SAND2011-2978C

Specialized Error Estimates for the Control of Transport Solver Iterations

Shawn D. Pautz
Sandia National Laboratories
Albuquerque, NM, U.S.

M&C 2011
Rio de Janeiro, Brazil
May 12, 2011

Sandia National Laboratories

Outline

- Motivation
- General form of error estimates
- Types of error norms
- Results
- Summary and Conclusions

Motivation

There is an increasing emphasis on error estimation and uncertainty quantification in computational physics

- Need sufficient computation to meet specific accuracy requirements
- Ensembles of calculations stress available computing resources

Need good error estimates to obtain sufficient, but not excessive, accuracy of results.

Types of computational errors

Computational results from a verified code will contain several types of errors

- iterative
- discretization
- model (missing physics)

This work addresses iterative errors: when has an iterative method performed a “sufficient” number of iterations?

Derivation of error estimates

Let $Ax = b$, where $A = L - R$

$$\longrightarrow \qquad x^{(l+1)} = L^{-1}Rx^{(l)} + L^{-1}b$$

Make the following definitions:

Error	Residual
$e^{(l)} \equiv x - x^{(l)}$	$r^{(l+1)} \equiv x^{(l+1)} - x^{(l)}$

$$\longrightarrow \qquad e^{(l+1)} = L^{-1}Re^{(l)} \qquad r^{(l+1)} = e^{(l)} - e^{(l+1)}$$

Asymptotic assumption

After sufficient iterations the error is related to the dominant eigenmode:

$$e^{(l+1)} \approx \lambda_{\max} e^{(l)}$$

The largest eigenvalue (spectral radius) and error may be computed as:

$$\lambda_{\max} \approx \lambda_{\max}^{(l+1)} = \frac{\left\| e^{(l)} - e^{(l+1)} \right\|}{\left\| e^{(l-1)} - e^{(l)} \right\|} = \frac{\left\| r^{(l+1)} \right\|}{\left\| r^{(l)} \right\|} \qquad e^{(l)} \approx r^{(l)} \frac{\lambda_{\max}^{(l)}}{1 - \lambda_{\max}^{(l)}}$$

Warning (false convergence): $e^{(l)} \neq r^{(l)}$

Relative error

Typically we need relative values rather than absolute values:

$$\left\| r_{rel}^{(l)} \right\| \equiv \frac{\left\| r^{(l)} \right\|}{\left\| x \right\|} \approx \frac{\left\| r^{(l)} \right\|}{\left\| x^{(l)} \right\|} \qquad \left\| e_{rel}^{(l)} \right\| \equiv \frac{\left\| e^{(l)} \right\|}{\left\| x \right\|} \approx \frac{\left\| e^{(l)} \right\|}{\left\| x^{(l)} \right\|}$$

$$\longrightarrow \quad \lambda_{\max}^{(l+1)} \approx \lambda_{\max,rel}^{(l+1)} \equiv \frac{\left\| r_{rel}^{(l+1)} \right\|}{\left\| r_{rel}^{(l)} \right\|} \qquad \left\| e_{rel}^{(l)} \right\| \approx \left\| r_{rel}^{(l)} \right\| \frac{\lambda_{\max,rel}^{(l)}}{1-\lambda_{\max,rel}^{(l)}}$$

Error norms for transport

The previous error estimates need a definition for $\| \quad \|$
We have defined numerous ones for transport with the following taxonomy:

- Form
- Order
- Signed/Absolute
- Discrete/Continuous
- Region of Integration

Error norms: form and order

$$L_n(\psi(r,\Omega)) \equiv \left[\int dV \int d\Omega \left|\psi(r,\Omega)\right|^n\right]^{1/n}$$

$$H_n(\psi(r,\Omega)) \equiv \left[\int dV \int d\Omega \left|\nabla \psi(r,\Omega)\right|^n\right]^{1/n}$$ (seminorm)

$$S_n(\psi(r,\Omega)) \equiv \left[\int dV \int d\Omega \left|\Omega \cdot \nabla \psi(r,\Omega)\right|^n\right]^{1/n}$$ (seminorm)

Error norms: signed vs. absolute values

For a "signed" norm we use ψ instead of $\left\|\psi\right\|$ (seminorm)

$$\longrightarrow \quad L_{n,signed}\left(\psi\left(r,\Omega\right)\right) \equiv \left[\int dV \int d\Omega\, \psi\left(r,\Omega\right)^{n}\right]^{1/n}$$

The signed norm is more directly related to integral quantities such as dose.

