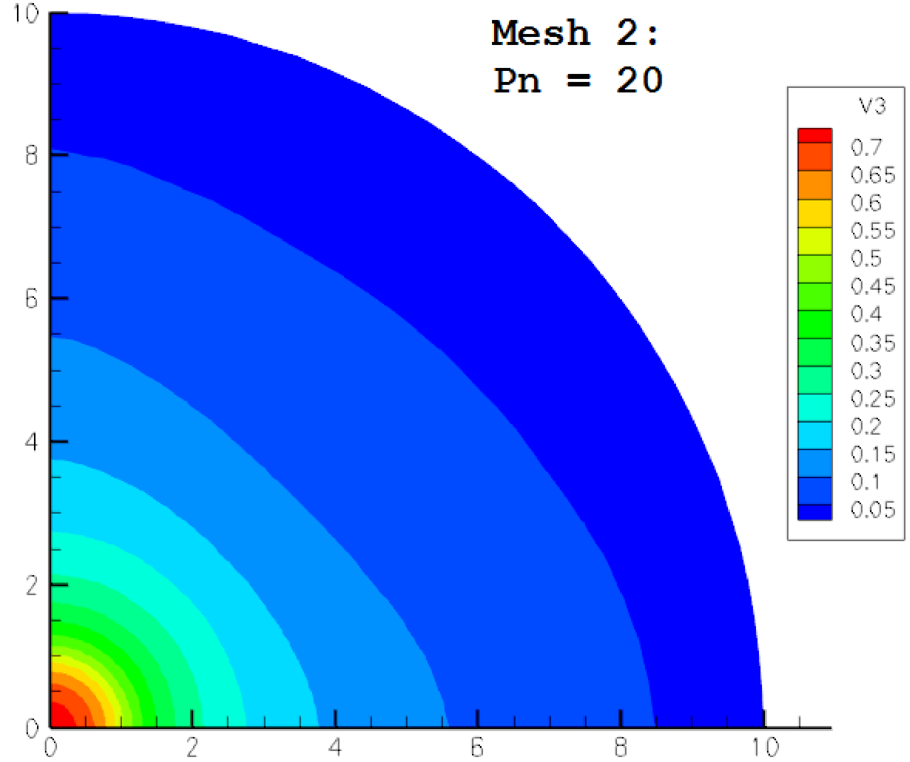


Sandia National Laboratories

Pn Method

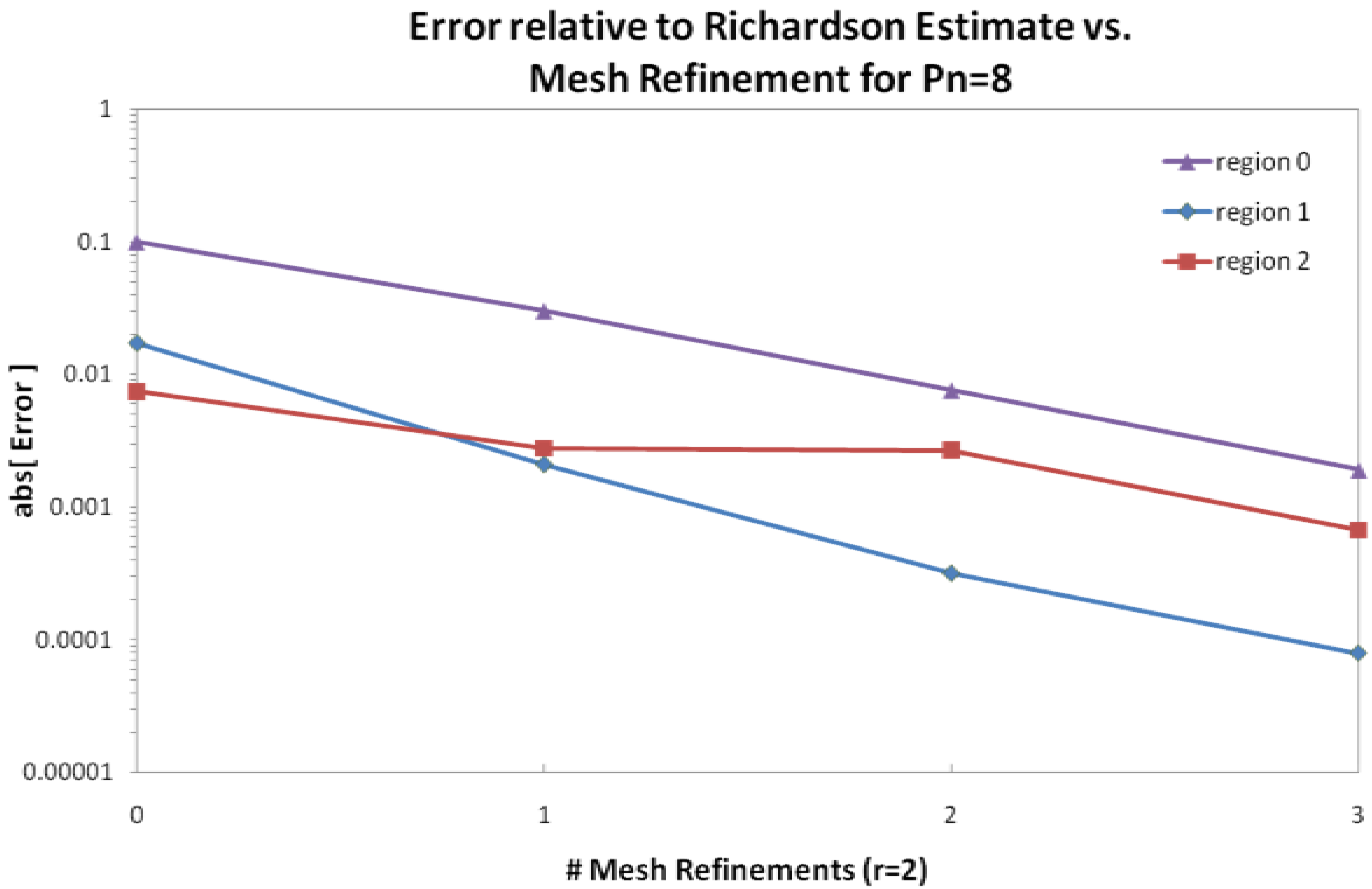
Pn method becomes less radial-symmetric at higher orders.





