Effectiveness of Various Error Metrics in SCEPTRE

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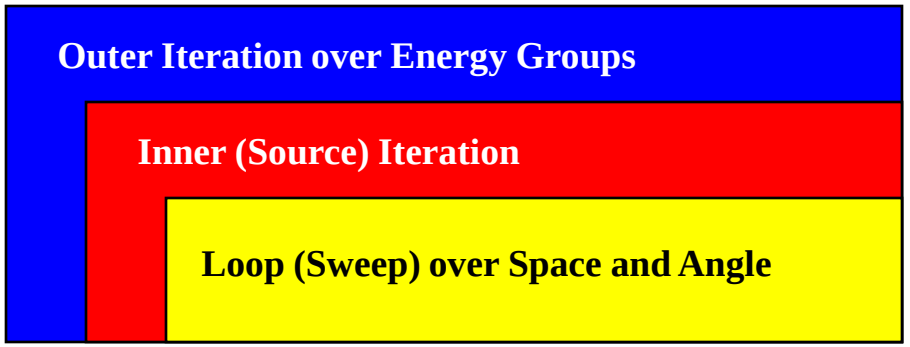
Objective

- **Investigate accuracy of error metrics in SCEPTRE and produce useful benchmarks**
  - **Identify metrics that do not work well**
  - **Identify metrics that do work well**
  - **Produce easy to reference results**

Background-Intro

- SCEPTRE - Sandia's Computational Engine for Particle Transport for Radiation Effects
  - Deterministic finite-element radiation transport code
  - Boltzmann transport equation

An Iteration		
Phase 1	Fixed	Compute
Phase 2	Compute	Fixed



- Error metrics determine number of iterations
  - Each iteration includes a sweep

$$\Omega \cdot \nabla + \sigma_t \bar{\psi}(r,\Omega) = M\Sigma D\psi(r,\Omega) + Q(r,\Omega)$$

Background-Metrics

- **Error Metrics consist of error norms what parameters are used in them**
  - **Error Norm/Semi-Norm**

$$\varepsilon_h(\mathbf{r},\Omega) = \phi(\mathbf{r},\Omega) - \phi_h(\mathbf{r},\Omega)$$

    - **L, H, or S**
    - **1, 2, or infinity**
    - **Absolute or Signed**

$$L_p\text{norm} = \left(\int\int \left|\varepsilon_h(\mathbf{r},\Omega)\right|^p d\mathbf{r}d\Omega \right)^{1/p}$$

$$H_p\text{energy norm} = \left(\int\int \nabla\varepsilon_h(\mathbf{r},\Omega) \cdot \nabla\varepsilon_h(\mathbf{r},\Omega)^{p/2} d\mathbf{r}d\Omega \right)^{1/p}$$

$$S_p\text{streaming norm} = \left(\int\int \left|\Omega \cdot \nabla\varepsilon_h(\mathbf{r},\Omega)\right|^p d\mathbf{r}d\Omega \right)^{1/p}$$

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Background-Norm Parameters

- **More error norm parameters**
  - **Region**
  - **Continuous or Discrete**
  - **Stopping Criteria**

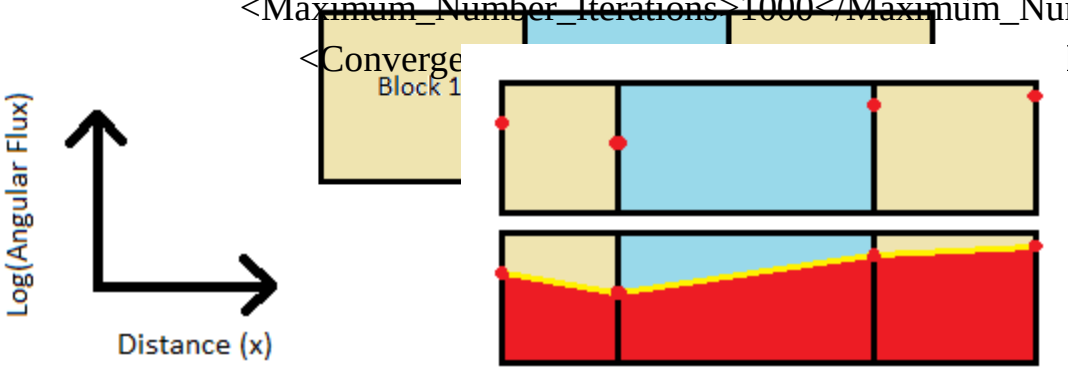
Region Type	Specific Region
Whole	all blocks
Region	block #
Leakage	right/left/etc. side
Surface	external boundary

