A NONLINEAR ITERATION METHOD BASED ON ONE NODE EXPANSION

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ABSTRACT

A nonlinear iterative method based on one node expansion is presented. In this method, we firstly solve the coarse mesh finite diffusion (CMFD) equations, in which the nonlinear coupling coefficients are involved, to obtain the nodal averaged fluxes. Then we compute the interface neutron currents in one node, instead of two nodes, to get the nonlinear coupling coefficients. After that we solve the CMFD equations with renewed coupling coefficients to obtain improved nodal average fluxes. After several iterations the nodal averaged fluxes and k_{eff} can be obtained accurately. The numerical results of two benchmark problems show that this new method has the potential to accurately solve multidimensional problems with less computing time compared with Nodal Green Function Method (NGFM).

1. INTRODUCTION

Since 1980's various nonlinear iterative methods have been developed and widely used in reactor physics computation [(1)]. In this paper, we present a nonlinear iterative method based on one node expansion. A multidimensional code POLY is developed based on this method. The numerical results of benchmark problems show that this new method has the potential to solve multidimensional diffusion equations accurately, while the computing time needed is significantly less than that of required by NGFM [(4,6)].

2. MODEL OF THE NONLINEAR ITERATIVE METHOD

The nonlinear iterative method based on one node expansion includes two parts: the solving of coarse mesh finite difference equations involving the nonlinear coupling coefficients and the solving of transverse integrated equations on a single node. Firstly we solve the CMFD equations and the nodal averaged fluxes are obtained. Then the interface neutron currents are computed on one node to get the nonlinear coupling coefficients. The CMFD equations with renewed coupling coefficients are solved to obtain improved nodal average fluxes. When this iteration is convergent the accurate nodal

averaged fluxes and k_{eff} are obtained.

2.1 CMFD equations

The neutron balance equation on node k is:

$$\sum_{u=x,y,z} \frac{1}{2a_u^k}[J_{g,u}^k(+a_u^k) - J_{g,u}^k(-a_u^k)] + \Sigma_g^{k,r} \bar{\Phi}_g^k = \bar{Q}_g^k \qquad (1)$$
$$k = 1,2,\cdots,K_u; g = 1,2,\cdots,G$$

where

$$\bar{\Phi}_g^k = \frac{1}{8a_u a_v a_w} \int_{-a_u}^{a_u}\int_{-a_v}^{a_v}\int_{-a_w}^{a_w} dudvdw\Phi_g^k(u,v,w)$$

$$J_{g,u}^k(\pm a_u^k) = \frac{1}{4a_v a_w} \int_{-a_v}^{a_v}\int_{-a_w}^{a_w} dvdw(-D_g^k)\frac{\partial}{\partial u}\Phi_g^k(u,v,w)\Big|_{u=\pm a_u^k}$$

$$\bar{Q}_g^k = \frac{1}{\lambda}\sum_{g'=1}^{G} \chi_g \nu \Sigma_{g'}^f \bar{\Phi}_{g'}^k + \sum_{\substack{g'=1 \\ g'\neq g}}^{G} \Sigma_{g'\to g}^s \bar{\Phi}_{g'}^k$$

We assume there is a relation between interface current and adjacent nodal averaged fluxes:

$$J_{g,u}^{k,k+1} = -DF_{g,u}^{k,k+1}(\bar{\Phi}_g^{k+1} - \bar{\Phi}_g^k) - DN_{g,u}^{k,k+1}(\bar{\Phi}_g^{k+1} + \bar{\Phi}_g^k) \qquad (2)$$

where

$$DF_{g,u}^{k,k+1} = \frac{1}{a_u^k / D_g^k + a_u^{k+1} / D_g^{k+1}} \qquad (3)$$

while $DN_{g,u}^{k,k+1}$ is the nonlinear coupling coefficient. Substituting Eq. (2) into Eq. (1), we get the CMFD equation with nonlinear coupling coefficients:

