Comparing *A Posteriori* Spatial Error Estimators for the S_N Neutron Transport Equation

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INTRODUCTION

The imposition of a spatial discretization onto the discrete ordinates (S_N) neutron transport equation results in a deviation from the spatially continuous equation that is defined as the spatial discretization error. Like the numerical solution itself, the spatial discretization error must be estimated, as knowledge of the true error would imply knowledge of the true solution.

Previous works [1–5] have developed *a posteriori* error estimators, but these are often in the context of adaptive mesh refinement (AMR), which places precedence on the ability to estimate the error spatial profile rather than the estimator's accuracy in quantifying the true error. Thereupon, we have previously developed the residual source estimator [6], a two-step error estimator in which: first, the residual, the deviation from particle balance when a spatial discretization is applied to the transport equation, is approximated using Taylor Expansions of the true solution; second, the residual is used as distributed source for a transport-like problem, in which the solution is the spatial discretization error.

We have tested the residual source estimator on a variety of fixed-source problems using the Method of Manufactured Solutions (MMS) [7] to generate true reference solutions. In this work comparison of the residual source estimator *versus* two estimators that have performed well in previous works, the Ragusa-Wang (RW) estimator [2] and the Duo-Azmy-Zikatanov (DAZ) estimator/indicator [1], is summarized and conclusions about the utility of the residual source estimator *vis-a-vis* the other two estimators are reached.

THEORY

We test the error estimators solving the one-speed S_N neutron transport equation in a two-dimensional Cartesian domain $\mathcal{D} = [0, X] \times [0, Y]$, comprising a homogeneous, non-multiplying, isotropic scattering medium,

$$\nabla \cdot \mathbf{\Omega}_n \psi_n(x, y) + \sigma_t \psi_n(x, y) = \sigma_s \sum_{m=1}^{M} w_m \psi_m(x, y) + q(x, y),$$
$$\text{for } n = 1, \ldots, M, \ \forall (x, y) \in \mathcal{D}, \quad (1)$$

with fixed source incoming boundary conditions (BCs),

$$\psi_m(x, y)|_{\hat{n}\cdot\mathbf{\Omega}_m<0} = \psi_{[BC]}(x, y),$$
$$\text{for } m = 1, \ldots, M, \ \forall (x, y) \in \partial\mathcal{D}. \quad (2)$$

For the purposes of this work, the solution to the above equation will be considered the "true" solution *versus* the solution to the spatially discretized equation. The spatial discretization method used in this work is Discontinuous Galerkin Finite Element Method of spatial order Λ (DGFEM-Λ), represented by Eq. 3, specifically DGFEM-0, which approximates the solution in discrete cell $K^{(i,j)} \subseteq \mathcal{D}$, $K^{(i,j)} = (x_{i-1}, x_i) \times (y_{j-1}, y_j)$, as a constant over space, generally discontinuous across neighboring cells.

$$L_h^\Lambda \psi_h^\Lambda = \mathcal{S}\psi_h^\Lambda + \Pi_h^\Lambda q \quad (3)$$

In the above equation, L_h^Λ is the bilinear form of the DGFEM-Λ transport operator, $\mathcal{S}$ is the S_N scattering operator, Π_h^Λ is the operator that projects a function onto the DGFEM-Λ h-mesh space, and ψ_h^Λ is the solution to the discrete S_N equation. We keep the cell size uniform across the domain, such that $i = 1, \ldots, N_X$ and $j = 1, \ldots, N_Y$, and X and Y are both fixed at 1 cm. The cell size h is equal to the maximum of the cell widths in the x- and y-dimension, Δx and Δy, respectively. The spatial discretization error is mathematically defined as

$$\varepsilon_h^\Lambda \equiv \psi_h^\Lambda - \Pi_h^\Lambda \psi, \quad (4)$$

where ψ is the true solution. The MMS is used to generate true reference solutions for comparison with the DGFEM-0 solutions and error estimators. The MMS reference solutions as developed by Duo in [7] sets the combined (fixed + scattering) source Q to a constant over the domain and solves Eq. 1 and 2 with *no* approximations in space. This solution is interfaced with DGFEM-0 by producing a resultant fixed source ($q = Q - \mathcal{S}\psi$) and using it as an input for the DGFEM-0 problem.

