

**ERROR ESTIMATION AND ADAPTIVE ORDER NODAL METHOD
FOR SOLVING MULTIDIMENSIONAL TRANSPORT PROBLEMS**

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Error Estimation and Adaptive Order Nodal Method for Solving Multidimensional Transport Problems

O. M. Zamonsky, C. J. Gho, Y. Y. Azmy

Abstract

We propose a modification of the Arbitrarily High Order Transport Nodal method whereby we solve each node and each direction using different expansion order. With this feature and a previously proposed *a posteriori* error estimator we develop an adaptive order scheme to automatically improve the accuracy of the solution of the transport equation. We implemented the modified nodal method, the error estimator and the adaptive order scheme into a discrete-ordinates code for solving monoenergetic, fixed source, isotropic scattering problems in two-dimensional Cartesian geometry.

We solve two test problems with large homogeneous regions to test the adaptive order scheme. The results show that using the adaptive process the storage requirements are reduced while preserving the accuracy of the results.

1. INTRODUCTION

Shielding problems are sometimes related to transport calculations in systems composed of few large homogeneous regions. The Discrete-Ordinates (S_N) method has been widely used principally for one and multidimensional systems. During the last several years a great effort has been pursued to improve the computational efficiency of different numerical methods under the S_N approach. In this sense, research has been focused mainly on the spatial treatment of the flux. The evolution from Finite Difference to High Order Nodal methods is motivated by the desire to obtain highly accurate solutions using less memory and shorter CPU time.

Usually the accuracy of the results is measured by the relative difference between average quantities obtained with the tested method versus reference converged solutions.^{1,2} This is not surprising because in reactor physics most of the quantities of interest are related to locally-averaged fluxes. On the other hand, high order nodal methods allow reconstruction of the flux at every point in a system even when the solution procedure is performed over large homogeneous regions.

The user of transport codes often does not have a complete knowledge of the uncertainties resulting from the numerical method used to solve the transport problem, even when referring only to the spatial treatment. In particular the different approximations used in nodal methods make this situation more difficult. To extract the basic information needed for a particular problem in high order nodal methods, the user has to provide not only a certain mesh but also the expansion order to be used.¹ More complicated are the differences between low order methods where it is necessary to understand most of the approximations of the scheme in order to select the "best" method for a particular problem.² The characterization and understanding of numerical difficulties in multidimensional S_N algorithms is very important not only to avoid poor interpretation of the results but also to provide fundamental means to improve the calculations.³

In this paper we propose a way to simplify the error estimation for the results of transport calculations. To do this, we estimate the errors produced by the Arbitrarily High Order Transport - Nodal Method¹ (AHOT-N) using an *a posteriori* error indicator based on the residual of the transport equation. Then we apply the error estimation on a per node per direction basis to develop an adaptive order scheme. Some modifications are proposed to the AHOT-N method in order to allow it to solve a system using a different approximation order in each node and direction.

Our aim is to perform the adaptive process automatically and to propose a simple scheme that could be easily included in codes that use nodal methods. The estimated errors could also be used to make mesh refinement in numerical methods where this is the only degree of freedom to improve the accuracy of the results.

We solve two test problems using the original AHOT-N method and one adaptive scheme to compare various average quantities. We conclude that this process decreases the user time rather than the CPU time and contributes to automatically improving the data quality rather than quantity. We conjecture that dynamic memory management must be implemented in the adaptive scheme to minimize the memory requirement.

2. THEORY

The adaptive order scheme proposed in this paper is directly applicable to arbitrarily high order transport methods. We selected the AHOT-N method due to its simple final equations.

In order to allow adapting the approximation order, we propose some modifications to the nodal method in which each node and each direction are solved using a different order. A review of the AHOT-N method and the modifications proposed are detailed in Section 2.1.

In Section 2.2 we introduce the estimator used to make *a posteriori* error estimation, and discuss the way we performed error calculations in problems with respect to analytical solutions. The way we conduct the adaptive order calculations is explained in Section 2.3.

