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Extension of AFEN Methodology to Multigroup Problems in Hexagonal-Z Geometry

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Abstract

The analytic function expansion nodal (AFEN) method has been successfully applied to two-group neutron diffusion problems. In this paper, the AFEN method is extended to solve general multigroup equations for any type of geometries. Also, a suite of new nodal codes based on the extended AFEN theory is developed for hexagonal-z geometry and applied to several benchmark problems. Numerical results obtained attest to their accuracy and applicability to practical problems.

I. Introduction

Recently, the analytic function expansion nodal (AFEN) method has been developed by Noh and Cho[1, 2]. The AFEN method, unlike the conventional nodal methods, does not suffer from the singularity problem resulting from the transverse integration in hexagonal geometry[3]. In this method, the intranodal flux is expanded in terms of analytic eigenfunctions of a Helmholz equation. Consequently, in multigroup (more than two groups) problems, it is necessary to use complex eigenmodes as basis functions. However, the original AFEN method cannot treat complex eigenfunctions effectively.

To overcome such a shortcoming of the AFEN method, an AFEN-PEN (Polynomial Expansion Method) hybrid method was developed[4]. Although this approach works well in two-dimensional rectangular geometry, it is complicated to use the hybrid method for the three-dimensional hexagonal-z geometry. In this paper, an algorithm which can treat the complex eigenmodes rigorously is proposed, which can be used in any type of geometry. Using the new AFEN algorithm, a suite of nodal codes for hexagonal-z geometry is developed and numerical results for several benchmark problems are reported.

II. Theory and Methodology

A key point of AFEN method is to find the analytical solution of the multi-group diffusion equations in a homogenized node. Although AFEN method is not restricted to the shape of the node, we assume in the following that the node is hexagonal. Without loss of generality, the G-group diffusion equations can be written as

$$-\nabla^2 \vec{\phi} + \boldsymbol{A}\vec{\phi} = 0, \quad \boldsymbol{A} = \boldsymbol{D}^{-1}\left[\boldsymbol{\Sigma} - \frac{1}{k_{eff}}\chi\nu\boldsymbol{\Sigma}_f\right], \tag{1}$$

where $\vec{\phi}$ is a $G\times 1$ vector and the notations are standard.

Let us introduce a new variable $\vec{\xi}$ defined by

$$\vec{\phi} = \boldsymbol{R}\vec{\xi}, \quad \boldsymbol{R} = [e_1, e_2, \ldots\ldots, e_G], \tag{2}$$

where e_g is an eigenvector of $\boldsymbol{A}$ with corresponding eigenvalue λ_g. Here, we assume that there is no eigenvalue deficiency. Then, Eq. (1) is decoupled as follows :

$$-\nabla^2\vec{\xi}+\Lambda\vec{\xi}=0,\quad \Lambda=\mathrm{diag}(\lambda_1,\lambda_2,\ldots,\lambda_G). \tag{3}$$

The general solution of Eq. (3) can be written easily as

$$\xi_g(\vec{r})=\sum_{l=1}^{\infty}[A_{g1}^{l}e^{\sqrt{\lambda_1}\vec{k}_l\cdot\vec{r}}+A_{g2}^{l}e^{-\sqrt{\lambda_1}\vec{k}_l\cdot\vec{r}}],\quad g=1,2,\ldots\ldots,G, \tag{4}$$

where $\vec{r}=(x,\ y,\ z)$ and $\vec{k}_l$ is an arbitrary unit vector satisfying $k_{lx}^2+k_{ly}^2+k_{lz}^2=1$

If the eigenvalues are all real, the eigenmodes of Eq. (4) can be used as the basis functions. If there are complex eigenvalues, efficient computation in AFEN method can hardly be achieved.