TABLE I. MMS Boundary Conditions

C^r	$\psi^{[N,S]}$	$\psi^{[W,E]}$
C^0	0	$(\sigma_t - \sigma_s)/\sigma_t$
C^1	0	0

The singular characteristics (SCs) are significant features of the true solution in the S_N method that impact the quality of the DGFEM-0 solution and resultant error estimators. SCs are rays that emanate from the intersection point of incoming boundaries for a given ordinate n with a slope η_n/μ_n, across which the solution is discontinuous in some derivative. The continuity order C^r represents the lowest order-r derivative of the solution that is discontinuous across the SCs, and r is dictated by the BCs as shown in Table I, where $\psi^{[N,S]}$ and $\psi^{[W,E]}$ are the incoming angular flux values on the north and south boundaries and west and east boundaries, respectively. The dependence of the C^0 BCs on the cross-sections ensures that the resultant fixed source does not attain negative (non-physical) values. Provided the mesh is not aligned with the SCs, the locations of which are known *a priori*, the discontinuities in the true solution cannot be accurately represented by a DGFEM-0 solution, which is locally continuous. Hence, poor accuracy results in SC-intersected cells and other cells downwind due to numerical spreading of error [8].

ERROR ESTIMATORS

An effective error estimator *must* go outside the function space of the discrete solution to capture some of true solution behavior that is truncated by the spatial discretization. Three estimators that accomplish this are compared in this work: the residual source estimator (LeR) [6], the RW estimator [2], and the DAZ estimator/indicator [1].

The three estimators are presented in the following subsection but first we introduce the quantities that will form the metrics of comparison. We facilitate analysis of the discretization error, which is in the same space as the numerical solution, by recasting it in local L_2 norms. The "angular" L_2 norm has been found to be more accurate for error estimator accuracy comparisons, and is given by,

$$E^{(i,j)}_{ang.} = \sqrt{\sum_{n=1}^{N} w_n \int_{\Delta x_i} dx \int_{\Delta y_j} dy \left(\varepsilon^{\Lambda}_{h,n}(x,y)\right)^2}. \qquad (5)$$

The global angular L_2 error norm is calculated by $E_{ang.} = \left(\sum_{i=1}^{N_X}\sum_{j=1}^{N_Y} E^{(i,j)2}_{ang.}\right)^{1/2}$. In the following sections, when an error estimate is implemented, the angular error estimate is represented by ϵ, and the error norm is represented with a lower-case e. It is commonplace to use another metric, the local "effectivity index", which represents the accuracy of an error estimator,

$$\theta^{(i,j)}_{ang.} = \frac{e^{(i,j)}_{ang.}}{E^{(i,j)}_{ang.}}, \qquad (6)$$

and the global effectivity index is calculated as $\theta_{ang.} = \frac{e_{ang.}}{E_{ang.}}$.

Residual Source Estimator

The residual source estimator (LeR) was developed by Hart and Azmy [6] based on a concept originally explored by O'Brien and Azmy [9]. When the true residual,

$$R^{\Lambda}_h \equiv \mathcal{S}\left[\Pi^{\Lambda}_h \psi\right] + \Pi^{\Lambda}_h q - L^{\Lambda}_h \left[\Pi^{\Lambda}_h \psi\right], \qquad (7)$$

is used as a fixed-source for a transport like problem,

$$L^{\Lambda}_h \varepsilon^{\Lambda}_h = \mathcal{S}\varepsilon^{\Lambda}_h + R^{\Lambda}_h, \qquad (8)$$

the true spatial discretization error is the solution. Of course, knowledge of the true residual implies knowledge of the true solution, so an *a posteriori* residual approximation method has been developed in which the true solution is approximated using a Taylor Expansion, and the DGFEM-0 solution is used to approximate point-wise derivatives in the resultant approximated residual expression [6]. The estimated Taylor Expansion with Approximated Derivatives (TE-AD) residual, $\mathcal{R}$, is used in conjunction with LeR to get the LeR/TE-AD estimator,

$$L^{\Lambda}_h \epsilon^{\Lambda}_h = \mathcal{S}\epsilon^{\Lambda}_h + \mathcal{R}^{\Lambda}_h, \qquad (9)$$

and estimate ϵ^{Λ}_h is inserted in place of ε^{Λ}_h in Eq. 5.

We also observe the behavior of the TE-AD residual as an error indicator due to its suspected conservatism and possibility to be calculated *en-route* to a LeR/TE-AD estimate. This is done by simply inserting the TE-AD residual, which is in the same space as the discretization error, into the error norm equations in place of ϵ^{Λ}_h.