Two test problems are solved in Section 3 where we compare the solutions obtained using the same approximation order in all the system with the solutions obtained adaptively, followed by a discussion in Section 4.

2.1. THE AHOT-N METHOD

Assuming one energy group and isotropic scattering the Discrete Ordinates, S_N , approximation of the transport equation in two-dimensional Cartesian homogeneous region can be written as

$$\bar{\Omega}_m \cdot \nabla \Psi_m(x, y) + \sigma \Psi_m(x, y) = S_m(x, y) \quad (1)$$

where the index m indicates the discrete direction.

The domain D is divided into N disjoint rectangular sub-domains (nodes) $D_n = [-a_n, a_n] \times [-b_n, b_n]$, $D = \cup D_n$. In each sub-domain the angular fluxes are expanded into a basis of dimensionless Legendre polynomials. Truncating these expansions at order Λ , the angular fluxes are expressed as

$$\Psi_n(x, y) = \sum_{i,j=0}^{\Lambda} (2i+1)(2j+1) \Psi_{n,ij} P_i(x) P_j(y) \quad (2)$$

where the index n indicates the node D_n of the local expansion of $\Psi(x, y)$, and the index m corresponding to the direction $\bar{\Omega}_m$ has been suppressed.

This method was originally derived¹ using the same truncation order Λ for every node and for all directions, and we will refer to this approximation as "homogeneous order".

In this work we use different truncation orders for each node and each direction, i.e. $\Lambda_{m,n}$ for the direction m in the node n , and we will refer to this approximation as "variable order." The set of Legendre polynomials from order zero to $\Lambda_{m,n}$ will be called the local basis. Since the method is applied to the solution of the transport equation in homogeneous nodes for each discrete direction the general form of the local equations is preserved with every occurrence of Λ replaced with $\Lambda_{m,n}$.

The local nodal moments of the angular flux, Ψ_{ij} , are the unknowns of the problem. Projecting Eq. (1) over a local basis, simultaneous algebraic equations for Ψ_{ij} are obtained in terms of the local transverse moments of the angular flux, $\Psi_{xj}(\pm a)$ and $\Psi_{iy}(\pm b)$, which emerge as new unknowns in the problem. The local transverse moment $\Psi_{xj}(x)$ [$\Psi_{iy}(y)$] is the "transversal" projection of the angular flux over the j [i]-component in the y [x] spatial coordinate. In order to clarify this definition the expression for $\Psi_{xj}(x)$ is expressed as follows:

$$\Psi_{n,m,xj}(x) = \frac{1}{2b_n} \int_{-b_n}^{b_n} \Psi_{n,m}(x, y) P_j(y) dy \Rightarrow \Psi_{n,m}(x, y) \approx \sum_{j=0}^{\Lambda_{m,n}} (2j+1) \Psi_{n,m,xj}(x) P_j(y) \quad (3)$$

Transversally projecting Eq. (1) over the y and x spatial coordinates and exactly solving the resulting one-dimensional differential equations for the transverse moments, relations between the nodal and transverse moments of the flux are obtained.

After large algebraic manipulations the discrete-variable equations representing the transport problem for each angular direction reduces to:

- a set of equations for the nodal moments Ψ_{ij} in terms of the incoming flux transverse moments, $\Psi_{xj}(-a)$ and $\Psi_{iy}(-b)$ if $\bar{\Omega}_m$ is in the positive octant, which are known from external boundary conditions, or are set equal to the outgoing flux transverse moments from corresponding neighboring cells, and
- simple relations to obtain the outgoing transverse moments using the incoming transverse moments and the nodal moments calculated by solving the above set of equations.