Sandia National Laboratories

Error norms: discrete vs. continuous

A computer code will of course only have a discrete set of solution values. But those discrete values may be sufficient to define the solution everywhere, e.g. in a finite element expansion. The integrals in the norms may be obtained through quadrature rules.

For a "discrete" norm we replace the integral over space and direction with a vector sum of the discretized variables.

$$\longrightarrow \quad L_{n,discrete}\left(\psi\left(r,\Omega\right)\right) \equiv \left[\sum_i \sum_k \left|\psi\left(r_i,\Omega_k\right)\right|^n\right]^{1/n}$$

- Continuous form more directly related to output quantities
- Continuous form performs volume/Jacobian weighting
- Continuous form more expensive

Sandia National Laboratories

Error norms: region of integration

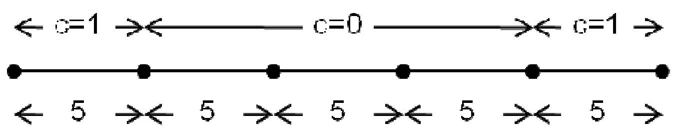
We may restrict the limits of integration in order to concentrate on important parts of the problem:

"global": entire spatial domain

"region": restricted to subdomain

"leakage": integration over a surface

Two test problems

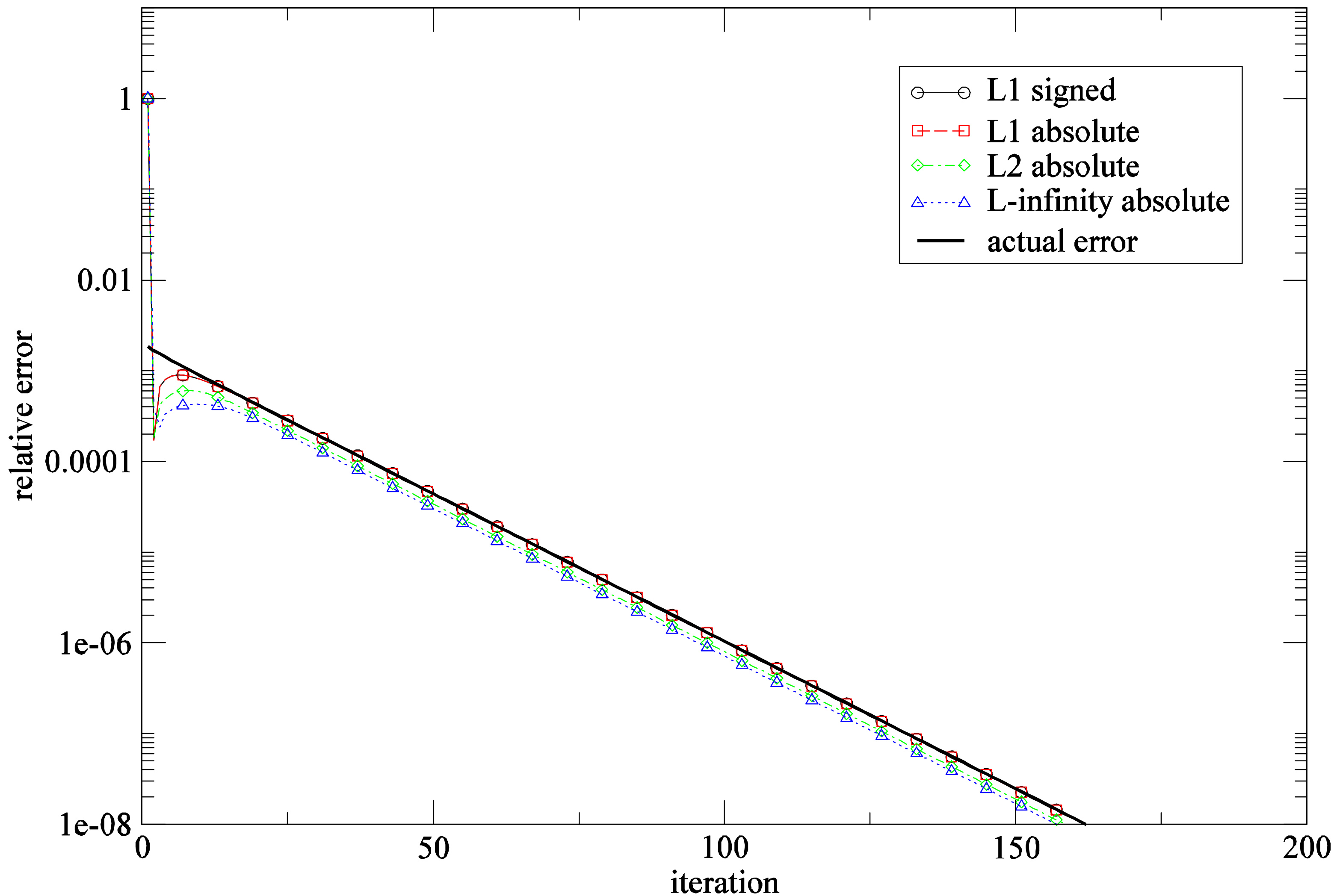


“Central source” and “boundary source” geometry

s	s	s	s	s
s	m	m	m	s
s	m	f	m	s
s	m	m	m	s
s	s	s	s	s

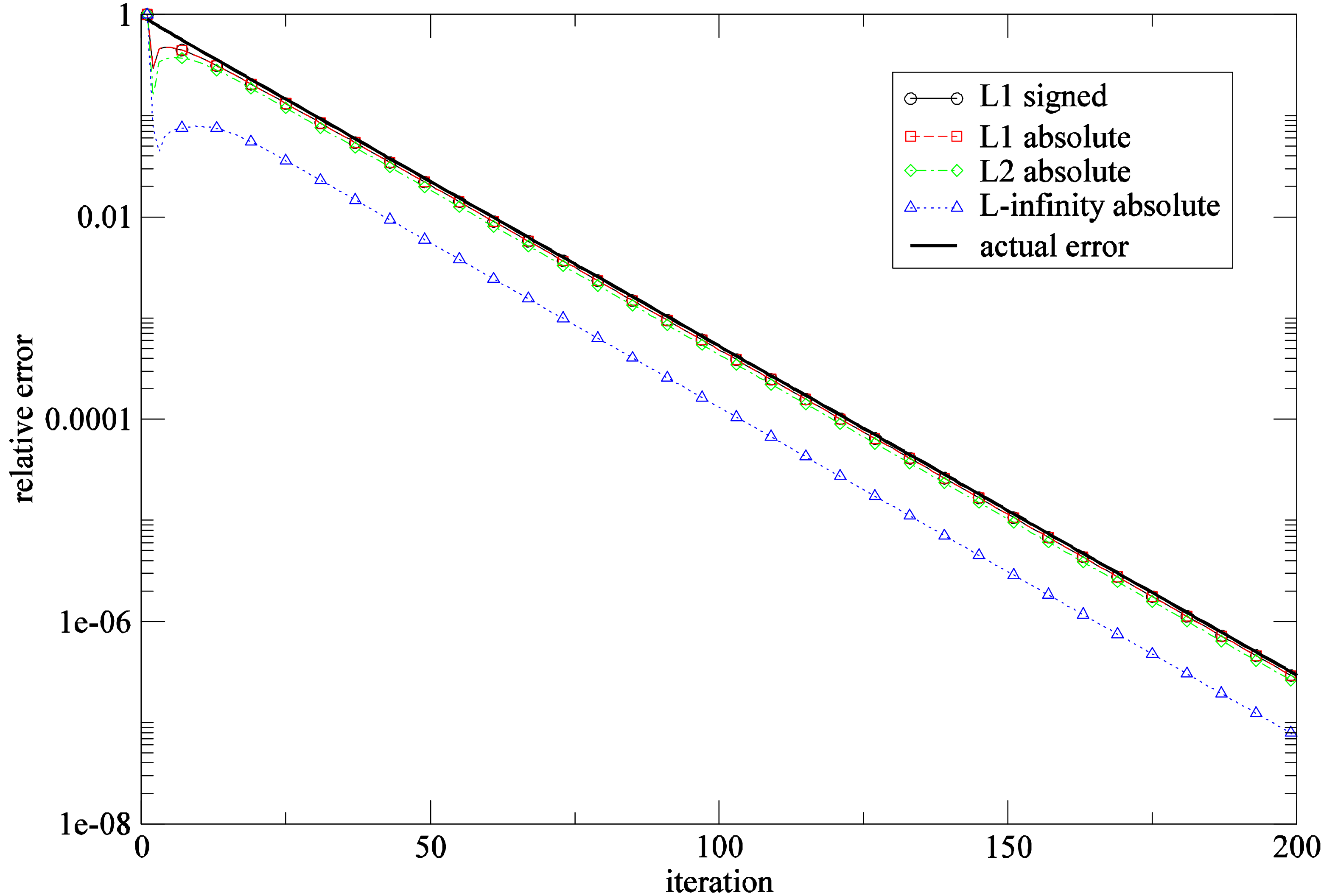
“Reactor” geometry

Global L-norm error estimates, "central source"



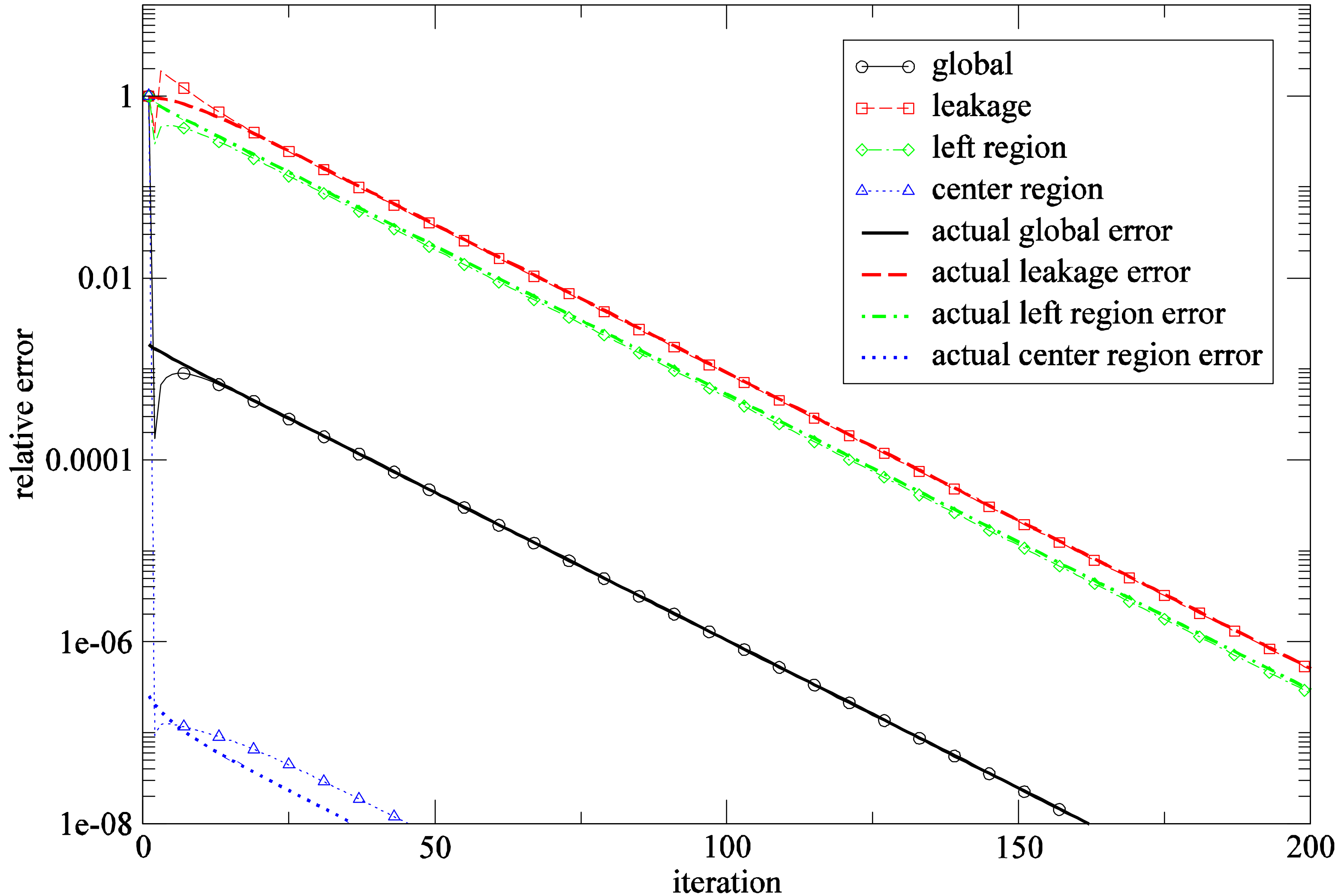
Sandia National Laboratories

L-norm error estimates in left region, "central source"