Ragusa-Wang Estimator

To obtain an estimate with the RW estimator, the mesh is uniformly refined and a new numerical solution is found on the refined $(h/2)$ mesh. This $h/2$-mesh solution is used as a reference solution for the original h-mesh solution in place of the true solution,

$$e^{(i,j)}_{RW,ang.} = \left(\sum_{n=1}^{N} w_n \int_{\Delta x_i} dx \int_{\Delta y_j} dy \Big(\psi^{\Lambda}_{h,n}(x,y) - \left[\Pi_h \psi^{\Lambda}_{h/2,n}\right](x,y)\Big)^2\right)^{1/2}. \qquad (10)$$

This method has been found to be accurate and precise [2, 9], but it comes at the cost of the memory and computation time required to solve an additional system of equations with 4 times as many unknowns (in 2D).

Duo-Azmy-Zikatanov Estimator

The DAZ estimator was derived from a dual argument estimator using discontinuous finite element theorems to bound the global error from above for C^1 or smoother problems [1, 7]. In the global sense it is given as

$$e_{DAZ,ang.} = C\left(\sum_{i=1}^{N_X}\sum_{j=1}^{N_Y}\sum_{n=1}^{N} \hat{h}^2_{K^{(i,j)}} w_n \times \int_{\Delta x_i} dx \int_{\Delta y_j} dy \left(\mathcal{R}^{(i,j)}_n(x,y)\right)^2\right)^{1/2} + C\left(\sum_{i=1}^{N_X}\sum_{j=1}^{N_Y}\sum_{n:\boldsymbol{\Omega}_n\cdot\hat{n}<0}^{N} 2\hat{h}_{K^{(i,j)}} w_n \times \int_{\partial K^{(i,j)}_-} dS \; |\hat{n}\cdot\boldsymbol{\Omega}_n| \left\{\psi^-_{\Lambda,n} - \psi^+_{\Lambda+l,n}\right\}^2\right)^{1/2}, \qquad (11)$$

where $\hat{h}$ is the cell diameter, $-$ and $+$ refer to the internal and external traces of the angular flux, respectively, and C is a constant related to the norm of the dual problem and the smoothness of the true solution, assumed in this work to be $C = 1$. The approximated residual and higher-order external trace are approximated by doing an additional higher-order sweep on a DGFEM-($\Lambda + l$) problem using the converged scattering source from the low order problem and the problem fixed source [1]. It is heuristically applied locally by removing the summation over cells and to C^0 problems, and in these contexts is referred to as an "indicator" rather than an estimator, by the fact that the bounding theorems no longer hold.

ESTIMATOR COMPARISON

We observe the varying estimator performance with scattering ratio c, optical thickness (*via* σ_t), and the continuity order, and have highlighted some cases here. For all problems Level-Symmetric S_4 quadrature is used, l is fixed at 1, and the mesh is fixed at $N_X = N_Y = 512$ as an ideal highly-converged problem. We condense the $N_X \times N_Y$ local estimates in each problem to several quantities: the number of cells with $\theta_{ang.} \geq 1$, an indicator of local conservatism, the number of cells with $|\theta_{ang.} - 1| \leq \beta$, where $\beta > 0$, an indicator of accuracy, and the standard deviation of $\log_{10} \theta_{ang.}$, an indicator of precision.