It is not relevant for the subject of this paper to reproduce here the detailed equations of the AHOT-N method but it is worth noting some properties that are affected when using variable order:

- In the homogeneous order case the equations are fully specified by only one spatial weight per node per dimension per distinct discrete ordinate. These weights are functions of the form $\alpha(\mu_m, a_n, \sigma_n, \Lambda)$ in the x-dimension, and they are odd functions of the direction cosines of the discrete ordinates. When variable order is used, the spatial weights have the form $\alpha_{m,n} = \alpha(\mu_m, a_n, \sigma_n, \Lambda_{m,n})$ and are not necessarily odd functions of the angle cosine even though α is still an odd function in its argument μ . This follows from the fact that for $\mu_{m'} = -\mu_m$ generally $\Lambda_{m',n} \neq \Lambda_{m,n}$ so that $\alpha_{m',n} \neq \alpha_{m,n}$. Thus the method requires the storage of more weights than in the homogeneous order case.
- Coupling between neighboring nodes is achieved by setting the incoming flux transverse moments to a cell, $\Psi_{nx-,xj}$, equal to the outgoing moments from its upstream neighbor along the direction of neutron travel, $\Psi_{n,xj}$. In the original AHOT-N method this coupling is made for all spatial moments from 0 to Λ . Using variable order per node per direction the coupling is made according to the prescription:

$$\begin{aligned} \Psi_{nx-,xj} &= \Psi_{n,xj} & , \quad j = 0, \dots, \Lambda_n & \text{ if } \Lambda_{nx-} \geq \Lambda_n \\ \Psi_{nx-,xj} &= \Psi_{n,xj} & , \quad j = 0, \dots, \Lambda_{nx-} & \left. \vphantom{\Psi_{nx-,xj}} \right\} \text{ if } \Lambda_{nx-} < \Lambda_n \\ \Psi_{nx-,xj} &= 0 & , \quad j > \Lambda_{nx-} \end{aligned} \quad (4)$$

- The scalar flux is evaluated in the usual way,

$$\phi_n = \sum_{m=1}^{\Lambda_{\max}} w_m \Psi_m \quad (5)$$

where $\Lambda_{\max} = \max.\{\Lambda_m, m=1, \text{NDIR}\}$ in the node n , where NDIR is the number of discrete directions corresponding to the order N of S_N .

- The set of discrete variables per node (n) per direction (m) is comprised of $(\Lambda_{n,m}+1)^2$ nodal moments and $2(\Lambda_{n,m}+1)$ transverse moments. If the problem to be solved does not require a uniform spatial approximation order for each direction and each node, the variable order distribution could reduce significantly the number of equations and unknowns evaluated.

2.2. ERROR ESTIMATION

In recent years several numerical methods have been proposed to solve the transport equation under the discrete ordinates approach. In most cases the computational efficiency of the new method is compared with classical finite differences schemes. This is usually done by observing the computing time and storage requirements to obtain a given accuracy of the results. To define the accuracy it is necessary to define the error of the approximate solution. In real problems, where analytical solutions are not available, numerical solutions obtained with the "best" approximations, e.g. using reasonably fine spatial mesh or high orders of approximation and shown to have converged with respect to them, are treated as the "exact" reference.

To the best of our knowledge no *a posteriori* error indicator has been proposed yet to estimate the error in the solutions produced by numerical transport methods with piece-wise polynomial approximations (spectral methods). In contrast, in finite element methods and in particular for the diffusion equation several error estimators have been proposed.⁴⁻⁸

In a previous work⁹ we proposed an *a posteriori* error estimator inspired by some indicators used in transport finite elements methods and in spectral methods for the diffusion equation.⁶