Sandia National Laboratories

Error Pn Method



Convergence Rates Pn Method

- **Differs from the expected value of 2**

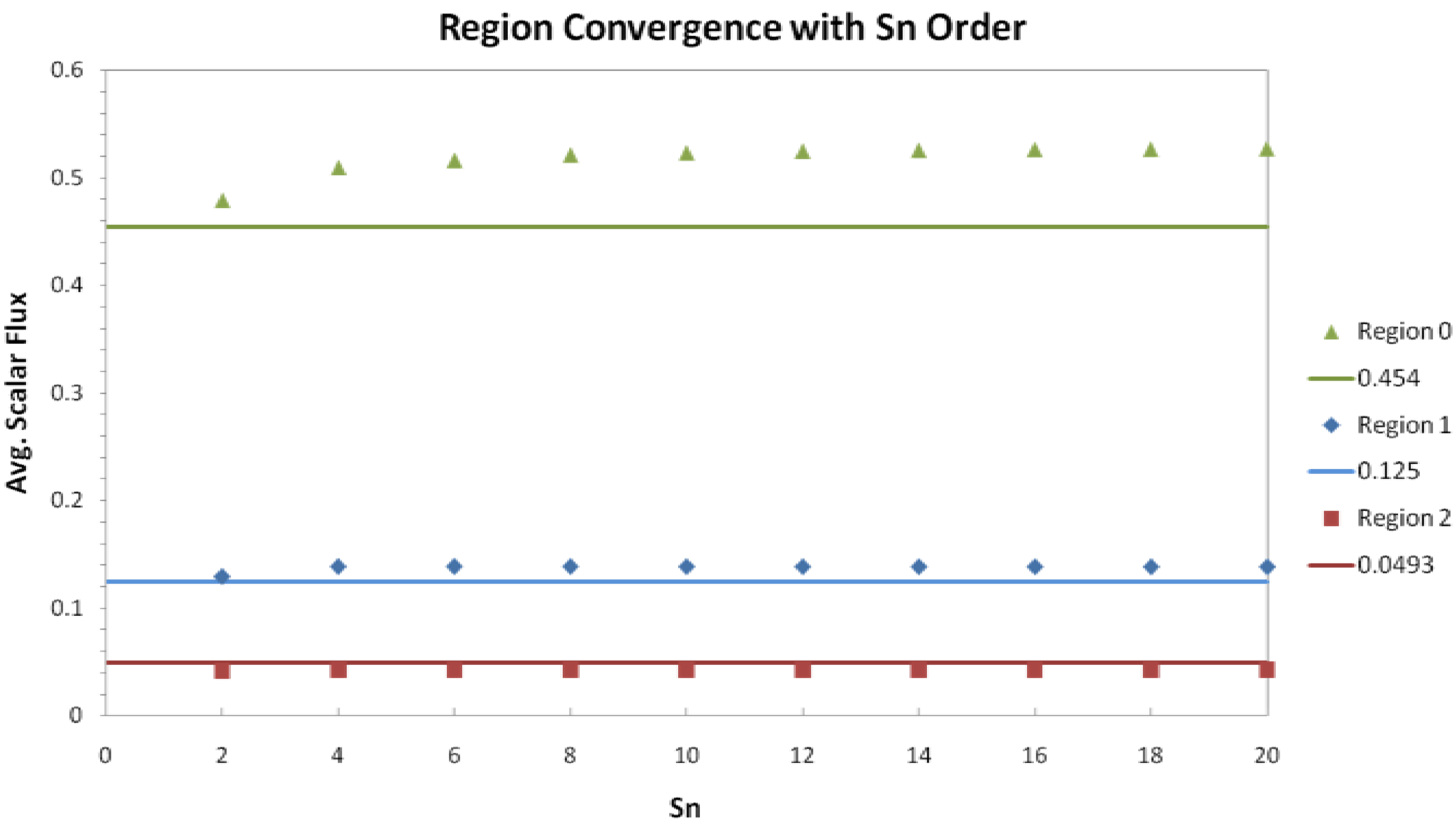
Convergence Rate			
Refinement	**Region 0**	**Region 1**	**Region 2**
0-1	1.73	3.04	1.42
1-2	1.99	2.74	0.0511
2-3*	2	2	2

