Transactions of the Korean Nuclear Society Autumn Meeting
Goyang, Korea, October 24-25, 2019

Numerical Performance of the Refined AFEN Response Matrix Method in the Two-Dimensional Hexagonal Geometry

Jae Man Noh
Korea Atomic Energy Research Institute
jmnoh@kaeri.re.kr

1. Introduction

A nodal method based on the Analytic Function Expansion Nodal (AFEN) method [1-5] in the hexagonal geometry has been implemented into CAPP [6] in order to improve the computational efficiency of its high order Finite Element Method (FEM). The AFEN version applied here is the refined AFEN method introduced in Reference [4].

As is generally known, numerical schemes based on the response matrix method are considered more numerically efficient than the original refined AFEN method. The response matrix method uses the interface partial currents as nodal unknowns instead of the interface fluxes used in the original refined AFEN method. There is an advantage in the response matrix method that the domain where the nodal unknowns and their coefficients matrixes are calculated is confined within the node independently of its neighbor nodes. This property is very favorable for parallel computation combined with the RGB sweeping scheme described in Reference [7].

In addition, the response matrix method has another advantage. It calculates the six outgoing interface partial currents of each node at once by solving a single-node problem with the boundary conditions of six incoming partial currents. On the other hand, the original refined AFEN method determines only one interface flux by solving a two-node problem with current continuity condition across each interface between two nodes. Considering that the number of nodes is three times less than the number of interfaces ideally, the response matrix method becomes at least three times more efficient than the original refined AFEN method theoretically if we assume that the number of iterations required to achieve a certain accuracy level is same for both methods.

Noting that the Finite Difference Method (FDM) nonlinear iteration scheme [8] is widely being used as an acceleration scheme for high-order neutron diffusion and transport methods, the nonlinear FDM response matrix method equivalent to the refined AFEN method was tried to reduce computational time.[7] However, unlike the hopeful expectation caused by a big success of the nonlinear FDM as an acceleration technique, the refined AFEN method equivalent FDM response matrix method could not provide a numerically stable solution.[7]

To assure numerical stability, we adopt finally a direct formulation of the response matrix of the refined AFEN with interface partial currents and their moments.[9] This method was tested against a benchmark problem in Reference [9]. The results showed that its computing speed is faster than that of the original refined AFEN method.

In order to generalize the conclusion of Reference [9], a numerical method to analyze the numerical performance of the refined AFEN response matrix method is presented in this paper. The numerical error analyses using this method are performed for several benchmark problems including the VVER-440 LWR benchmark problem and the MHTGR-350 HTGR benchmark problem to show the numerical performance of the refined AFEN response matrix method.

2. Methodology

The readership of this paper is kindly recommended to refer Reference [9] for the refined AFEN response matrix method in the two-dimensional hexagonal geometry. Only a numerical method for its numerical performance analysis is describe here.

The performance of an iterative numerical scheme to solve a linear elliptic partial differential equation is shown by a numerical error analysis in a general textbook on numerical methods.[10] The iterative method applied to solve the AFEN response matrix in the hexagonal geometry by the power method is given by

$$\mathbf{s}^{(t+1)} = \frac{1}{k^{(t)}} \mathbf{A}\, \mathbf{s}^{(t)} \tag{1}$$

$$k^{(t+1)} = \frac{\|A\, \mathbf{s}^{(t)}\|}{\|\mathbf{s}^{(t)}\|} = k^{(t)} \frac{\|\mathbf{s}^{(t+1)}\|}{\|\mathbf{s}^{(t)}\|} \tag{2}$$

where $\mathbf{s}^{(0)} = \mathbf{s}_0$, $k^{(0)} = k_0$, and $t = 0,1, \ldots$ $\mathbf{s}$ is an $1 \times \mathrm{n}$ iteration vector and $\mathbf{A}$ is the $\mathrm{n} \times \mathrm{n}$ corresponding iteration matrix. The nodal neutron source vector can be the iteration vector in this discussion and the sum of absolute values of the elements of the source vector can serve as the norm for the iteration vector in Eq. (2). Assume that $\mathbf{A}$ is a complete matrix and that it has a single dominant eigenvalue and a second dominant eigenvalue. Le $\lambda_1, \ldots, \lambda_n$ ($|\lambda_1| > |\lambda_2| > |\lambda_j|$ for all j) denote the eigenvalues of $\mathbf{A}$ and $\mathbf{u}_1, \ldots, \mathbf{u}_n$ the corresponding eigenvectors, which form a complete basis set.

