Conf-941102--29

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Invited for presentation at the *Tutorial Review of Solution Methods and Applications of the One-Group Transport Equation*, organized by Dr. John Garth in the 1994 Winter Meeting of the American Nuclear Society, Washington, D.C., November 13–17, 1994.

*Research sponsored by the U.S. Department of Energy under contract No. DE-AC05-84OR21400 with Martin Marietta Energy Systems, Inc.

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As part of an effort to develop an adaptive mesh refinement strategy for use in state-of-the-art nodal diffusion codes[1], we derive error bounds on the solution variables of the quadratic Nodal Expansion Method(NEM) in slab geometry. The discrete variables utilized by the quadratic NEM for cell $i = 1, \ldots, N$, are the node average flux $\langle\phi\rangle^i$, the east surface flux ϕ^i_- and the west surface flux ϕ^i_+. Use of the nodal basis functions described in [2] results in a system of nodal balance equations similar to that of a central finite difference approximation,

$$6\left[\frac{\phi^i_+ - 2\langle\phi\rangle^i + \phi^i_-}{\Delta x^2}\right] - \frac{1}{L^2}\langle\phi\rangle^i = -\frac{\langle s\rangle^i}{D} \tag{1.a}$$

and current continuity constraints,

$$\frac{D^i}{\Delta x}\left[-2\phi^i_+ + 6\langle\phi\rangle^i - 4\phi^i_-\right] = \frac{D^{i-1}}{\Delta x}\left[4\phi^{i-1}_+ - 6\langle\phi\rangle^{i-1} + 2\phi^{i-1}_-\right] \tag{1.b}$$

where D is the diffusion coefficient, L is the diffusion length, Δx is the mesh spacing and $\langle s\rangle^i$ is the average neutron source in cell i. Closure of the system is obtained through flux (dis)continuity relationships and boundary conditions.

First we establish the uniqueness of the solution to the NEM equations via a "Maximum Principle"[3]. For this purpose it is necessary to assume a uniform mesh and homogeneous

[1]Supported by the Department of Energy Computational Science Graduate Fellowship administered through Ames Laboratory. This work was completed while on practicum assignment in the Engineering Physics & Mathematics Division of the Oak Ridge National Laboratory. Permanent address is P.O. Box 7909 NCSU Campus, Raleigh, NC 27695-7909.

nuclear properties, as well as continuity of the flux across the cell boundaries. Thus the notation will now reflect that ϕ^i is the flux at the surface located at x_i on the right boundary of node i.

Hypothesize the existence of two solutions to the discrete equations $\{\langle\phi\rangle^i, \phi^i\}$ and $\{\langle\psi\rangle^i, \psi^i\}$, and let $\langle\xi\rangle^i = \langle\phi\rangle^i - \langle\psi\rangle^i$ and $\xi^i = \phi^i - \psi^i$. If we now form the difference of the two sets of NEM equations in these two solutions, we obtain an analogous homogeneous set in the difference variables with homogeneous boundary conditions $\xi^0 = 0$ and $\xi^N = 0$. Close inspection of the coefficients in (1.a) reveal that $\mid \langle\xi\rangle^i \mid \leq max\{\mid \xi^{i-1} \mid, \mid \xi^i \mid\}$ implying the maximum absolute difference occurs at a cell boundary, say cell k, hence $|\xi^k| \geq |\xi^i|$ and $|\xi^k| \geq |\langle\xi\rangle^i|$ for all i. Solving the current continuity expression for ξ^k and substituting for the node-average quantities we obtain a 3-point difference scheme involving only surface quantities, $\xi^k = \alpha(\xi^{k-1} + \xi^{k+1})$, $\alpha \equiv [6 - \frac{\Delta x^2}{L^2}]/[12 + 4\frac{\Delta x^2}{L^2}]$. Note that $|\alpha| \leq \frac{1}{2}$, and $\alpha \geq 0$ for $\Delta x \leq \sqrt{6}L$, a condition that must be satisfied in the limit $\Delta x \to 0$ that is necessary for the error analysis. Applying the Triangle Inequality[4], $|\xi^k| \leq |\alpha| \left(|\xi^{k-1}| + |\xi^{k+1}| \right)$. If $|\xi^{k+1}| \geq |\xi^{k-1}|$ then we conclude, $|\xi^k| \leq 2|\alpha|\ |\xi^{k+1}| \leq |\xi^{k+1}|$, and it follows that $|\xi^k| = |\xi^{k+1}|$. Similarly $|\xi^{k+1}| \leq |\xi^{k-1}|$ yields $|\xi^k| = |\xi^{k-1}|$ so that $|\xi^k| = max\left\{|\xi^{k+1}|, |\xi^{k-1}|\right\}$. Now suppose $|\xi^k| = |\xi^{k+1}| > |\xi^{k-1}|$, then $|\xi^k| \leq |\alpha|(|\xi^{k-1}| + |\xi^{k+1}|) < |\xi^{k+1}| = |\xi^k|$, a contradiction that implies $|\xi^{k-1}| = |\xi^k| = |\xi^{k+1}|$. We conclude that if a maximum does in fact occur in the interior of the interval then $|\xi^i|$ is constant, $i = 0, \ldots, N$. The boundary conditions, $\xi^0 = 0$ and $\xi^N = 0$, then imply that ξ is identically zero at all surfaces and for all node averages, and the solution of the NEM equations is unique.