*Identically Equal to 2 due to extrapolation method

Pn Method

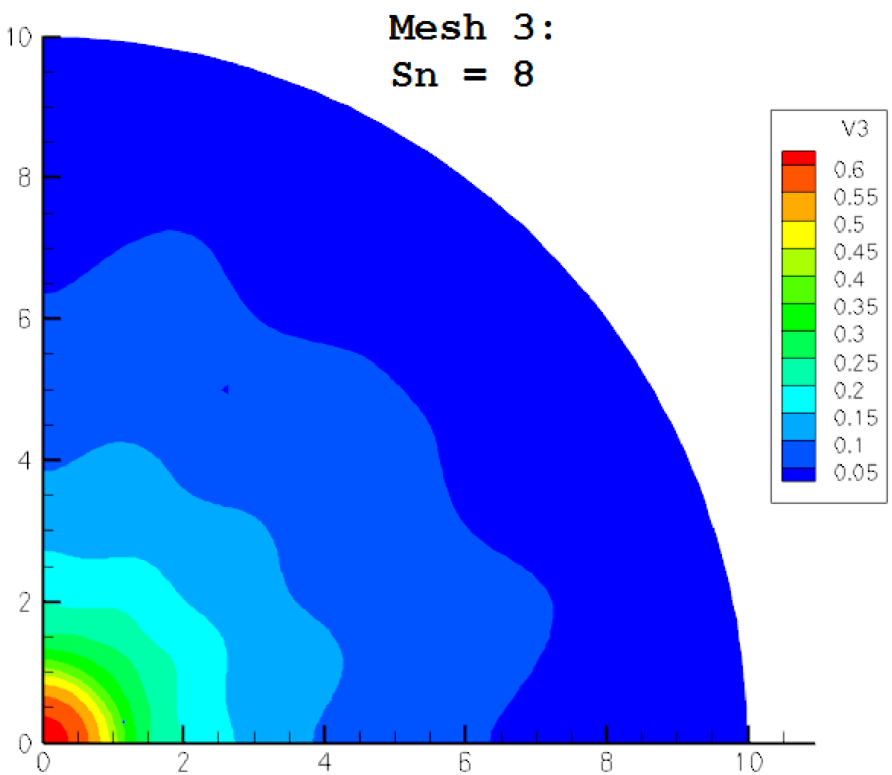
- **Conclusions**
  - Appears to have stable convergence until high order is reached
    - Possibly due to Sn (Fully Symmetric) only available up to 20
  - Error drops off exponentially with refinement
  - Smooth radially symmetric solution is obtained
  - Region 0 value higher than expected