$$L_p\text{norm} = \left(\sum \iint \left| \varepsilon_h(\mathbf{r},\Omega) \right|^p d\mathbf{r}d\Omega \right)^{1/p}$$

$$L_p\text{norm} = \left(\iint \left| \varepsilon_h(\mathbf{r},\Omega) \right|^p d\mathbf{r}d\Omega \right)^{1/p}$$

<Maximum_Number_Iterations>1000</Maximum_Number_Iterations>

<Converge lerance>



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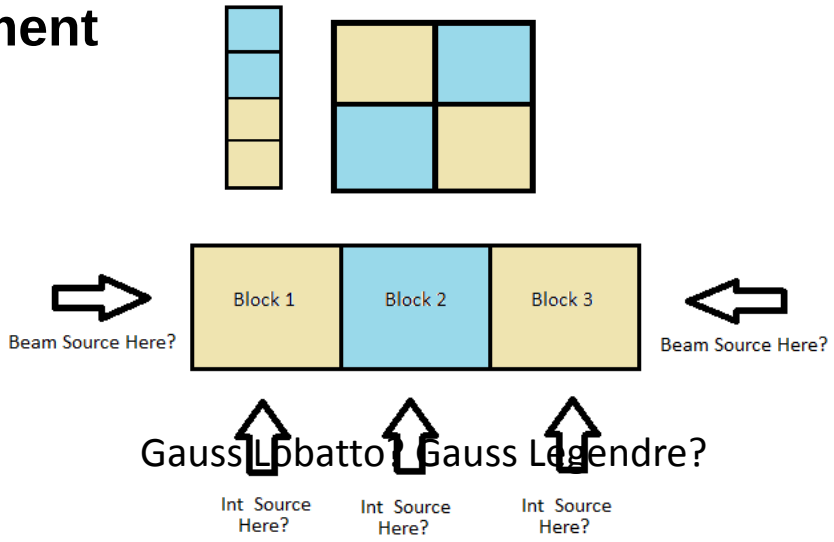
Background-Geometry

- **Physical geometry and the discretization method used also affects norm operation**
  - **Physical**
    - **Source Type & Placement**
    - **Dimensionality**
    - **Size & Shape**
    - **c, scattering ratio**
    - **Optical Thickness**
  - **Discretization**
    - **Quadrature method**



Background-Estimated Error

- **Accuracy of estimated error governs accuracy of quantities of interest**
  - **Estimated error is error according to norm at iteration**
  - **Stop iterating when estimated error below tolerance**
  - **Number of iterations determines accuracy of physical quantities (and therefore actual error of them)**