Turning now to the question of bounding the error in the solution, start with the nodal balance equation and subtract from each side $-6\Phi^i + 12\langle\Phi\rangle^i - 6\Phi^{i-1}$ where Φ implies the exact solution. The error in the NEM solution is then $\langle e\rangle^i = \langle\phi\rangle^i - \langle\Phi\rangle^i$, $e^i = \phi^i - \Phi^i$. The nodal balance and current continuity analogs in the error variable are given by,

$$-6e^i + 12\langle e\rangle^i - 6e^{i-1} = \Delta x^2 \tau_1(i, \Delta x), 1 \leq i \leq N \qquad (2.a)$$

$$-2e^{i-1} + 6\langle e\rangle^i - 8e^i + 6\langle e\rangle^{i+1} - 2e^{i+1} = \Delta x \ \ \tau_2(i,\Delta x), 1 \le i \le N-1 \qquad (2.b)$$

where the components of the discretization error are defined by,

$$\tau_1(i,\Delta x) \equiv 6\frac{\Phi^i - 2\langle\Phi\rangle^i + \Phi^{i-1}}{\Delta x^2} - \frac{1}{\Delta x}\int_{x_{i-1}}^{x_i} \frac{d^2}{dx^2}\Phi(x)dx \qquad (3.a)$$

$$\tau_2(i,\Delta x) \equiv \frac{2\Phi^{i-1} - 6\langle\Phi\rangle^i + 4\Phi^i}{\Delta x} + \frac{4\Phi^i - 6\langle\Phi\rangle^{i+1} + 2\Phi^{i+1}}{\Delta x} \qquad (3.b)$$

We now show that the truncation errors in the node average and surface fluxes are bounded by a combination of the components of the discretization error. We solve (2.a) for the node average flux error in nodes i and $i+1$ then substitute into (2.b) to get an expression in only the surface flux errors,

$$\left[8 - \frac{72}{12 + \frac{\Delta x^2}{L^2}}\right] e^i = \left[-2 + \frac{36}{12 + \frac{\Delta x^2}{L^2}}\right](e^{i+1} + e^{i-1}) + \frac{6\Delta x^2}{12 + \frac{\Delta x^2}{L^2}}[\tau_1(i,\Delta x) + \tau_1(i-1,\Delta x)] - \Delta x\tau_2(i,\Delta x) \qquad (4)$$

The most important property of $\tau_n(i,\Delta x)$ to establish is that it approahes zero in the limit as $\Delta x \to 0$ since this guarantees the truncation error will also approach zero. We also determine in the case that the exact flux solution is sufficiently smooth the rate at which the local discretization error components approach zero. Expanding the exact flux in a Taylor series assuming it is sufficiently smooth about the surface at x_i the discretization error components can be written exclusively in terms of the exact solution derivatives at x_i. Substituting these expressions into (4), then using the Triangle Inequality, we obtain

$$\left[8 - \frac{72}{12 + \frac{\Delta x^2}{L^2}}\right] e^i \le \left|-4 + \frac{72}{12 + \frac{\Delta x^2}{L^2}}\right| |e| + \frac{M^{iv}\Delta x^4}{12 + \frac{\Delta x^2}{L^2}} \qquad (5)$$

where $M^{(iv)} = \max_{0<x<a} \mid \Phi^{(iv)}(x_i) \mid$.

This expression is true for all nodes including the node where the maximum absolute surface flux error,$|e|$, is actually attained. There are two branches we can follow depending on the magnitude of the term inside the absolute value. We will only examine the inequality under

the assumption that this term is positive, $\Delta x^2 \leq 6L^2$ since this is true in the limit of small Δx. We may solve for the maximum surface flux error bound as,

$$|e| \leq \left[\frac{M^{iv}L^2}{12}\right] \Delta x^2 \tag{6.a}$$

Returning to (2.a) and applying the Triangle Inequality, we complete our analysis by finding an upper bound on the node average flux error,

$$| \langle e \rangle^i | \leq \frac{M^{(iv)}L^2}{12} \Delta x^2 \tag{6.b}$$

implying second order convergence of the quadratic NEM.