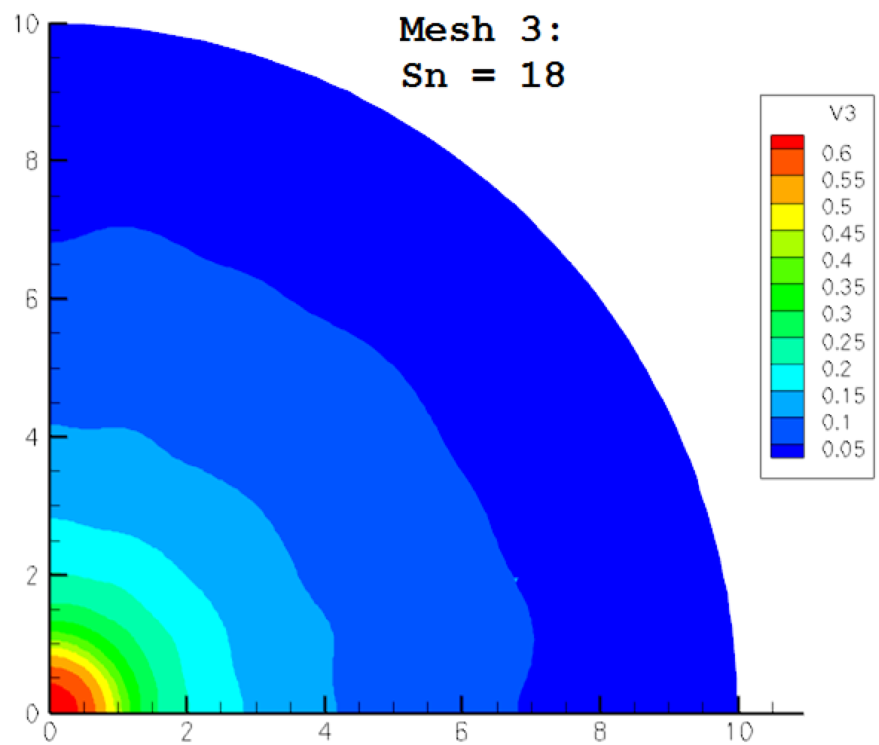
Sn (Level Symmetric) Method



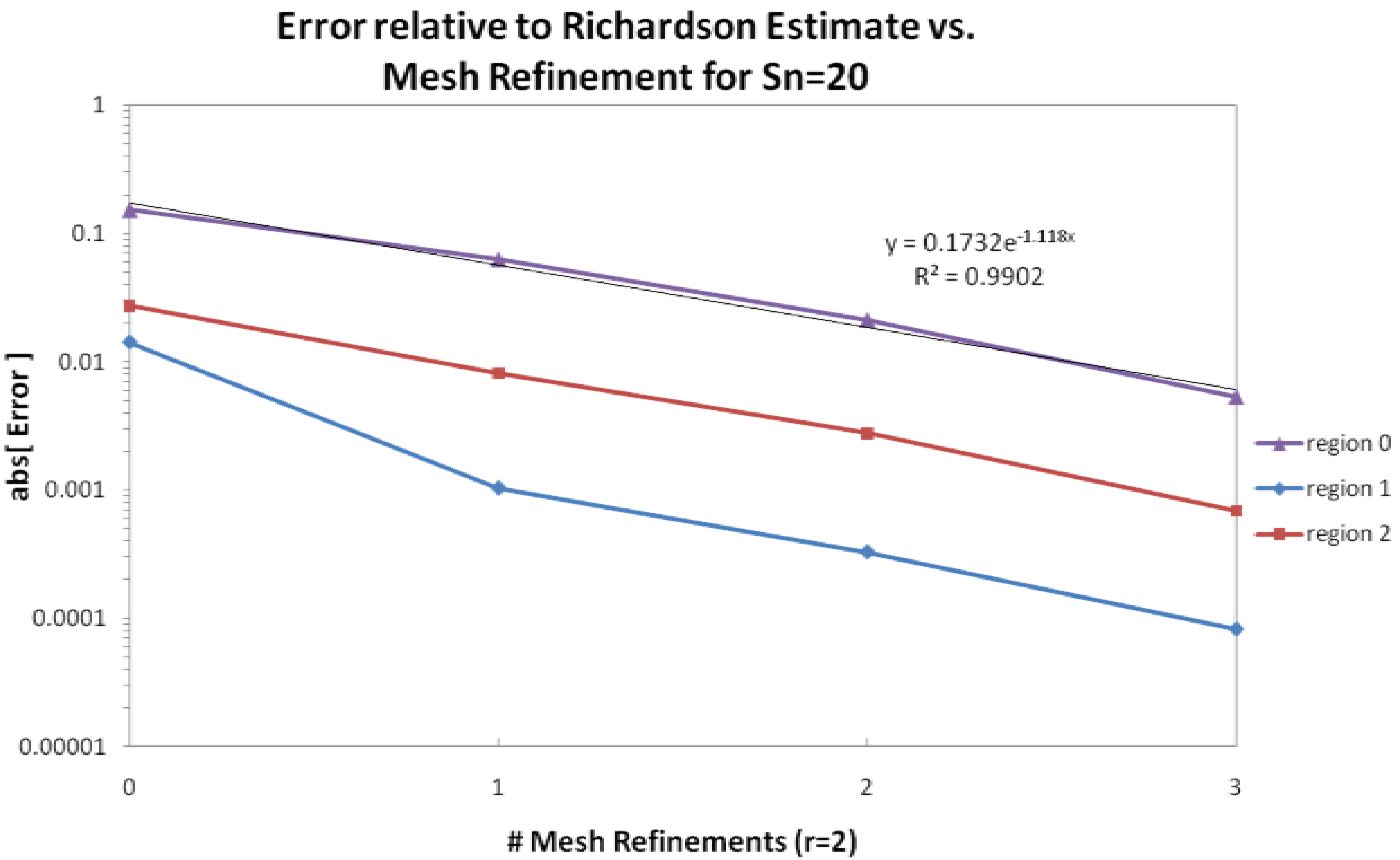
Sn Method

- Sn method becomes more radially symmetric for higher order





Error Sn Method