The proposed local error estimator $E_{n,m}$ for node n in direction m is composed of a residual term plus a discontinuity term:

$$E_{n,m} = \sqrt{R_{n,m}^2 + D_{n,m}^2} \quad (6)$$

where the local residual of Eq. (1) is expressed as:

$$R_{n,m}^2 = \frac{V_n}{(\Lambda_{n,m} + 1)^2} \int_{V_n} (\bar{\Omega}_m \cdot \nabla \Psi_{n,m}(x, y) + \sigma_n \Psi_{n,m}(x, y) - S_n(x, y))^2 dv \quad (7)$$

and the discontinuity term as:

$$D_{n,m}^2 = \frac{2b_n}{(\Lambda_{n,m} + 1)} \int_{-b_n}^{b_n} (\Psi_{n,m}(-a_n, y) - \Psi_{nx,m}(a_{nx}, y))^2 dy + \frac{2a_n}{(\Lambda_{n,m} + 1)} \int_{-a_n}^{a_n} (\Psi_{n,m}(x, -b_n) - \Psi_{ny,m}(x, b_{ny}))^2 dx \quad (8)$$

where nx [ny] is the index of the neighboring cell in the x - [y]-dimension. The total estimator in the system is given by $E_m = \sqrt{\sum_n E_{n,m}^2}$.

There is no rigorous proof that the proposed estimator is actually an error estimator. However, some comparisons were made of this estimator to the exact error measured in L_2 norm for some problems that possess analytical solutions.⁹

The local and total errors, e_n and e are expressed as:

$$e_n = \sqrt{\int_{V_n} (\Psi_n^{an} - \Psi_n)^2 dv} \quad ; \quad e = \sqrt{\sum_n e_n^2} \quad (9)$$

The evolution of the estimator and the error with increasing spatial approximation order and mesh refinement was observed in Ref. 9. In all cases it was found that the ratio of the estimator to the error asymptotically approaches a constant value. For example, we solved problems of the kind proposed in Ref. 10 where the singular characteristics always pass through a cell vertex and others where they pass through cell edges, and the behavior of the ratio mentioned above remained the same. We also observed in some nodes of some problems that the solutions got worse with increasing spatial approximation order, an unexpected behavior. This feature was exhibited equally by the estimator, as well as the error.

These observations motivated us to implement this error estimator in an AHOT-N code for solving more realistic problems, and to apply the estimated errors into an adaptive order scheme.

2.3. ADAPTIVE EXPANSION ORDER

Local mesh refinement is the most popular technique when dealing with adaptivity in finite elements. In finite difference as well as in nodal methods, local mesh refinement is accomplished by approximations at the interfaces between fine and coarse meshes.

The AHOT-N method has two degrees of freedom to modify the accuracy in the results, mesh and order of the spatial approximation. Conceptually, mesh refinement in this method has the same characteristics as the finite difference method. In particular when it is necessary to make mesh refinement in part of the system, mesh refinement in other parts or surface approximations must be made.

In contrast adaptive expansion order in the AHOT-N method needs only local approximations. These are the approximations mentioned before to couple neighboring nodes with different approximation orders and to calculate scalar fluxes from directions with different order.

In this work we use a simple adaptive strategy based on the following adaptive iteration scheme:

1. Input initial order distribution per node per direction:
Uniform order distribution is the simplest first approach considering that adaptivity will modify the orders depending on the estimated errors. At this point, it is interesting to note that even-order approximations usually produce fewer negative scalar fluxes than odd-order approximations.¹¹
2. Perform the inner iterations until convergence is reached:
We use for the inner iterations the standard pointwise convergence criterion on the scalar fluxes with the same accuracy in all adaptive stages.
Once the inner iterations converge an additional sweep of the system allows storage of the nodal and transverse angular flux moments needed to perform the error estimation.
3. Estimate errors per node per direction:
This step is performed using the converged angular moments in Eq. (6) to (8).
4. Convergence test of the adaptive scheme:

Convergence is reached when the maximum estimator for all the nodes and all the directions is less than a predefined value.