By defining the error vector as follows and writing it in terms of these basis vectors, we can derive the expression for the dominance ratio, $|\lambda_2/\lambda_1|$ by which the rate of convergence of the iteration system is governed:

$$\begin{aligned} \mathbf{e}^{(t)} &= \mathbf{s}^{(t)} - \mathbf{s}_\infty \\ &= T^{(t)} \left(c_2 \left(\frac{\lambda_2}{\lambda_1}\right)^t \mathbf{u}_2 \cdots + c_n \left(\frac{\lambda_n}{\lambda_1}\right)^t \mathbf{u}_n \right) \\ &\approx T^{(t)} c_2 \left(\frac{\lambda_2}{\lambda_1}\right)^t \mathbf{u}_2 \qquad \textit{for all } t \gg 0 \end{aligned} \tag{3}$$

where $\mathbf{s}_\infty$ is the converged source vector and is approximated by iteration until $\mathbf{s}^{(t)}$ converges within almost the truncation error level. Once we get $\mathbf{s}_\infty$, we repeat the iteration from the beginning to compute the dominance ratio by using the following equation:

$$\frac{\|\mathbf{e}^{(t)}\|}{\|\mathbf{e}^{(t-1)}\|} \approx \frac{\lambda_2}{\lambda_1} \quad \textit{for all } t \gg 0 \tag{4}$$

3. Numerical Results and Discussion

The numerical performance of the refined AFEN response matrix method was verified against several benchmark problems including small and large light water reactor (LWR) and high temperature gas-cooled reactor (HTGR) cores. The verification here focuses primarily on showing computational efficiency rather than accuracy. The excellent accuracy of the refined AFEN method has already shown in Reference [4].

3.1. Mini Core Problem

A mini core problem having seven fuel assemblies in the first and second rings of the hexagonal core and twelve non-power generating control assemblies in the third ring was derived from VVER-440 problem. [4,11]

The numerical error analysis was performed with two energy groups in a sixth core and the results of the refined AFEN response matrix method were compared with those of the original refined AFEN method and the FDM response matrix method without any nonlinear correction factors. Fig. 1 shows a pattern in which the fission source vector converges as the iteration progresses. Each of the three solid lines in this figure is the logarithmic scale normalized norm of the error vector of the source vector given in Eq. (3) (See the left-y axis.) and each of dotted lines is the dominance ratio estimated by the equation (4) (See the right-y axis). Red, green and blue colors on both solid and dotted lines indicate the quantity for the refined AFEN response matrix, the original refined AFEN method and the FDM response matrix, respectively.

This figure clearly illustrates the excellence of the refined AFEN response matrix method in numerical performance beyond comparison with the other two methods. This method with a much lower dominance ratio converges more than twice as fast as the other two methods. This method reaches asymptotic convergence state after only a few initial iterations, which is characterized by a flat dominance ratio and a linearly decreasing error in logarithmic scale. In this state, the error is reduced by the power of the dominance ratio as each iteration progresses. Therefore, an acceleration by extrapolation of the iterative vector becomes possible.

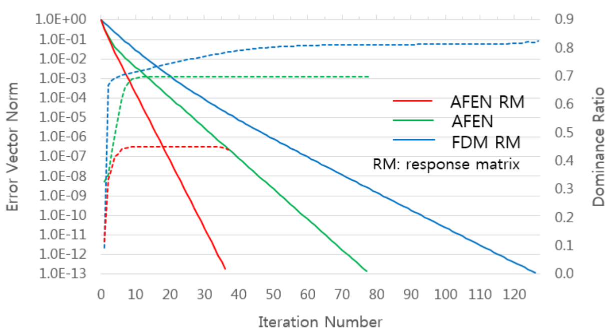

Fig. 1 Convergence Pattern (Mini Core)

Some numerical performance related parameters calculated by the three methods are compared in Table I. The k-effective difference between the two refined AFEN methods is purely due to the different boundary conditions because the two methods are mathematically equivalent. Therefore, this difference does not mean that one is better in accuracy than the other. The boundary condition applied is the zero incoming partial current for the two response matrix methods and the zero flux for the conventional form of the refined AFEN method. The numerical performance of a method is not significantly affected by the difference between these two boundary conditions. (See the footnote below Table II.)