Convergence Rates Sn Method

- **Differs from the expect value of 2**

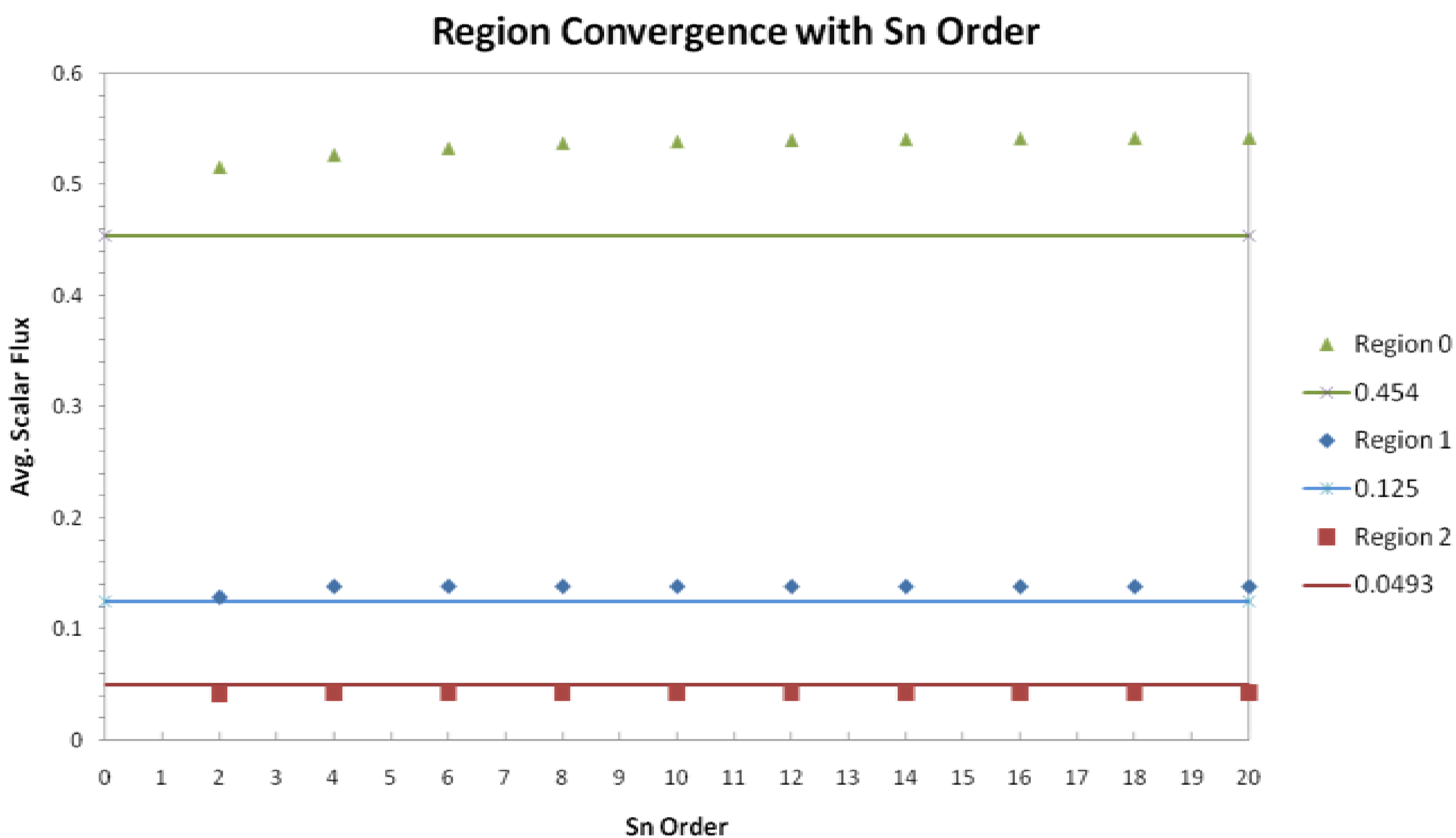
Convergence Rate			
Refinement	**Region 0**	**Region 1**	**Region 2**
0-1	1.29	3.78	1.75
1-2	1.57	1.65	1.55
2-3*	2	2	2