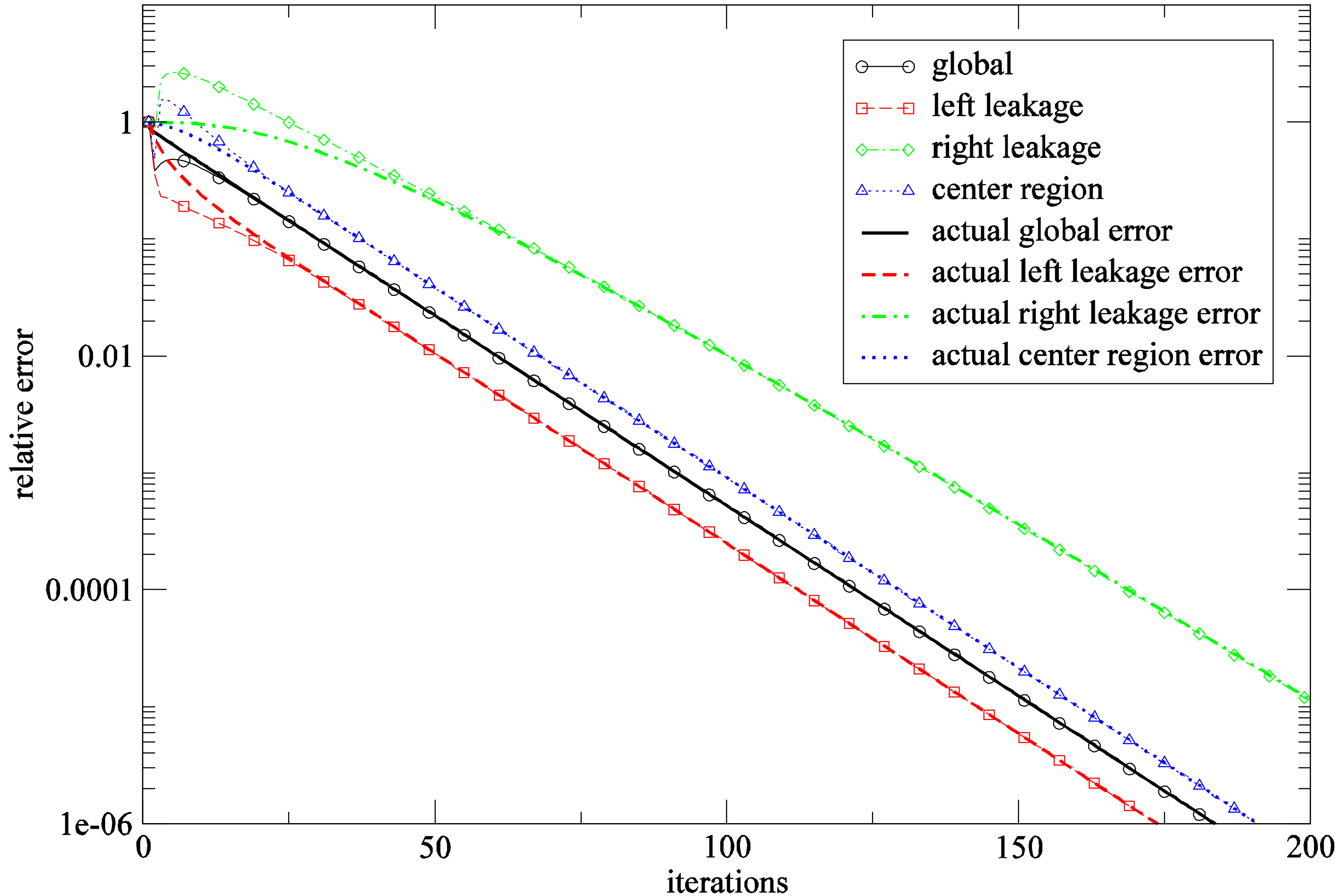
Sandia National Laboratories

L1-signed error estimates, "central source"