In order to verify the analysis presented above, we compare the quadratic NEM to the analytic solution of a test problem. The test problem for this investigation is a one-dimensional slab $[0, 20cm]$ with $L^2 = 6.495cm^2$ and $D = 0.1429cm$. The slab has a unit neutron source distributed uniformly throughout and zero flux boundary conditions. The analytic solution to this problem is used to compute the node-average fluxes over a variety of meshes, and these are used to compute the NEM maximum error on each mesh. The system of NEM equations is solved in double precision using established double precision LU factorization (DGECO) and solver (DGESL) routines from the LINPACK library[5]. The number of nodes used in the solution was increased until the behavior of the error was observed to be asymptotic. Results of this comparison are presented in Figure 1 and comfirm our analysis of the error order as quadratic. The error bound predicted is larger than the computed value by a factor greater than five in the asymptotic region. This is due to the "worst case" assumed bythe analysis. Work is underway extending this analysis to higher order nodal methods in multi-dimensions.

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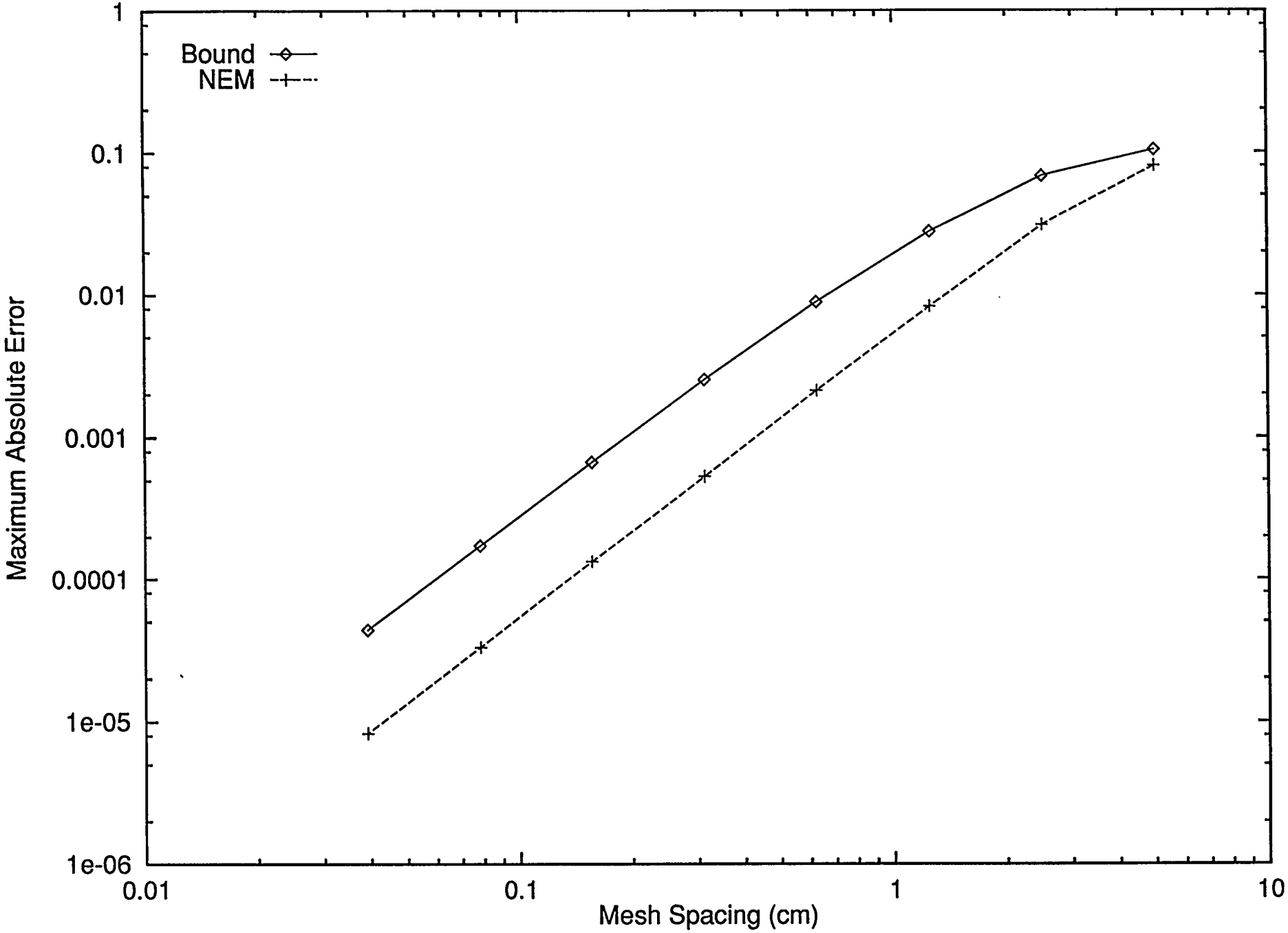
Figure 1: Comparison of the computed maximum absolute error and the upper bound on the node-average flux error for the quadratic NEM solution to the test problem on various uniform meshes.


Bound
NEM
Maximum Absolute Error
Mesh Spacing (cm)
1
0.1
0.01
0.001
0.0001
1e-05
1e-06
0.01
0.1
1
10