$$\begin{aligned}
&[\Sigma_g^{k,r} + \sum_{u=x,y,z} \frac{1}{2a_u^k}(DF_{g,u}^{k,k+1} - DN_{g,u}^{k,k+1} + DF_{g,u}^{k-1,k} + DN_{g,u}^{k-1,k})]\bar{\Phi}_g^k - \\
&\sum_{u=x,y,z} \frac{1}{2a_u^k}(DF_{g,u}^{k-1,k} - DN_{g,u}^{k-1,k})\bar{\Phi}_g^{k-1} - \sum_{u=x,y,z} \frac{1}{2a_u^k}(DF_{g,u}^{k,k+1} + DN_{g,u}^{k,k+1})\bar{\Phi}_g^{k+1} \qquad (4) \\
&= \sum_{\substack{g'=1 \\ g'\neq g}}^{G} \Sigma_{g'\to g}^{k,s} \bar{\Phi}_{g'}^k + \frac{1}{k_{eff}} \sum_{g'=1}^{G} \chi_g \nu \Sigma_{g'}^{k,f} \bar{\Phi}_{g'}^k
\end{aligned}$$

Eq.(4) can be solved by using source iteration method to get the nodal averaged fluxes and k_{eff}.

Some traditional convergence acceleration methods can be used to speed up the process of calculation.

2.2 Nodal transverse integrated equation

The transverse integrated equation on node k is:

$$-D_g^k \frac{d^2}{du^2}\Phi_{g,u}^k(u) + \Sigma_g^{r,k}\Phi_{g,u}^k(u) = Q_{g,u}^k(u) - L_{g,u}^k(u) \tag{5}$$

$$u \in \left[-a_u^k, a_u^k\right], \quad k = 1,2,\cdots,K_u; g = 1,2,\cdots,G$$

The first four Legendre polynomial functions are applied in the nodal fluxes expansion, and the transverse leakage term is expanded with quadratic polynomials:

$$\Phi_{g,u}^k(u) = \bar{\Phi}_g^k + \sum_{i=1}^{4}\Phi_{g,i}^k \cdot f_i(\frac{u}{a_u^k}) \tag{6}$$

$$L_{g,u}^k(u) = \bar{L}_g^k + \sum_{i=1}^{2}L_{g,i}^k \cdot f_i(\frac{u}{a_u^k}) \tag{7}$$

where

$$f_1(x) = x$$

$$f_2(x) = \frac{1}{2}(3x^2 - 1)$$

$$f_3(x) = \frac{1}{2}(5x^3 - 3x)$$

$$f_4(x) = \frac{1}{8}(35x^4 - 30x^2 + 3)$$

Fluxes expanded coefficients are determined by weighted residual method, using the following three weight functions respectively:

$$W_0 = 1$$

$$W_1 = f_1(x)$$

$$W_2 = f_2(x)$$

and noting

$$J_{g,u}^k(u) = -D_g^k \frac{d}{du}\Phi_{g,u}^k(u) \tag{8}$$

We can obtain three equations (Eq.(9), (10), (11))

the neutron balance equation is:

$$J_g^{k,u+} - J_g^{k,u-} = 2a_u^k(\sum_{g'=1}^{G}\gamma_{g'\to g}^k \bar{\Phi}_{g'}^k - \bar{L}_g^k) \tag{9}$$

the first order moment equation is:

$$J_g^{k,u+} + J_g^{k,u-} + \frac{D_g^k}{a_u^k}(\Phi_g^{k,u+} - \Phi_g^{k,u-}) = \frac{2}{3}a_u^k(\sum_{g'=1}^{G}\gamma_{g'\to g}^k \Phi_{g',1}^k - L_{g,1}^k) \tag{10}$$

the second order moment equation is:

$$J_g^{k,u+} - J_g^{k,u-} + \frac{3D_g^k}{a_u^k}(\Phi_g^{k,u+} + \Phi_g^{k,u-} - 2\bar{\Phi}_g^k) = \frac{2}{5}a_u^k(\sum_{g'=1}^{G}\gamma_{g'\to g}^k \Phi_{g',2}^k - L_{g,2}^k) \tag{11}$$

where

$$\gamma_{g'\to g}^k = \begin{cases} \dfrac{\lambda_g \nu\Sigma_{g'}^{f,k}}{k_{eff}} + \Sigma_{g'\to g}^{k,s} & g' \neq g \\ \dfrac{\lambda_g \nu\Sigma_{g'}^{f,k}}{k_{eff}} + \Sigma_{g'\to g}^{k,s} - \Sigma_g^{k,r} & g' = g \end{cases}$$