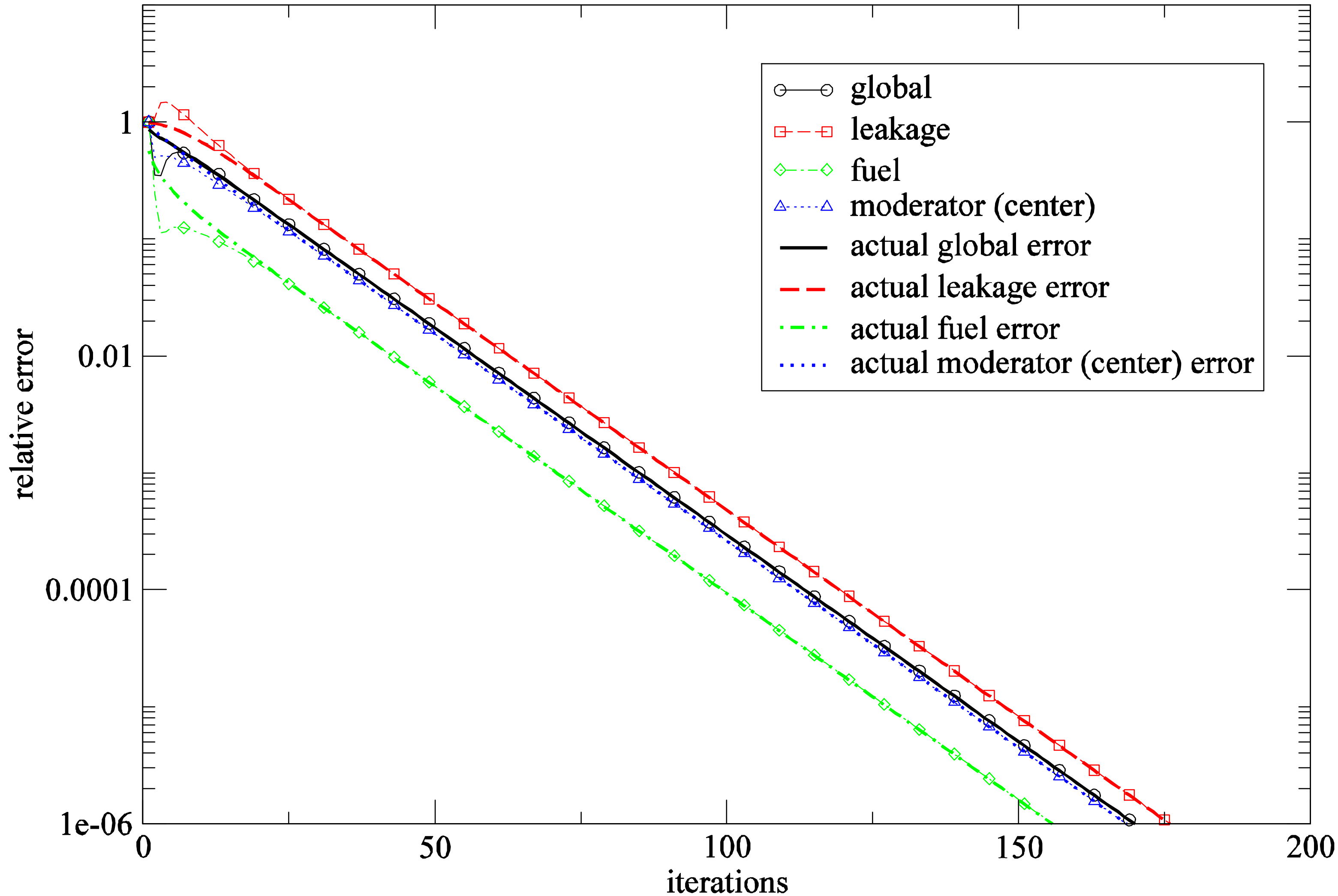
Sandia National Laboratories

L1-signed error estimates, "boundary source"