*Identically Equal to 2 due to extrapolation method

Conclusions Sn Method

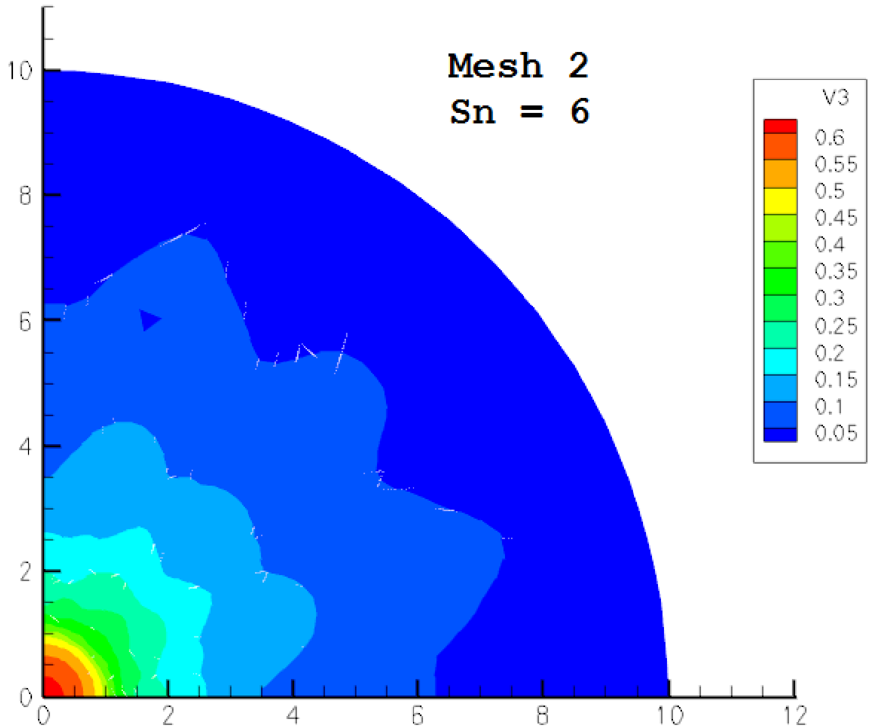
- Conclusions
  - Appears to have stable value of average scalar flux for all orders
  - Ray Effects are present which can distort the solution
  - Error drops off exponentially with refinement
  - Region 0 value higher than expected