The second column of the table is the dominance ratio estimated numerically, where the value for the refined AFEN response method is the smallest. The third column is the number of iterations expected to achieve a less than 10^{-7} accuracy in node-wise sources if the source error decreases in an asymptotic manner as described above. This is the value calculated by the following equation:

$$-\frac{7}{\log_{10}(\frac{\lambda_2}{\lambda_1})} \qquad (5)$$

The next column is the number of iterations performed to achieve the same accuracy in the actual calculation. Not only does the refined AFEN response matrix method have the smallest number of iterations, but it also has the smallest deviation between the prediction and the actual value. This means it reaches the asymptotic state very early, which is advantageous for acceleration by asymptotic extrapolation. The last column is time consumed for the calculation. This value is obtained by averaging three measurements from a PC with Intel® Core™ i7-4930K CPU using the functions of the MS Visual Studio™ Chrono library. The refined AFEN response matrix method is 2.5 times faster than the original refined AFEN method. It is a little faster considering the number of iterations, but slower considering the efficiency of the response matrix aforementioned in Introduction. This is probably due to the fact that the size of the core and the number of energy groups are so small that the proportion of auxiliary operations other than the iteration matrix related operations becomes not small within a single iteration.

Table I. Numerical Performance Parameters (Mini Core)

	k-eff	λ_2/λ_1	Expected Iterations	Actual Iterations	Time (μsec)
AFEN RM	0.778735	0.45164	20	20	389
AFEN	0.776642	0.69846	45	41	944
FDM RM	0.865688	0.81307	78	51	293

3.2. VVER-440 Problem

The refined AFEN response matrix method were further verified against the VVER440 benchmark problem [4,11] , which is a commercial size LWR core simulating an old Soviets PWR. It consists of 342 fuel assemblies, 7 non-power generating control rod assemblies, and 72 surrounding reflector assemblies.

The results of the numerical error analysis are shown in Fig. 2 and Table II. All the components of the figure and the table have a completely same meaning as described in the previous section. Note that there exists the same boundary condition difference among the three methods as described in the section.

The error vector of the refined AFEN response matrix method is smaller than that of the FDM response matrix method at the early stage of iteration. But eventually it gets caught up with the FDM response matrix method near the 1,000th iteration (near 10^{-11} error). This is because the refined AFEN response matrix method has a very comparable but slightly larger dominance ratio compared with the FDM response matrix method.

The deviation between the predicted and the actual number of interactions widens as the problem size increases. Therefore, attention is required to accelerate calculation with asymptotic extrapolation. An adequate under-relaxation factor in extrapolation may be desirable.

Comparing the refined AFEN response matrix method and the original refined AFEN method is more exciting. Although the refined AFEN response matrix method has a much smaller dominance ratio (The criterion is how far from one.), it seems to be inferior to the original refined AFEN method in terms of the error size at the early stage of iteration. However, eventually, it requires three times shorter computing time to achieve 10^{-7} accuracy. Considering that it does not seem to be overwhelmingly faster (3.4 times faster) than the number of iterations has reduced (3.2 times), the proportion of auxiliary operations is still too significant to show the advantage of the calculational efficiency of the response matrix.