$$e(\Psi) = \frac{\int \Psi(\infty) - \int \Psi(\Psi)}{\int \Psi(\infty)}$$

  - **Trick to balance computational time and accuracy**

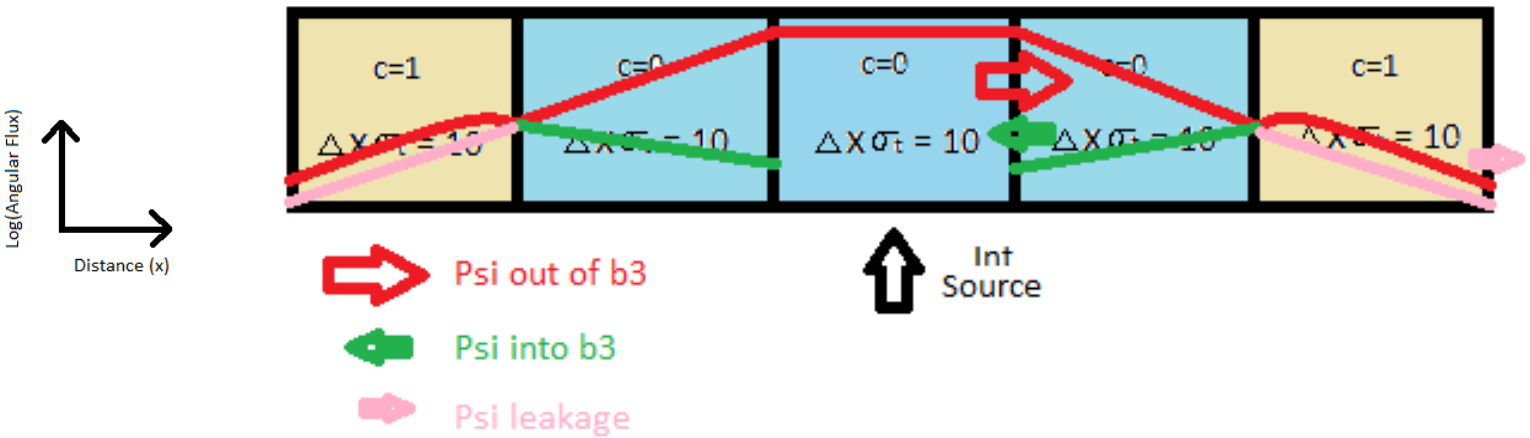
Background-Review

- **Error Metric**
  - **Consists of:**
    - **Norm**
    - **Parameters**
  - **Affected by:**
    - **Physical geometry & discretization method**

- **Estimated Error**
  - **Accuracy determines accuracy of quantities of interest**
  - **Don’t over or under iterate**

Results-Beam 3

Geometry for the Beam 3 Test Set



Evolving Angular Flux

	Psi out of b3	Psi into b3	Psi leakage
1 iteration	0.999954606	0	2.060502E-09
10 iterations	0.999954606	1.334365E-09	1.189094E-06
50 iterations	0.999954606	1.694030E-09	7.057503E-06
100 iterations	0.999954606	1.716267E-09	7.547262E-06
454 iterations	0.999954606	1.717085E-09	7.565288E-06

Investigating: Masked Errors/Choosing Metric Regions & Tolerance

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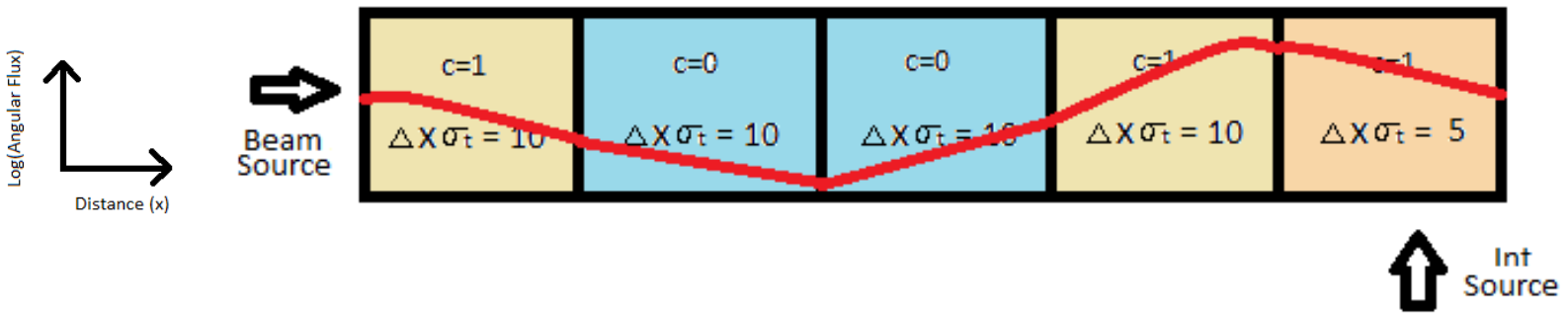
Results-Beam 10