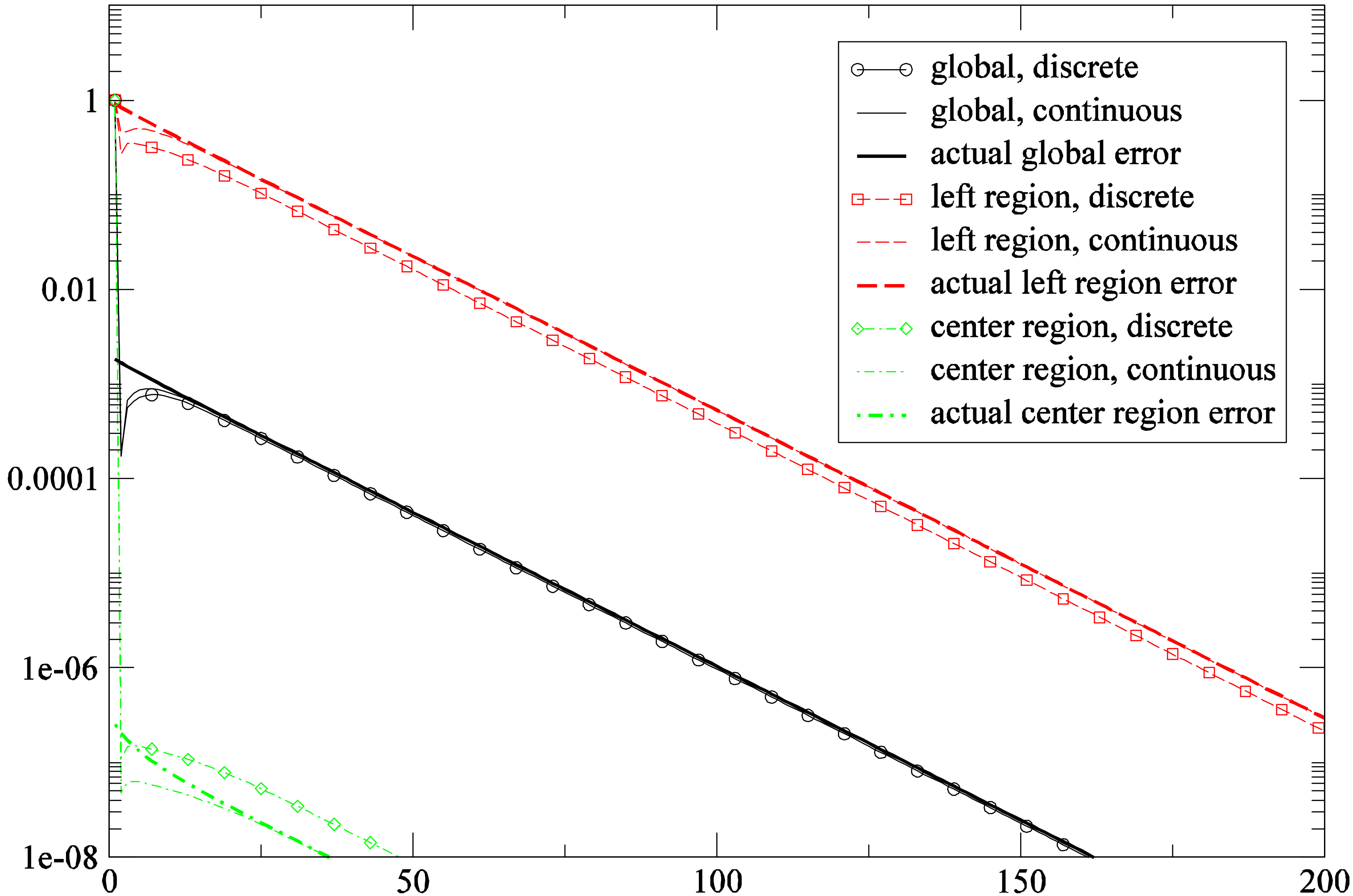
Sandia National Laboratories

L1-signed error estimates, “reactor”



Sandia National Laboratories

L1-signed error estimates, "distorted central source"



Sandia National Laboratories

Summary and Conclusions

- Iterative errors are not directly known, so they must be estimated
- Our estimates are derived from the iterative residuals
- Numerous options available for defining the norms used in the estimates
- Norms that are most closely related to the desired quantity of interest are the most accurate
- The region of integration affected the error estimates the most in our tests
- Our results are for source iteration – need to examine problems with preconditioning