5. IF convergence is reached, or maximum number of adaptive iterations reached, STOP,

6. ELSE, automatically modify the order distribution.

For a given direction the order of the approximation increases in the nodes whose estimator lies within a given range above the maximum estimator. This criterion, that we call "bound criterion" is expressed as follows:

$$\text{If } \frac{E_{\max,m}^{(t)}}{E_{n,m}^{(t)}} \leq B > 1 \text{ then } \Lambda_{n,m}^{(t+1)} = \Lambda_{n,m}^{(t)} + 1,$$

$$\text{Else } \Lambda_{n,m}^{(t+1)} = \Lambda_{n,m}^{(t)},$$

where m and n indicate the direction and node respectively, t the iteration of the adaptive process, and $E_{\max,m}^{(t)}$ is the maximum estimator over the nodes of the system for the direction m in the iteration t .

It is important to notice that this criterion applies to each discrete direction independent of the estimated errors in other directions. It allows local increase of the order of approximation that is driven in part by the estimated errors in other parts of the system through the influence of $E_{\max,m}^{(t)}$.

7. GO TO 2.

3. NUMERICAL TESTS

We implemented the adaptive AHOT-N method in a discrete-ordinates steady-state code for solving monoenergetic, fixed source, isotropic scattering problems in two-dimensional Cartesian geometry. We use the algorithm described in Ref. 1 in which the simultaneous algebraic equations for the nodal flux moments are solved at the beginning of the calculation process. We execute this code on a Silicon Graphics computer with all variables defined in double precision.

We solved two test problems with uniform order distribution and with the adaptive scheme to compare the number of unknowns used in each method to obtain the same accuracy. In order to investigate the evolution of the solutions in the adaptive process, we did not apply the convergence test, STEP 4 of the adaptive scheme; instead we allowed the system to evolve until reaching a prefixed number of adaptive iterations.

The first test problem we solved is presented in Ref. 1. It is a 0.1 m square with reflective left and bottom, and vacuum right and top boundary conditions. The system contains a unit source region located in a 0.05 m square at the lower left corner (Region I) with total cross section and scattering ratio 100 m^{-1} and 0.5, respectively, surrounded by a source-free region with total cross section and scattering ratio 200 m^{-1} and 0.05, respectively.

We solved this test problem using an S_4 angular quadrature and a pointwise relative convergence criterion of 10^{-4} for the calculated scalar flux spatial moments to test convergence of the inner iterations.

To validate the programming of our code we solved this test problem with uniform order distribution using meshes ranging from 2×2 to 128×128 and approximation orders from 0 to 9 and the results obtained are identical to the results presented in Ref. 1.

We also solved this problem adaptively using the bound criterion with $B=10^2$ and $B=10^4$ on a 4×4 mesh.

The relative error in the Region-averaged scalar flux obtained using uniform order distribution and both adaptive cases vs. the number of unknowns used to solve the problem are shown in Fig. 1 for the lower left corner (Region I), the lower right corner (Region II) and the upper right corner (Region IV).

No great advantage is observed in this problem when solving it adaptively. The number of unknowns used to obtain a given accuracy in the Region-averaged scalar fluxes is similar in all the cases. The adaptive $B=10^4$ case uses in general less unknowns than the uniform order case to obtain the same accuracy, but this saving does not justify the programming effort and the longer execution times involved to solve the problem adaptively.

These observations do not apply to the adaptive process in general but to the application of the adaptive process to this particular test problem. The system solved possesses high angular flux gradients for all the discrete directions in the nodes neighboring the region material (and source) discontinuities and in the lower left node of Region IV. These nodes represent 50% of the total number of nodes in the system. Therefore it should not be expected that any adaptive process applied to this test problem will produce great improvement with respect to the uniform order distribution scheme.