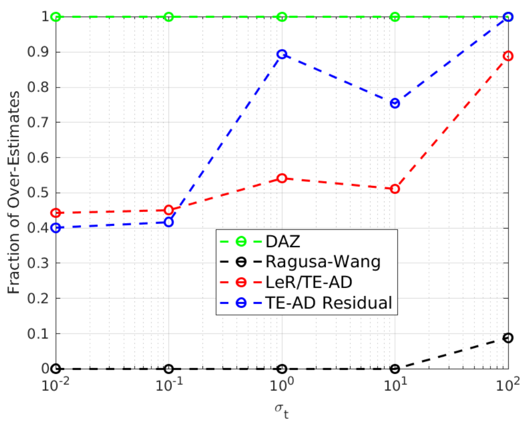

Fig. 1. Fraction of Cells that have $\theta_{ang.} \geq 1$, $c = 0.9$, C^1

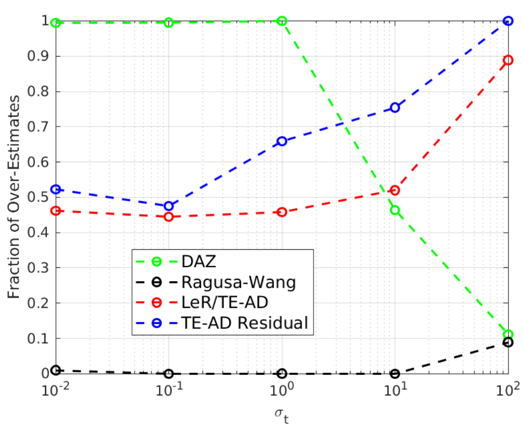

Fig. 2. Fraction of Cells that have $\theta_{ang.} \geq 1$, $c = 0.9$, C^0

Figures 1-2, which plot the fraction of cells with conservative error estimates for $c = 0.9$, show the DAZ indicator is most locally conservative, generally. The TE-AD residual shows promise as an indicator as well, as it is quite conservative at larger optical thicknesses. The LeR/TE-AD estimator is only moderately conservative, though, and the RW estimator has a tendency to underestimate due to the theoretical under-estimation of an h-refinement error estimator for already converged meshes.

Figures 3-4, which plot the fraction of cells within some

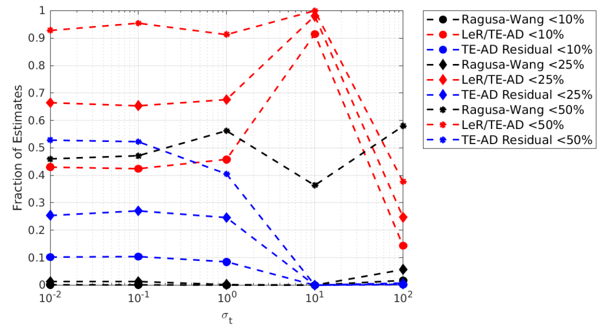

Fig. 3. Fraction of Cells that have $|\theta_{ang.} - 1| \leq \beta$, $c = 0.1$, C^1

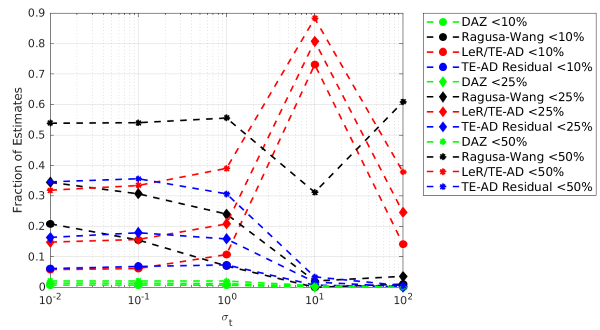

Fig. 4. Fraction of Cells that have $|\theta_{ang.} - 1| \leq \beta$, $c = 0.1$, C^0

accuracy range fraction β for $c = 0.1$, highlight that the LeR/TE-AD estimator is most accurate for C^1 problems regardless of problem parameters, but suffers in C^0 problems where SCs break assumptions that lead to the TE-AD residual. The RW estimator is inaccurate by most of these β metrics for C^1 problems because it underestimates too much, but in C^0 problems it has slightly better accuracy because the distribution of effectivity values is altered due to the discontinuities in the true solution. The TE-AD residual is somewhat accurate, but the DAZ indicator is not accurate by these β metrics, in direct correlation to its bounding theorems derivation assumption.