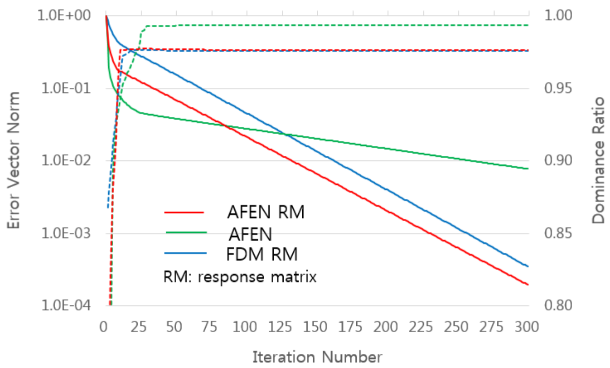

Fig. 2 Convergence Pattern (VVER-440)

Table II. Numerical Performance Parameters (VVER-440)

	k-eff	λ_2/λ_1	Expected Iterations	Actual Iterations	Time (msec)
AFEN RM	1.009645	0.97672	684	460	64
AFEN*	1.008632	0.99358	2501	1454	216
FDM RM	1.018224	0.97583	659	463	31

* The original AFEN method with the vacuum boundary condition computed the effective multiplication factor equal to the value of the AFEN RM method after 1483 iterations.

3.3. MHTGR-350 Problem

The MHTGR-350 problem[12] is a 350MWth hexagonal prismatic block type HTGR core with graphite moderator and helium coolant. It has an active core of 66 fuel blocks in the fourth, fifth and sixth rings of the core, surrounded by graphite reflectors with about three rings thick inward and outward. Due to spectrum shift in the graphite-moderated reactor, the ten-energy group system rather than the two- group system is used for the analysis of the MHTGR-350 core.

Fig. 3 and Table III illustrate the results of the numerical error analysis. The results of the error analysis show that the convergence patterns for the VVER-440 problem, such as the order of the three methods in convergence speed driven by the dominance ratio size, remain the same for this problem. The error of the original refined AFEN method is the smallest in the early iteration stage but eventually caught by the refined AFEN response matrix method. However, the big difference from the results of the error analysis of VVER-440 is also shown: The dominance ratio deviation between the two AFEN methods has greatly narrowed, which in turn leads to a big reduction in the difference in the number of iterations (from 3.2 times for VVER-440 to 1.2 times for MHTGR-350).

This should have meant less reduction in computing time but, there is another reversal, so the reduction is almost the same as for the VVER-440 problem (3.4 times faster). This is because the proportion of the iterative matrix related operations increases significantly compared to that of the auxiliary operations as the number of energy groups increases from two to ten. The calculational efficiency of the refined AFEN response matrix method, which is at least three times higher per iteration, becomes easier to be realized for this problem. The results showed again that a careful asymptotic acceleration is required with under-relaxation factors.

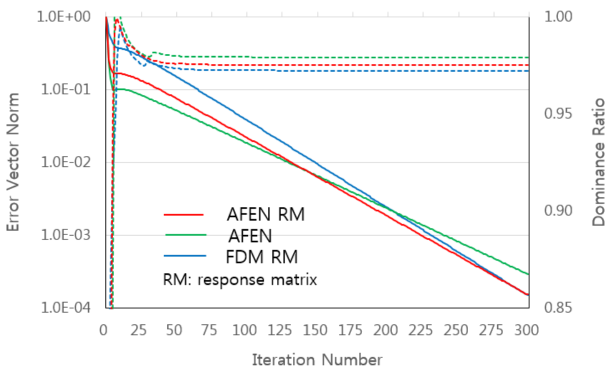

Fig. 3 Convergence Pattern (MHTGR-350)

Table III. Numerical Performance Parameters (MHTGR-350)

	k-eff	λ_2/λ_1	Expected Iterations	Actual Iterations	Time (msec)
AFEN RM	1.093230	0.97531	645	450	290
AFEN	1.092759	0.97936	773	545	971
FDM RM	1.050210	0.97248	578	413	55

4. Conclusions

In order to improve efficiency of the CAPP code in the analysis of the hexagonal reactor cores, we have tried to implement a refined AFEN method in the hexagonal geometry whose accuracy has been well proven. The numerical method for the refined AFEN method adopted here is the response matrix method that uses the interface partial currents as nodal unknowns instead of the interface fluxes. This method has an advantage that all iterative matrix calculations are single-node based, which is not only very efficient but also very favorable for parallel computation.