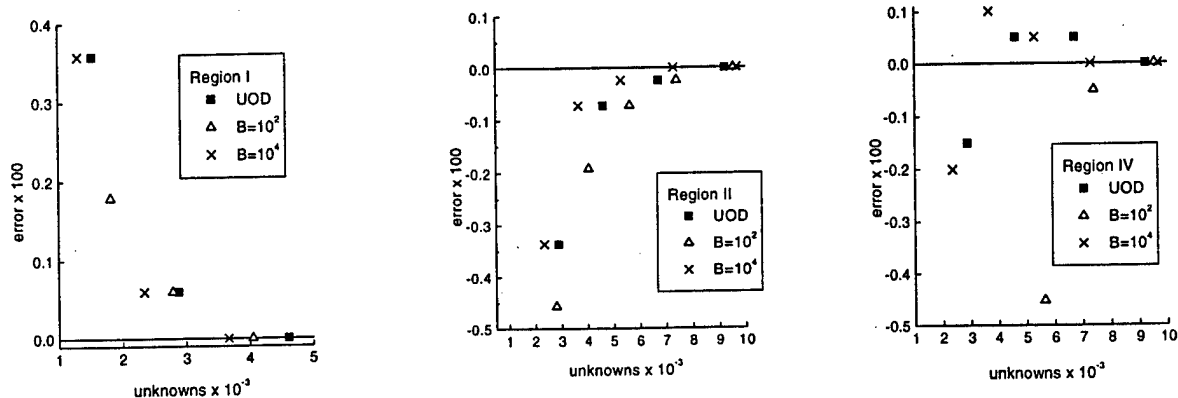


Fig. 1. Relative error in Region-averaged scalar fluxes of the first test problem.

In order to numerically test the advantages of the adaptive process we solved a modified version of the first problem. This is a homogeneous 0.4 m. square composed by the material of Region I of the first test problem with a unit source in the lower left 0.35 m. square. We solved this problem using the same S_4 angular quadrature and pointwise convergence criterion as before on an 8x8 mesh.

Fig. 2 shows schematically the Region-averaged scalar fluxes obtained with $\Lambda=6$ in the uniform distribution order case, where the shadow cells indicate the source region. These fluxes were considered as reference values for the errors depicted in Fig. 1 since they are converged in the increasing uniform order process.

0.1515	0.1515	0.1515	0.1515	0.1515	0.1513	0.1338	0.0176
1.848	1.848	1.848	1.848	1.848	1.848	1.715	0.1338
1.999	1.999	1.999	1.999	1.999	1.998	1.848	0.1513
2.000	2.000	2.000	2.000	2.000	1.999	1.848	0.1515
2.000	2.000	2.000	2.000	2.000	1.999	1.848	0.1515
2.000	2.000	2.000	2.000	2.000	1.999	1.848	0.1515
2.000	2.000	2.000	2.000	2.000	1.999	1.848	0.1515
2.000	2.000	2.000	2.000	2.000	1.999	1.848	0.1515

Fig. 2. Region-averaged scalar fluxes of test problem 2 with $\Lambda=6$.

The square root of the quadratic sum of the relative error obtained in the Region-averaged scalar fluxes divided by the number of nodes of the system vs. the number of unknowns used to solve the problem with uniform order distribution and with the B=10² and B=10³ adaptive schemes are depicted in Fig. 3.

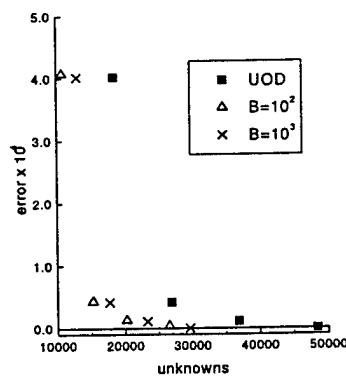


Fig. 3. Relative error in System-averaged scalar fluxes of the second test problem.

In this problem the adaptive $B=10^3$ case uses 61% of the number of unknowns that the uniform order case uses to reach to the same final Region-averaged scalar fluxes, while the adaptive $B=10^2$ case uses 55%. Moreover, the differences in the Region-averaged scalar fluxes obtained with the adaptive $B=10^3$ case and with uniform order distribution when solving the system with the same maximum order Λ_{\max} are less than the required accuracy for the inner iterations.