From Eq.(6) we know:

$$\begin{aligned} &\bar{\Phi}_g^k - \Phi_{g,1}^k + \Phi_{g,2}^k - \Phi_{g,3}^k + \Phi_{g,4}^k = \Phi_g^{k,u-} \\ &\bar{\Phi}_g^k + \Phi_{g,1}^k + \Phi_{g,2}^k + \Phi_{g,3}^k + \Phi_{g,4}^k = \Phi_g^{k,u+} \end{aligned} \tag{12}$$

Differentiating Eq.(6) we get the currents on the left and right surfaces of node k:

$$\begin{aligned} &\Phi_{g,1}^k - 3\Phi_{g,2}^k + 6\Phi_{g,3}^k - 10\Phi_{g,4}^k = -\frac{a_u^k}{D_g^k}J_g^{k,u-} \\ &\Phi_{g,1}^k + 3\Phi_{g,2}^k + 6\Phi_{g,3}^k + 10\Phi_{g,4}^k = -\frac{a_u^k}{D_g^k}J_g^{k,u+} \end{aligned} \tag{13}$$

From Eqs.(12) and Eqs.(13), $\Phi_{g,1}^k$ and $\Phi_{g,2}^k$ can be obtained as follows:

$$\begin{aligned} \Phi_{g,1}^k &= \frac{3}{5}(\Phi_g^{k,u+} - \Phi_g^{k,u-}) + \frac{a_u}{10D_g^k}(J_g^{k,u+} + J_g^{k,u-}) \\ \Phi_{g,2}^k &= \frac{5}{7}(\Phi_g^{k,u+} + \Phi_g^{k,u-} - 2\bar{\Phi}_g^k) + \frac{a_u}{14D_g^k}(J_g^{k,u+} - J_g^{k,u-}) \end{aligned} \tag{14}$$

Through substitution of Eqs.(14) into Eq.(10) and Eq.(11), Eq.(9), (10), (11) can be rewritten as:

$$J_g^{k,u+} - J_g^{k,u-} = 2a_u^k(\sum_{g'=1}^{G}\gamma_{g'\to g}^k \bar{\Phi}_{g'}^k - \bar{L}_g^k) \tag{15}$$

$$\left(J_g^{k,u+}+J_g^{k,u-}\right)+\frac{D_g^k}{a_u^k}\left(\Phi_g^{k,u+}-\Phi_g^{k,u-}\right)= \frac{2}{3}a_u^k\left\{\sum_{g'=1}^{G}\gamma_{g'\to g}^k\left[\frac{3}{5}\left(\Phi_{g'}^{k,u+}-\Phi_{g'}^{k,u-}\right)+\frac{a_u^k}{10D_g^k}\left(J_{g'}^{k,u+}+J_{g'}^{k,u-}\right)\right]-L_{g,1}^k\right\} \tag{16}$$

$$\left(J_g^{k,u+}-J_g^{k,u-}\right)+\frac{3D_g^k}{a_u^k}\cdot\left(\Phi_g^{k,u+}+\Phi_g^{k,u-}-2\bar{\Phi}_g^k\right)= \frac{2}{5}a_u^k\left\{\sum_{g'=1}^{G}\gamma_{g'\to g}^k\left[\frac{5}{7}\left(\Phi_{g'}^{k,u+}+\Phi_{g'}^{k,u-}-2\bar{\Phi}_{g'}^k\right)+\frac{a_u^k}{14D_g^k}\left(J_{g'}^{k,u+}-J_{g'}^{k,u-}\right)\right]-L_{g,2}^k\right\} \tag{17}$$