- **Beam 10- Test each region with the matching metric region**
  - **L_2**
  - **Compare at critical points: tol e^{-n}, n={2,3,4,5,6,7}**

Geometry for the Beam 10 Test Set



Investigating: Accuracy of Reported Error

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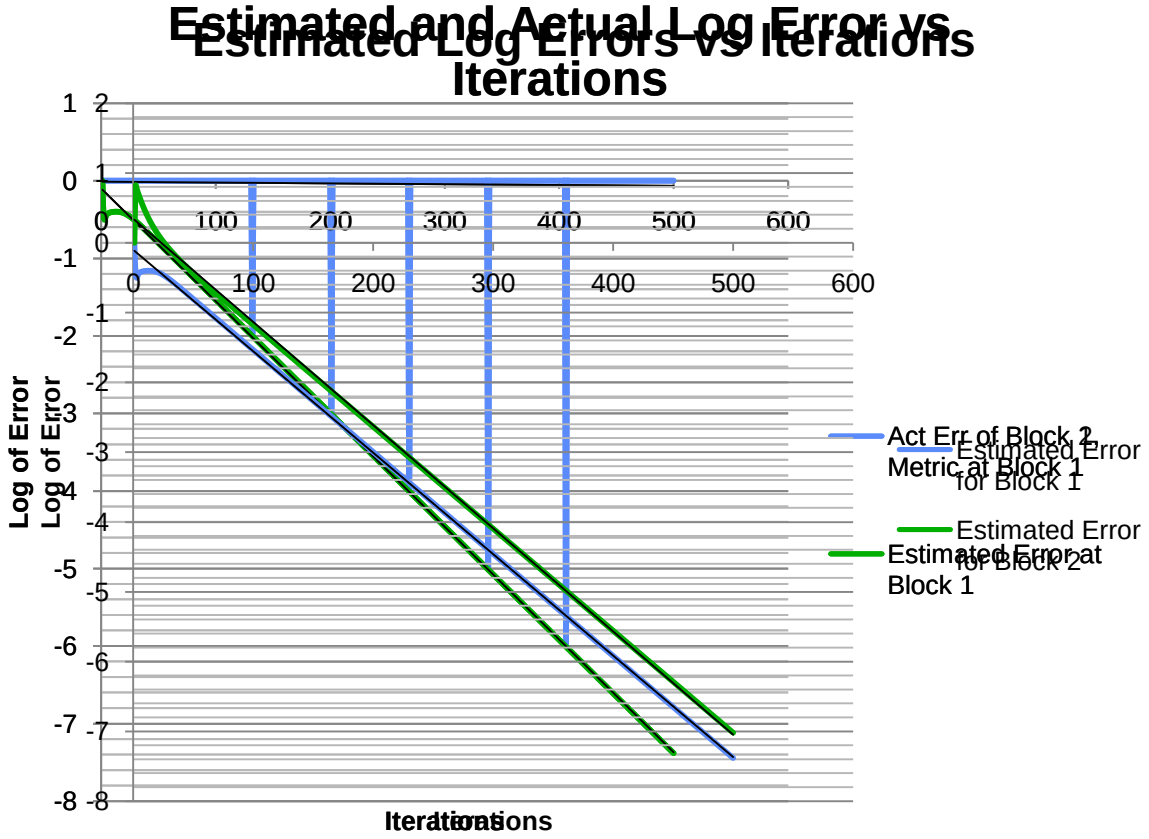
Results-Beam 10