We also calculated the average leakage at the right surface of the upper right quadrant using the homogeneous and adaptive order schemes.

The angular fluxes at the surfaces of the nodes can be obtained using the angular flux transverse moments which are calculated explicitly by the AHOT-N method, or they can be reconstructed from the angular nodal moments. In general different values are obtained for the leakage in each node depending on the way it is calculated. In the following we refer to the leakage reconstructed from nodal moments as "reconstructed leakage" and the leakage obtained using transverse moments as "direct leakage".

These results are shown in Table 1 where Λ refers to the order in the homogeneous order scheme and to the adaptive step when using variable order.

Table 1. Average leakage at the upper right Region.

Λ	Uniform order distribution			$B=10^2$			$B=10^3$		
	number of unkn.	Leakage		number of unkn.	Leakage		number of unkn.	Leakage	
		rec.	dir.		rec.	dir.		rec.	dir.
0	2304	1.007E-02	5.986E-03	2304	1.007E-02	5.986E-03	2304	1.007E-02	5.986E-03
1	6144	-3.943E-03	-1.829E-03	4314	-3.530E-03	-1.347E-03	4929	-3.943E-03	-1.829E-03
2	11520	1.347E-03	1.103E-03	7143	1.242E-03	9.683E-04	8604	1.347E-03	1.103E-03
3	18432	2.897E-03	1.131E-03	10782	9.729E-04	3.978E-04	13005	9.657E-04	3.770E-04
4	26880	-3.012E-05	1.052E-03	15231	-1.435E-05	5.256E-04	17702	-1.507E-05	5.260E-04
5	36864	8.939E-04	5.017E-04	20204	8.947E-04	5.008E-04	23291	8.939E-04	5.017E-04
6	48384	2.958E-04	5.046E-04	26541	2.938E-04	5.047E-04	29645	2.958E-04	5.046E-04

The adaptive $B=10^3$ case produces the same leakage as the uniform order case when the system is solved with the maximum order greater than 4. This feature can be explained by observing that the distribution of orders in the adaptive $B=10^3$ case is very close to the order of approximation in the uniform order distribution case in all the directions and nodes where no flat fluxes appears.

4. CONCLUSIONS

In this work we applied an adaptive scheme to automatically increase the expansion order in regions of a system depending on the estimated errors of the solution when solving the system using the AHOT-N method. The errors have been obtained using an *a posteriori* error estimator that could also be used in other polynomial nodal methods as well as in finite difference schemes.

To accomplish this we proposed simple approximations to modify the nodal method in order to calculate with different spatial approximation orders each node of the system and each direction of the angular quadrature. This technique could be applied not only for the purposes used in this paper but also to avoid negative scalar fluxes in some nodes of a system by locally increasing the expansion order.

The two-dimensional numerical test problems solved in this paper constitute a sample analysis of the modified nodal method and the local adaptive scheme. The results obtained are in agreement with the concept that adaptive schemes are advantageous when applied to systems with smooth solutions in large regions.

The search for an optimal range above the maximum estimator for increasing the approximation order is one of the areas worthy of further investigation. In this sense, the second test problem solved is an example of when the bound B increases the solutions are more accurate in each adaptive step but the saving in the number of unknowns decreases compared to lower B values.

We also conclude that the criterion used to modify the approximation orders in the adaptive process must be investigated in more detail to provide alternative means for adapting the order based on the error in quantities whose accuracy is most important for a given application.

For example to control the scalar flux accuracy in some particular node of the system with the adaptive process, a local bound criterion could be used rather than the bound criterion proposed above to automatically increase the approximation order. This local criterion can be implemented by increasing the approximation order in the directions where the estimated error lies within a range of the maximum estimated error over all directions for a given node.

A more elaborate criterion to modify the approximation orders can take into account the relationship between the estimated errors and the errors in other quantities of interest as scalar fluxes or leakage. While doing this we will continue to investigate different applications of the error estimation.

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