For this purpose, we need a new transform matrix T instead of R. Let $\lambda_1=\alpha+\beta j$ and $\lambda_2=\alpha-\beta j$, where j denotes $\sqrt{-1}$. In this case, the following transform matrix T is introduced :

$$T=[Re(e_1),\ Im(e_1),\ e_3,\ldots\ldots,e_G], \tag{5}$$

If the new transform 'matrix T is used, i.e., $\vec{\phi}=T\vec{\xi}$, we get a loosely coupled system of equations similar to Eq. (3) :

$$-\nabla^2\vec{\xi}+\Lambda'\vec{\xi}=0.\ \Lambda'=\begin{pmatrix}\alpha & \beta & & & & & \\ -\beta & \alpha & & & & & \\ & & \lambda_3 & & & & \\ & & & \lambda_4 & & & \\ & & & & \ddots & & \\ & & & & & \lambda_G & \end{pmatrix}. \tag{6}$$

Letting $\sqrt{\lambda_1}=\sqrt{\alpha+\beta j}=\pm(p+qj)$ and $\sqrt{\lambda_2}=\pm(p-qj)$, after some algebraic manipulations, one can find the following general solutions :

$$\begin{aligned}\xi_1(\vec{r})=\sum_{l=1}^{\infty}[\ & a_1^l\cosh(p\vec{k}_l\cdot\vec{r})\cos(q\vec{k}_l\cdot\vec{r})+a_2^l\sinh(p\vec{k}_l\cdot\vec{r})\sin(q\vec{k}_l\cdot\vec{r})+\\ & a_3^l\sinh(p\vec{k}_l\cdot\vec{r})\cos(q\vec{k}_l\cdot\vec{r})+a_4^l\cosh(p\vec{k}_l\cdot\vec{r})\sin(q\vec{k}_l\cdot\vec{r})\ ],\end{aligned} \tag{7}$$

$$\begin{aligned}\xi_2(\vec{r})=\sum_{l=1}^{\infty}[\ & -a_1^l\sinh(p\vec{k}_l\cdot\vec{r})\sin(q\vec{k}_l\cdot\vec{r})+a_2^l\cosh(p\vec{k}_l\cdot\vec{r})\cos(q\vec{k}_l\cdot\vec{r})\\ & -a_3^l\cosh(p\vec{k}_l\cdot\vec{r})\sin(q\vec{k}_l\cdot\vec{r})+a_4^l\sinh(p\vec{k}_l\cdot\vec{r})\cos(q\vec{k}_l\cdot\vec{r})\ ].\end{aligned} \tag{8}$$

It should be noted that real eigenmodes ξ_i, $i\geq 3$, can be obtained in the form of Eq. (4) since they are completely decoupled.

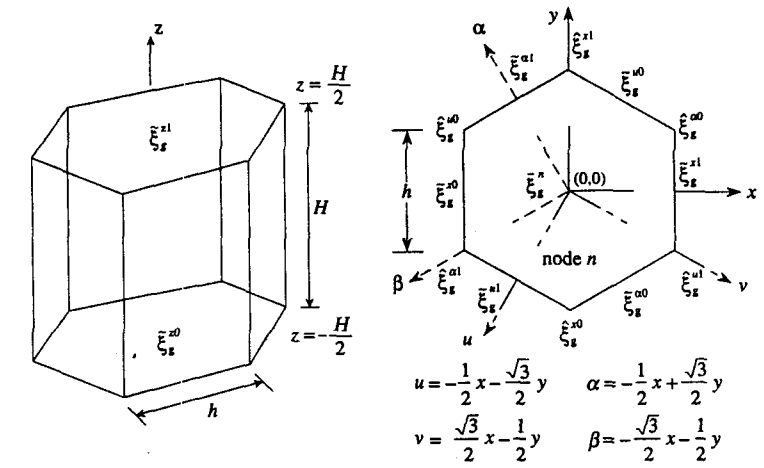
III. Nodal Coupling Equations

The methodology described in the previous section can be applied to any geometry. However, in this paper, hexagonal-z geometry is considered. Once the basis functions $\xi_g(\vec{r})$, $g=1,2,\ldots,G$, are obtained, the next step in AFEN method is to expand the intranodal flux in terms of these basis functions.

The number of basis functions depends on the number of node boundary conditions to use. For hexagonal-z geometry shown in Fig. 1, we consider 14 boundary conditions, which consist of 8 surface-averaged fluxes and 6 axial edge-averaged fluxes. Note that radial edge-averaged fluxes are not considered to reduce the number of unknowns. In two-dimensional calculations, 6 surface-averaged and 6 corner-point fluxes are nodal unknowns.

Considering the coordinate system in Fig. 1, we may choose seven direction vectors $\vec{k}$, which correspond to x-, y- α-, β-, u-, v-, and z-direction. Then, for a real eigenvalue, $\xi_g(\vec{r})$ in Eq.