Investigating: Accuracy of Reported Error

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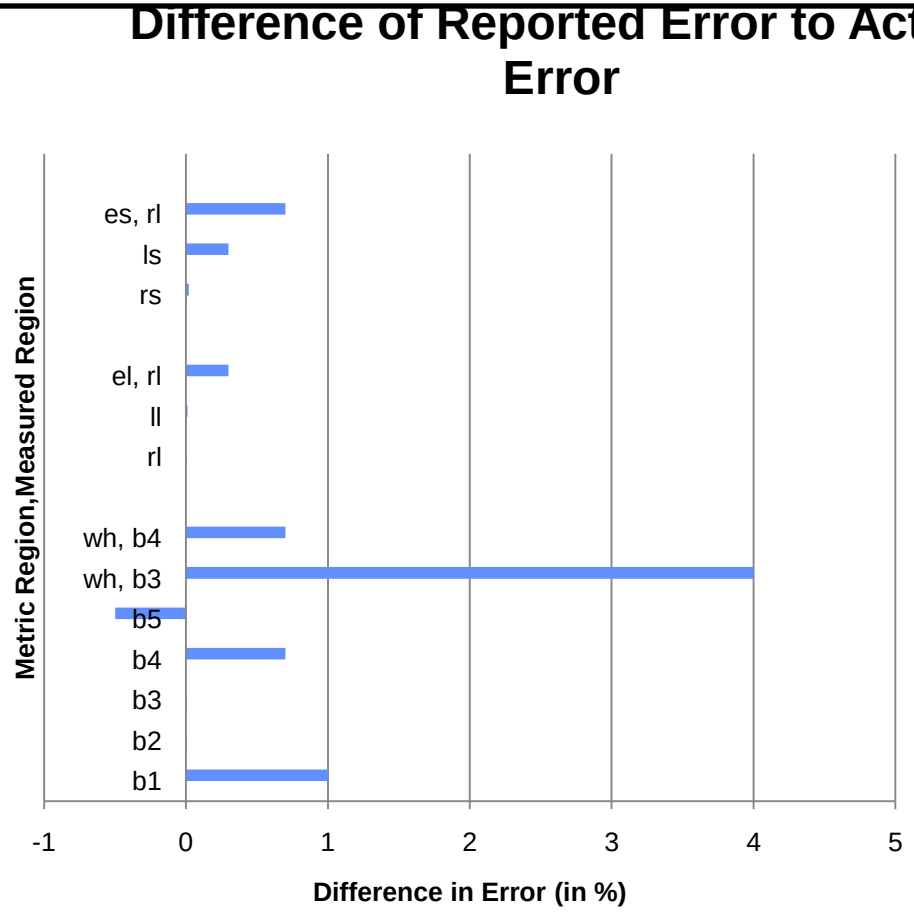
Results-Beam 10



Positive - too soon

Negative – could stop sooner

Designation	Meaning
b#	block #
wh	whole
r_	right side
l_	left side
e_	external boundary
_l	leakage
_s	surface