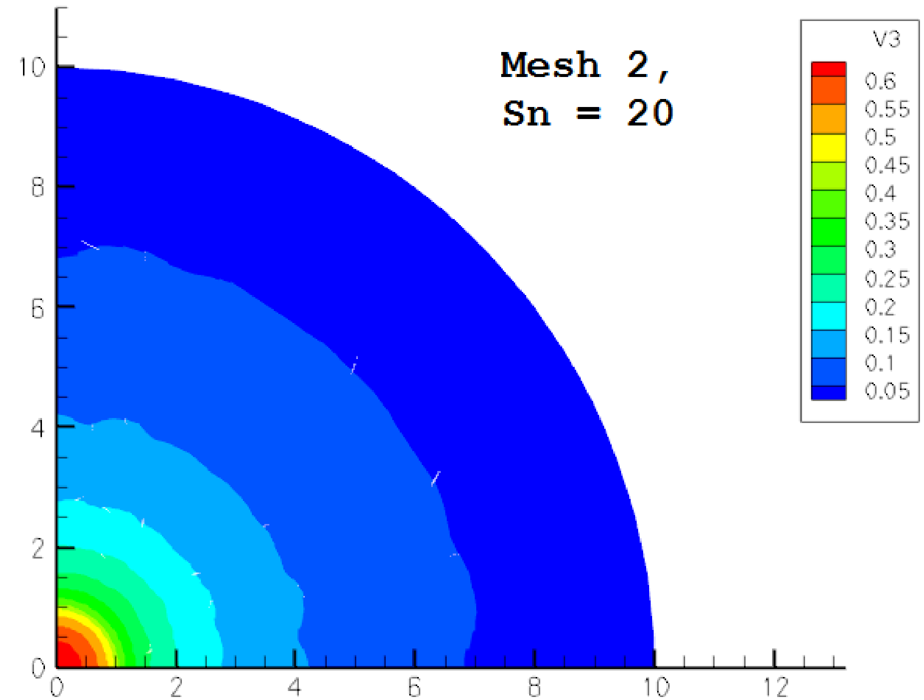
1st Order Solver



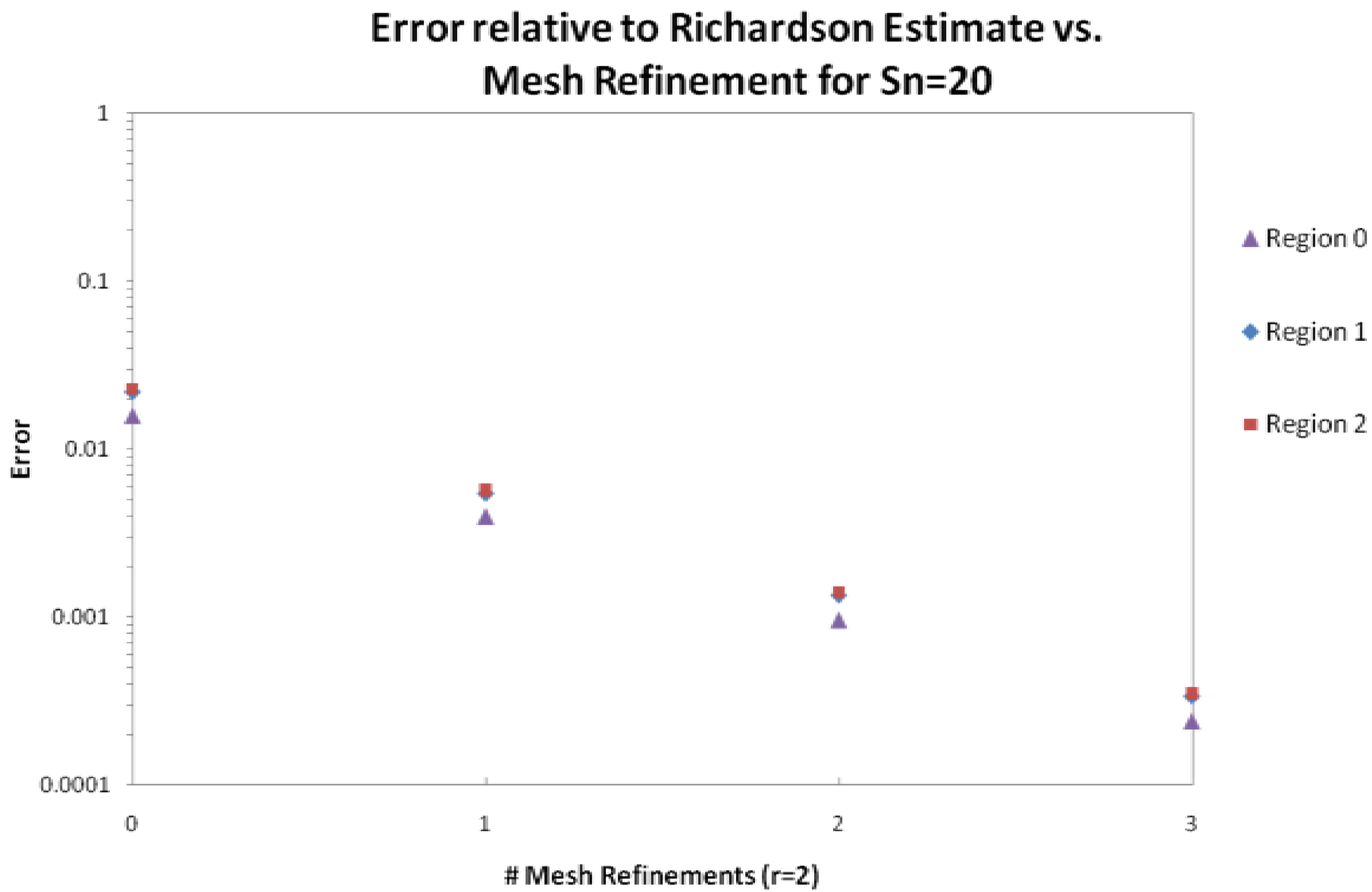
1st Order Solver

- **Ray Effects Present**





Error 1st Order Solver



Convergence Rates 1st Order Solver

- **Good agreement with expected rate of 2.**

Convergence Rate			
Refinement	**Region 0**	**Region 1**	**Region 2**
0-1	1.99	2.01	2.00
1-2	2.04	2.02	2.02
2-3*	2.00	2.00	2.00

*Identically Equal to 2 due to extrapolation method

Conclusions 1st Order Solver

- Conclusions
  - Appears to have stable value of average scalar flux for all orders
  - Ray Effects are present which can distort the solution
  - Error drops off exponentially with refinement
  - Region 0 value higher than expect

Comparison of Methods (Mesh 3)

Sn/Pn=18, Mesh 3	Region0	Region 1	Region 2	% Diff 0	% Diff 1	% Diff 2
Sn	0.536	0.138	0.0427	18.0%	10.7%	-13.4%
Pn	0.551	0.143719	0.0463	21.4%	15.0%	-6.05%
1st	0.541	0.138	0.0427	19.3%	10.6%	-13.3%

Sn/Pn=8, Mesh 3	Region0	Region 1	Region 2	% Diff 0	% Diff 1	% Diff 2
Sn	0.530719	0.139	0.0427	16.9%	10.9%	-13.5%
Pn	0.478	0.140	0.0414	5.35%	11.6%	-16.0%
1st	0.537	0.138	0.0427	18.3%	10.8%	-13.4%

Sn Quadrature Sets

- Quadrature sets exactly integrate spherical harmonics up to an order
- Level Symmetric
  - Pros: Closed form formula
  - Cons: only goes up to order 20 due to unphysical negative weights at higher order.
- Lebedev
  - Pros: ½ the directions for same benefit, higher orders up to 130 available
  - Cons: no closed form formula for Lebedev.