(4) with seven terms is used in the intranodal flux expansion, while two coupled real functions in Eqs. (7) and (8) with seven terms are used for complex eigenvalues.



bird-eye view of hexagonal-z node top view of hexagonal-z node

Fig. 1. Coordinate system and nodal quantities in hexagonal-z geometry

Now, we should express the expansion coefficients in terms of the nodal unknowns. This can easily be done using the definitions of the nodal unknowns. Once all the coefficients used in the intra-nodal flux expansion are determined, nodal coupling equations are needed to update node-averaged flux, surface-averaged (radial and axial) fluxes, and edge-averaged (or corner-point) fluxes in the multi-node problem.

Integration of the diffusion equation over a node leads to the nodal balance equation. The second nodal coupling equations for the radial surface-averaged fluxes are derived by applying the current continuity condition across interface between two neighbouring two nodes. The third nodal coupling equations are derived by imposing current continuity condition on the axial interface. The fourth nodal coupling equations are required to update the edge-averaged (or corner-point) fluxes. These equations can be derived on the basis of the source free condition around an edge (or corner).

IV. Application to Benchmark Problems

Based on the generalized multigroup AFEN methodology, two nodal codes named AFEN-H1 and AFEN-H2 were developed. In the AFEN-H1 code, both surface-averaged and edge-averaged fluxes in addition to volume-averaged flux are solved. To circumvent the longer computing time, we also developed AFEN-H2, where edge-averaged fluxes are not considered as the nodal unknowns. As can be expected, numerical results show that AFEN-H1 can provide more accurate solutions than AFEN-H2.

To improve accuracy of AFEN-H2, we introduce a semi-empirical factor which modifies an eigenmode in AFEN method. From the numerical experiments, it is observed that the negative eigenmode plays an important role in accuracy of AFEN method. Especially, truncation error resulting from the large negative eigenvalue may have large effect on the AFEN solution since negative eigenvalue usually appears in the multiplying medium with high reactivity. On the basis of the above observations, we relax the negative eigenmode such as $x_g \rightarrow 0.78 x_g$ for radial directions and $x_g \rightarrow 0.71 x_g$ for axial direction. The relaxation factors were obtained via numerical tests on various kinds of benchmark problems.

Using the above modifications, two variants of AFEN-H1,2 are developed, which are denoted as AFEN-H1R and AFEN-H2R, respectively. For AFEN-H1, relaxation is implemented only for axial direction, since radial approximation in AFEN-H1 is already accurate.

The codes treat albedo boundary condition, which is defined as the ratio of net current to scalar flux, i.e., J/ϕ. The codes uses Chebyshev extrapolation scheme in outer iterations and SOR (Successive Over-Relaxation) in inner iterations. To test performance of the newly developed codes, many benchmark calculations were done and several results are reported here. Results of AFEN method are compared with those of other codes such as DIF3D[5] and VENTURE[6]. All calculations were done using the 1/6 symmetry (reflective and rotational) and convergence criteria were 1.E-07 for reactor eigenvalue and 1.E-06 for fission source. The computational time includes input- and output-processing times.

The first benchmark problem is a two-dimensional 4-group VVER-1000 core, which is defined in Makai's paper[7]. Numerical results for this problem are given in Table I. The results show that agreement of AFEN-H1,2 and AFEN-H2R solutions with the reference solution is excellent. Table II contains the eigenvalues of matrix A of this problem when k_{eff} = 1.11204.

Table I. Results for 4-group VVER-1000 problem

method	k_{eff}	k_{eff} error(%)	node power error(%)		CPU time* (sec)
			max.	avg.	
reference	1.11192	--	--	--	--
AFEN-H1	1.11204	0.011	0.64	0.27	20.9
AFEN-H2	1.11207	0.014	0.60	0.27	5.8
AFEN-H2R	1.11182	-0.009	0.62	0.15	5.8
DIF3D-Nodal	1.10693	-0.449	N.A.	N.A.	N.A.
VENTURE (96△/hex)	1.11157	-0.031	-2.12	0.72	191.2