After we found that the refined AFEN method equivalent nonlinear FDM response matrix method could not provide a numerically stable solution, we developed the direct formulation of the refined AFEN response matrix to assure numerical stability.

To show the numerical performance of the refined AFEN response matrix method against the original AFEN method, the numerical error analyses were performed for several benchmark problems including the two-group VVER-440 problem representing the LWR core and the ten-group MHTGR-350 problem representing the HTGR core. Although the difference varies depending on the problem, the refined AFEN response matrix method consistently shows a smaller dominance ratio for the benchmark problems. It also shows a more than three times speedup in computing time for both problems. The reason of the speedup is explained differently for each of them: that for the VVER-440 problem is mainly due to a big cut in the number of iterations caused by a far smaller dominance ratio, on the other hand, that for MHTGR-350 problem is mainly due to the advantage of the computational efficiency of the response matrix method.

In addition, it was found from the results of the error analyses that the dominance ratio of this method is smaller than or at least comparable to that of the FDM response matrix. This can be presented as a cause of poor performance of the nonlinear FDM schemes in accelerating the refined AFEN response matrix method.

In short, it can be concluded that the refined AFEN response method significantly outperforms the conventional AFEN method in analyzing the hexagonal reactor cores.

Acknowledgements

This work was supported by the National Research Foundation of Korea (NRF) grant funded by the Korea government (No. 2017M2A8A1014757).

References

1. J. M. NOH and N. Z. CHO, "A New Approach of Analytic Basis Function Expansion to Neutron Diffusion Nodal Calculation," *Nucl. Sci. Eng.*, **116**, 165 (1994).
2. N. Z. CHO and J. M. NOH, "Analytic Function Expansion Nodal Method for Hexagonal Geometry," *Nucl. Sci. Eng.*, **121**, 245 (1995).
3. N. Z. CHO, Y. H. KIM, and K. W. PARK, "Extension of Analytic Function Expansion Nodal Method to Multigroup Problems in Hexagonal-Z Geometry," *Nucl. Sci. Eng.*, **126**, 35 (1997).
4. S. W. WOO, N. Z. CHO, and J. M. NOH, "The Analytic Function Expansion Nodal Method Refined with Transverse Gradient Basis Functions and Interface Flux Moments," *Nucl. Sci. Eng*., **139**, 156 (2001).
5. N. Z. CHO and J. J. LEE, "Analytic Function Expansion Nodal (AFEN) Method in Hexagonal-z Three Dimensional Geometry for Neutron Diffusion Calculation," *J. Nucl. Sci. and Tech*., **43**, 1320 (2006).
6. H. C. LEE, T. Y. HAN, C. K. JO and J. M. NOH, "Development of the HELIOS/CAPP code system for the analysis of pebble type VHTR cores," Ann. Nucl. Eng., 71, 120 (2014).
7. J. M. NOH, "An AFEN Equivalent Hexagonal Nodal Method based on the Single-Node Nonlinear FDM Response Matrix," *Trans. KNS Autumn Mtg.* Yeosu, Korea, October 25-26, (2018).
8. K. S. Smith, "Nodal Method Storage Reduction by Non-Linear Iteration," *Trans. Am. Nucl. Soc*., 44, 265 (1983).
9. J. M. NOH, "A Response Matrix Formulation of the Refined AFEN Method with Interface Flux Moments in the Two-dimensional Hexagonal Geometry," *Trans. KNS Spring Mtg* Jeju, Korea, May 23-24, (2019).
10. S, Nakamura, *Computational methods in engineering and science, with applications to fluid dynamics and nuclear systems*, John Wiley & Sons, Inc. (1977).
11. Y. A. CHAO and Y. A. SHATILLA, "Conformal Mapping and Hexagonal Nodal Methods-II; Implementation in the ANC-H Code," *Nucl. Sci. Eng.*, **121**, 210 (1995).
12. *CAPP v3.0 Verification Report*, KAERI/TR-7647/2019, Korea Atomic Energy Research Institute KAERI (2019).