Lebedev

- **Moment to Discrete Matrix**
  - **Rows are quadrature directions, Columns are spherical harmonics evaluated at the direction**
  - **Needs to have spherical harmonics chosen in order to be invertible.**
  - **Used a Gram-Schmidt Process to determine linear independence of the columns.**

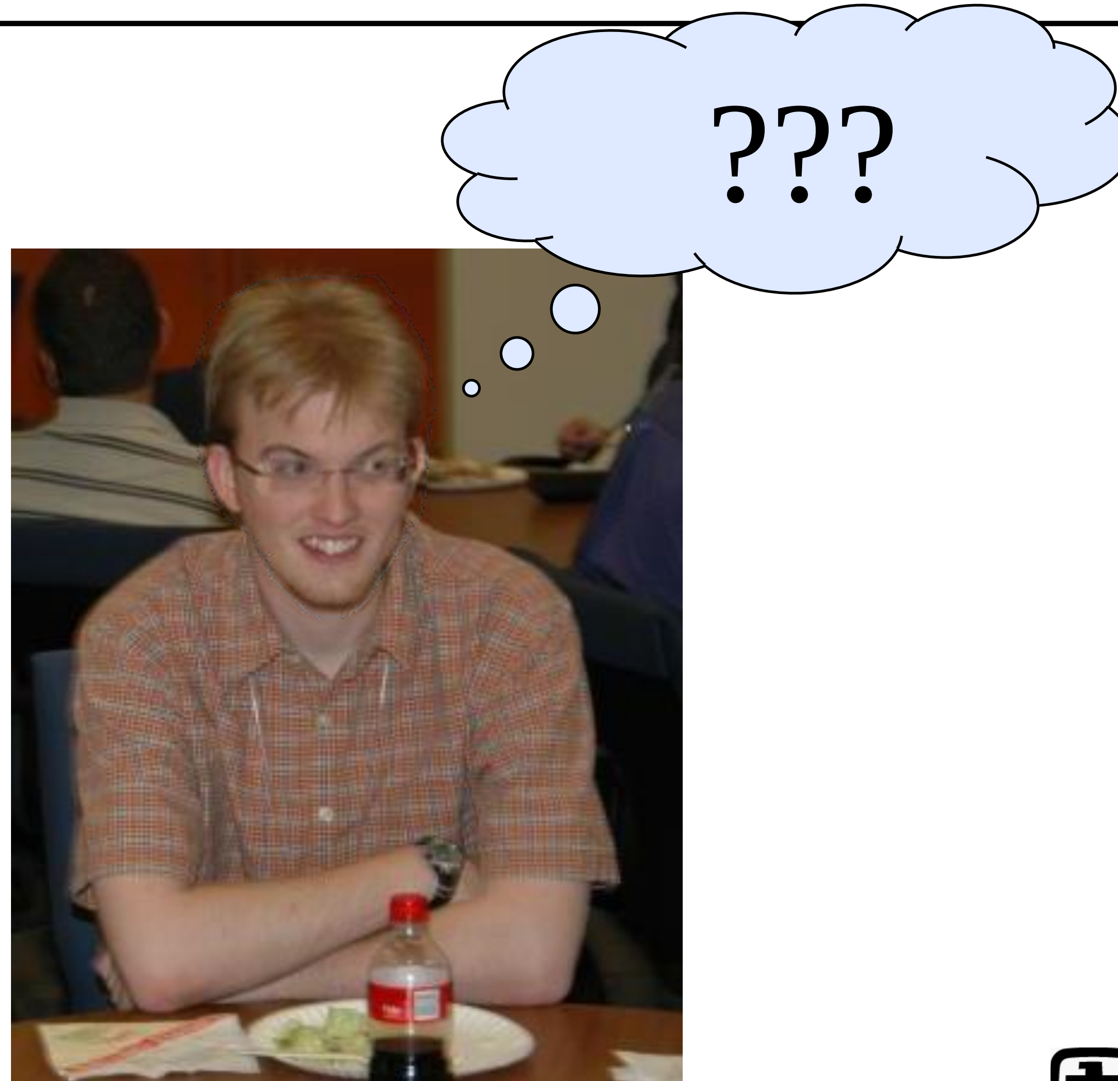
$$\boldsymbol{u}_1 = \boldsymbol{v}_1 / \|\boldsymbol{v}_1\|$$

$$\boldsymbol{u}_k = \left(\boldsymbol{v}_n - \sum_{k=1}^{n-1} \langle \boldsymbol{v}_n , \boldsymbol{u}_k \rangle \cdot \boldsymbol{u}_k \right) \Big/ \left\| \boldsymbol{v}_n - \sum_{k=1}^{n-1} \langle \boldsymbol{v}_n , \boldsymbol{u}_k \rangle \cdot \boldsymbol{u}_k \right\|$$

Lebedev Results?

- Work in Progress

Questions?



The End