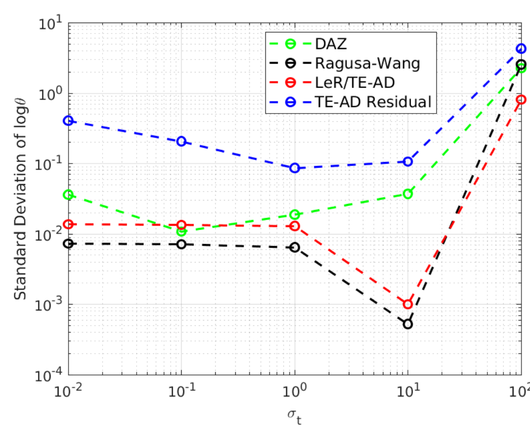

Fig. 5. Standard Deviation of $\log_{10} \theta_{ang.}$, $c = 0.1$, C^1

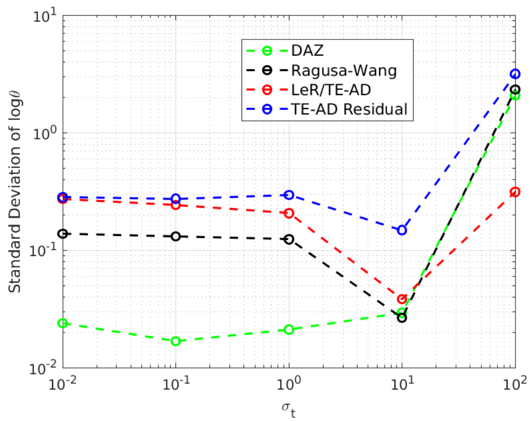

Fig. 6. Standard Deviation of $\log_{10}\theta_{ang.}$, $c = 0.1$, C^0

Figures 5-6 plot the standard deviation of $\log_{10}\theta_{ang.}$ as an indicator of precision for $c = 0.1$. Note that effectivities are not distributed following a normal curve, but we have found that they nonetheless look normal-distribution-like in $\log_{10}$-scale. The RW estimator provides an excellent estimate of the error profile for C^1 problems, and the LeR/TE-AD estimator is competitive in this regard. However, for C^0 problems, both estimators perform poorly relative to their performance in C^1 problems, and the DAZ indicator is generally the best error profile estimator for these C^0 problems. The TE-AD residual does not show promise as a shape estimate, as it is consistently the worst in this respect.

CONCLUSIONS

Each local estimator is highly dependent on the continuity order of the problem. The LeR/TE-AD estimator is most accurate for C^1 problems regardless of problem parameters, but in C^0 problems its accuracy relative to other estimators is dependent on the impact of the solution discontinuities (which is dependent on scattering ratio and optical thickness). The RW estimator suffers from inaccuracy due to its propensity to underestimate the true error, but it underestimates very precisely, and is superior to all estimators as an error profile estimate for C^1 problems, though the LeR/TE-AD estimator is competitive in this regard. However, for C^0 problems this advantage is nullified. The DAZ indicator is inaccurate by the metrics used in this work, but it is locally conservative for most problems examined due to its origin as a bound on the global error. Because it does not suffer from worsened precision in C^0 problems, it is advantageous as an error profile estimate. The TE-AD residual is moderately locally conservative and somewhat accurate when used as an error indicator, but it is poor as an error profile estimate, and we have found that the true (and TE-AD) residual has a different convergence order than the error, making its use as a global or local indicator questionable.

Future work will focus on modifying residual approximations in cells intersected by SCs to enhance accuracy and precision for C^0 problems. We also seek to expand this analysis to $\Lambda = 1$ or higher problems, as DGFEM-0 is considered insufficient for most problems.

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REFERENCES

1. J. I. DUO, Y. Y. AZMY, and L. T. ZIKATANOV, “A Posteriori Error Estimator and AMR for Discrete Ordinates Nodal Transport Methods,” *Annals of Nuclear Energy*, **36**, 268–273 (2009).
2. Y. WANG and J. C. RAGUSA, “Standard and Goal-Oriented Adaptive Mesh Refinement Applied to Radiation Transport on 2D Unstructured Triangular Meshes,” *Journal of Computational Physics*, **230**, 763–788 (2011).
3. D. FOURNIER ET AL., “Analysis of a hp-Refinement Method for Solving the Neutron Transport Equation Using Two Error Estimators,” in “International Conference on Mathematics and Computational Methods Applied to Nuclear Science & Engineering (M&C 2011),” Rio de Janeiro, RJ, Brazil (May 2011).
4. R. JEFFERS, “Goal-Based h-Adaptivity of the 1-D Diamond Difference Discrete Ordinate Method,” *Journal of Computational Physics*, **335**, 179–200 (2017).
5. D. LATHOUWERS, “Goal-Oriented Spatial Adaptivity for the S_N Equations on Unstructured Triangular Meshes,” *Annals of Nuclear Energy*, **38**, 1373–1381 (2011).
6. N. H. HART and Y. Y. AZMY, “A Residual-based *A Posteriori* Estimator of the Spatial Approximation Error for Discrete Ordinates Solutions of the Transport Equation,” in “International Conference on Mathematics & Computational Methods Applied to Nuclear Science & Engineering,” Jeju, Korea (April 2017).
7. J. I. DUO, *Error Estimates for Nodal and Short Characteristics Spatial Approximations of Two-Dimensional Discrete Ordinates Method*, Ph.D. thesis, The Pennsylvania State University (2008).
8. J. I. DUO and Y. Y. AZMY, “Error Comparison of Diamond Difference, Nodal and Characteristics Methods for Solving Multidimensional Transport Problems with the Discrete Ordinates Approximation,” *Nucl. Sci. Eng.*, **156**, *2*, 139–153 (2007).
9. S. O’BRIEN and Y. Y. AZMY, “*A Posteriori* Error Estimators for the Discrete Ordinates Approximation of the One-Speed Neutron Transport Equation,” in “International Conference on Mathematics & Computational Methods Applied to Nuclear Science & Engineering,” Sun Valley, ID, USA (2013).