* SUN Sparc/2

Table II. Eigenvalues of matrix A in VVER-1000 problem (k_{eff} =1.11204)

fuel 1	fuel 2	fuel 3	reflector
0.2546E-3	-0.2674E-2	-0.3258E-2	0.4398E-1
0.1452E+0 + 0.1029E-1j	0.1470E+0 + 0.3661E-02j	0.1436E+0	0.1734E+0
0.1452E+0 - 0.1029E-1j	0.1470E+0 - 0.3661E-02j	0.1514E+0	0.2166E+0
0.4242E+0	0.5240E+0	0.5518E+0	0.1204E+0

As the second problem, SNR300 is considered. SNR300 is a 4-group problem modeling a small LMFBR core. Geometry of the three-dimensional core is shown in Ref. 9. Two two-dimensional calculations were performed: rod-in and rod-out case. Numerical results are summarized in Table III.

From the two-dimensional results, one can see that both AFEN-H1 and AFEN-H2 provide accurate k_{eff} and power distribution. It should be noted that computation time of AFEN-H1 is almost the same as the FDM calculation with 24 triangles/hexagon. One can note that AFEN-H2R can accurately analyze both rod-in and rod-out cases of the SNR300 benchmark problem.

Three-dimensional calculations for the SNR300 problem were done with AFEN-H1,2 and were compared with those of DIF3D-nodal. The results are summarized in Table IV. Table V contains numerical results of AFEN-H1R and AFEN-H2R. Clearly, it can be observed that the negative eigenmode relaxation in this three-dimensional problem provides much better solutions.

Table III. Two-dimensional SNR300 calculations

	method	k_{eff}	k_{eff} error(%)	node power error(%)		CPU time* (sec)
				max.	avg.	
rod-in	VENTURE (1536△/hex)	1.12375	--	--	--	--
	AFEN-H1	1.12376	0.001	-0.82	0.13	59.6[a]
	AFEN-H2	1.12474	0.088	0.55	0.22	14.5[a]
	AFEN-H2R	1.12430	0.049	0.75	0.31	14.5[a]
	DIF3D-nodal	1.12529	0.137	N.A.	N.A.	1.4[b]
	VENTURE (24△/hex)	1.12475	0.089	-0.42	0.16	47.5[a]
rod-out	VENTURE (1536△/hex)	1.22413	--	--	--	--
	AFEN-H1	1.22427	0.011	-0.84	0.20	54.8[a]
	AFEN-H2	1.22504	0.074	-0.60	0.18	15.3[a]
	AFEN-H2R	1.22466	0.043	-0.54	0.21	15.3[a]
	DIF3D-nodal	1.22527	0.093	N.A.	N.A.	1.4[b]
	VENTURE (24△/hex)	1.22461	0.039	-0.45	0.12	44.2[a]

[a] SUN Sparc/2, [b] IBM 370/195, * 1 IBM 370/195 sec ≃ 7.5 SUN Sparc/2 sec

Table IV. Three-dimensional SNR300 results

group	DIF3D-fdm max.error(%)	AFEN-H1 max. error(%)		AFEN-H2 max. error(%)		DIF3D-nodal max. error(%)	
	24△/hex, 36 planes	8 planes	16 planes	8 planes	16 planes	8 planes	18 planes
1	-1.94(0.63)†	-2.21(0.60)	-0.69(0.23)	-2.24(0.78)	-0.72(0.40)	-1.04(0.56)	-0.55(0.36)
2	-0.69(0.27)	-1.56(0.50)	-0.63(0.24)	-1.45(0.52)	-0.60(0.31)	+0.94(0.38)	+0.95(0.32)
3	-1.21(0.38)	-1.39(0.57)	-0.66(0.28)	-1.66(0.73)	+1.02(0.47)	+1.90(0.80)	+1.91(0.71)
4	-2.31(0.92)	-2.11(0.84)	-1.29(0.48)	-2.12(0.85)	+1.63(0.54)	-4.43(1.62)	-3.76(1.38)
k_{eff} (ref=1.00989)	1.01118	1.01334	1.01134	1.01376	1.01176	1.01151	1.01125
k_{eff} error (%)	0.128	0.342	0.144	0.383	0.185	0.160	0.135
CPU time (min)*	6.4	8.91	19.89	2.54	6.53	0.24	0.64
Computer	IBM 370/195	SUN Sparc/2				IBM 370/195	