*"wh, b5“, "el, ll“, and "es, ll“ had over 100% negative difference

Investigating: Accuracy of Reported Error

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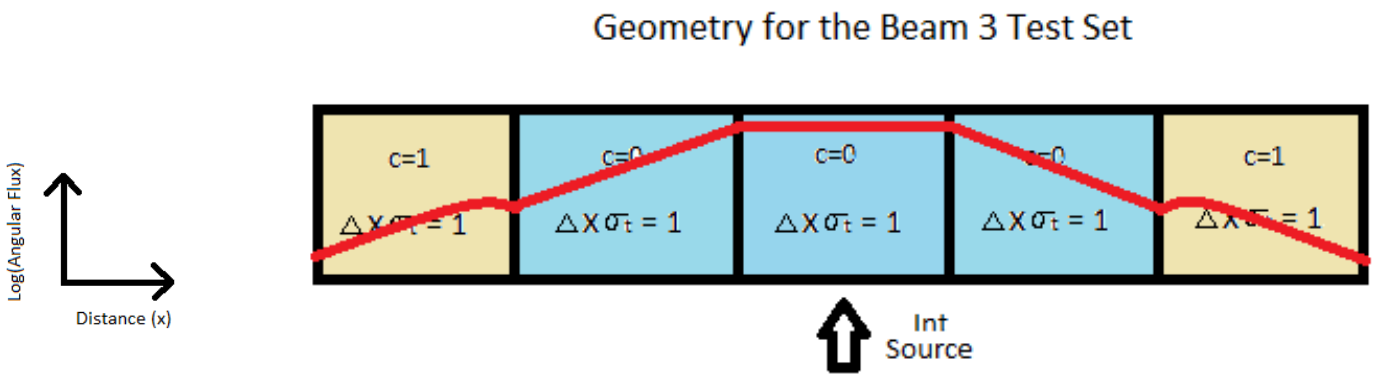
Results-Abs vs Sign



		Region of Metric, then Measurement								
		whole, b3	whole, b5	b3	b4	b5	rs	el, rl	b4 e-13	b5 e-13
L1 S1	it	17	17	15	16	19	18	18	31	33
	rep err	5.31E-08	5.31E-08	5.90E-08	9.29E-08	4.01E-08	8.96E-08	5.46E-08	4.98E-14	5.28E-14
	Act Err	8.2384E-09	6.942E-08	5.73E-08	5.68E-08	9.99E-09	3.34E-08	3.34E-08		
L1signed	it	18	18	2	16	2	2	18	31	2
S1signed	rep err	5.46E-08	5.46E-08	0	9.29E-08	0	0	5.46E-08	4.41E-14	0
	Act Err	3.1247E-09	2.633E-08	0.017193	5.68E-08	0.143516	0.180168	3.34E-08		

Investigating: Absolute vs Signed Norms

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Other Documented Tests

Test Inventory		
Test Set	Runs of SCEPTRE	Runs of Post Processing Code
Exploratory Testing	131	5
Email Prob	273	273
Beams 1-5	65	65
Beam 6	213	572
Beam 10	457	721
bridgeToReality	140	593
Total	**1279**	**2229**
Grand Total	**3508**	

- **Tests Exploring…**
  - **L vs H vs S norms**
  - **Continuous vs discrete**
  - **Dimensionality (1, 2, and 3D)**
  - **Actual error calculated using total integral, average integral, and internal and external boundary angular flux values**

Other Documented Tests

- **Tests Exploring…**
  - **Total cross sections and values of C**
  - **Phasing out of less dominant eigen modes in weakly coupled systems**
  - **Quadrature type (gauss lobatto vs gauss legendre)**
  - **Accuracy of reported error versus number of iterations trends**
  - **Symmetry of results in multi-D with varied S_n orders**

Conclusions

- **Choose an appropriate metric for what you are interested in**
  - **Norm**
  - **Region**
  - **Tolerance**
  - **Based on geometry**
- **Reported error largely reliable in common range of tolerances**
  - **If must have within tolerance, set input tolerance slightly finer**

Acknowledgements

- Shawn Pautz
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- Patricia St. John

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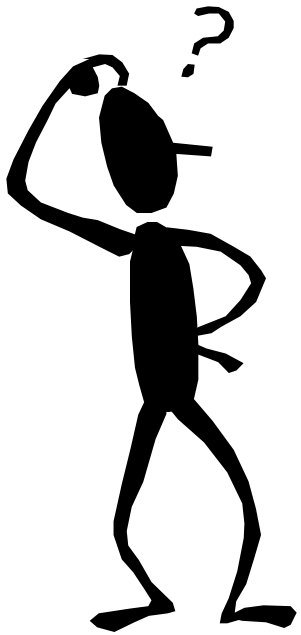
Questions



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