* 1 IBM 370/195 sec ≃ 7.5 SUN Sparc/2 sec , † average error (%)

Table V. Results of AFEN-H1R and AFEN-H2R in three-dimensional SNR300

g	AFEN-H1R error(%)				AFEN-H2R error(%)			
	8 planes		16 planes		8 planes		16 planes	
	max	avg	max	avg	max	avg	max	avg
1	-0.47	0.19	-0.34	0.13	-0.50	0.32	-0.44	0.28
2	-0.42	0.18	-0.33	0.16	+0.75	0.26	+0.78	0.30
3	-0.76	0.27	-0.46	0.22	+1.30	0.54	+1.30	0.45
4	-1.28	0.66	-1.21	0.22	+2.00	0.92	+1.92	0.61
k_{eff} (ref=1.00989)	1.01124		1.01081		1.01121		1.01079	
k_{eff} error (%)	0.133		0.09		0.131		0.089	
CPU time (min)	8.91		19.89		2.54		6.53	
Computer	SUN Sparc/2							

V. Conclusions

Four types of computer codes based on the new AFEN method were developed to solve the general multigroup diffusion equations in the hexagonal reactor core. The first is AFEN-H1 which considers both interface and edge fluxes as nodal unknowns and the second AFEN-H2 where only interface fluxes are solved. AFEN-H2 is much faster than AFEN-H1 but at the cost of some loss of accuracy. The other two codes are variants of AFEN-H1 and AFEN-H2, which are named AFEN-H1R and AFEN-H2R, respectively. AFEN-H1R and AFEN-H2R are based on the eigenmode relaxation, where the negative eigenmode, if exists, is relaxed by a factor which is empirically determined.

Application to several benchmark problems shows that the new AFEN-H1 can provide accurate solutions for both two- and three-dimensional problems but requires relatively long computing time. Also, it is observed that AFEN-H2 runs 2 or 3 three times faster than AFEN-H1, but gives a little less accurate solution. From the results, it may be concluded that AFEN-H1 is useful for thermal reactor analysis which requires very fine-mesh FDM calculation and AFEN-H2 can be used for fast reactors which are analyzed usually with relatively coarse-mesh FDM calculation.

Numerical results also show that the negative eigenmode relaxation in both AFEN-H1 and AFEN-H2 results in improved solutions, especially, improvement is significant in three-dimensional calculation. Although the eigenmode relaxation is based on numerical experiments and needs stronger theoretical basis, we think that both AFEN-H1R and AFEN-H2R can be effectively used for multigroup analysis of nuclear reactors with hexagonal geometry.

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**, 165-180 (1994).

[2]. N. Z. Cho and. J. M. Noh, "Analytic Function Expansion Nodal Method for Hexagonal Geometry," Nucl. Sci. Eng., **121**, 245-253 (1995).

[3]. Y. A. Chao, "Comments on the Treatment of Transverse Leakage in Advanced Nodal Codes for Hexagonal Nodes," Nucl. Sci. Eng., **109**, 423 (1991).

[4]. N. Z. Cho and J. M. Noh, "Hybrid of AFEN and PEN Methods for Multigroup Diffusion Nodal Calculation," Trans. Am. Nucl. Soc., **73**, 438 (1995).

[5]. R. D. Lawrence, "The DIF3D Nodal Neutronics Option for Two- and Three-Dimensional Diffusion Theory Calculations in Hexagonal Geometry," ANL-83-1, Argonne National Laboratory (Mar. 1983).

[6]. D. R. Vondy et al.,"VENTURE: A Code Block for Solving Multigroup Neutronic Problems Applying the Finite-Difference Diffusion-Theory Approximation to Neutron Transport - Version II," ORNL-5062/R1, Oak Ridge National Laboratory (1977).

[7]. M. Makai, "Response Matrix of Symmetric Nodes," Nucl. Sci. Eng., **86**, 302-314 (1984).

[8]. K. Singh and V. Kumar, "Solution of the Multigroup Diffusion Equation in Hex-Z Geometry by Finite Fourier Transformation," Annals of Nuclear Energy, **20**, 153-161 (1993).

[9]. ANL Benchmark Problem Book, ANL-7416, Suppl. 3, Argonne National Laboratory (1985).