For each node there are 3G (G: the number of energy group) equations (Eq.(15), (16), (17)) and 4G unknowns ($\Phi_g^{k,u+},\Phi_g^{k,u-},J_g^{k,u+},J_g^{k,u-}$). For two adjacent nodes there are 8G unknowns and 6G equations. Considering the continuity of neutron fluxes and currents in the interface, we have two other equations:

$$\Phi_g^{k,u+}=\Phi_g^{k+1,u-}\quad g=1,2,\cdots,G \tag{18}$$

$$J_g^{k,u+}=J_g^{k+1,u-}\qquad g=1,2,\cdots,G \tag{19}$$

So there are 8G equations and 8G unknowns totally, these unknowns can be determined uniquely.
For left and right boundaries, boundary condition can be written as:

$$\alpha_g\Phi_g^b+\beta_g J_g^b=\gamma_g \tag{20}$$

where Φ_g^b and J_g^b are flux and current respectively on the boundary, α_g, β_g and γ_g are constants. Taking left boundary as the example, the values of α_g, β_g and γ_g for some common used boundary conditions are listed in Table I.

Table I . α_g, β_g and γ_g for some common used boundary conditions

Boundary condition	α_g	β_g	γ_g
Reflect	0	1	0
Free boundary and incoming current is zero	1	2	0
Free boundary and flux in the boundary is zero	1	0	0

Therefore when dealing with boundary current we still have 4G equations (Eq.(15), (16), (17), (20)) and 4G unknowns, and these unknowns can be determined uniquely also.

Some authors have developed two node nonlinear iterative method [1,5], in which they solve the 8G equations on two adjacent node directly to get the interface current. However, in our method, we use a iterative method. The process of iteration is shown in Fig. 1.

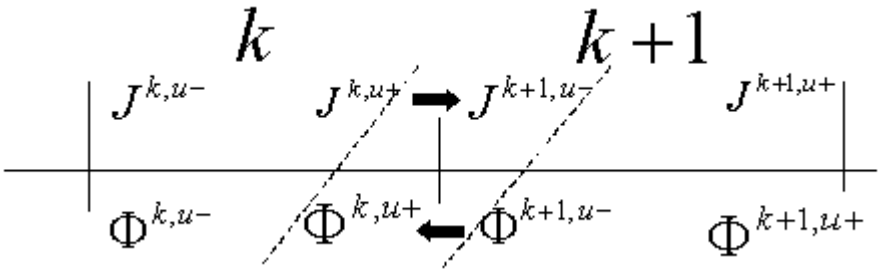

Fig. 1 Diagram of iterative method

In fact, for node k $\Phi_g^{k,u+}$ can be regarded as known because of the flux continuity, namely:

$$\Phi_g^{k,u+} \Leftarrow \Phi_g^{k+1,u-}$$

For node k+1 $J_g^{k+1,u-}$ can be regarded as known because of the current continuity, namely:

$$J_g^{k+1,u-} \Leftarrow J_g^{k,u+}$$

So each node has 3G equations and 3G unknowns, these unknowns can be determined uniquely. To ensure the continuity of interface currents and fluxes, we must iterate between two adjacent nodes.

we define some auxiliary variable as follows:

$$(J_g^{k,u+} - J_g^{k,u-}) = CJ_g^k \tag{21}$$

$$(\Phi_g^{k,u+} + \Phi_g^{k,u-} - 2\bar{\Phi}_g^k) = C\Phi_g^k \tag{22}$$

$$(J_g^{k,u+} + J_g^{k,u-}) = DJ_g^k \tag{23}$$

$$(\Phi_g^{k,u+} - \Phi_g^{k,u-}) = D\Phi_g^k \tag{24}$$

$$k = 1,2,\cdots,K_u; g = 1,2,\cdots,G$$

Before iteration, for each node we get the value of CJ_g^k from Eq.(15), and then get the value of $C\Phi_g^k$ from Eq.(17).

Now we describe the procedure of the iteration, taking the interface of node k and node k+1 as example. In following each step, operations are performed for all energy group. l is the mark of iterative process.

1) Take the interface current obtained from coarse mesh calcualtion as the initial value of $J_g^{k,u+}(l)$, $l = 0$;

2) Let $J_g^{k+1,u-}(l) = J_g^{k,u+}(l)$;

3) Compute DJ_g^{k+1} from $J_g^{k+1,u-}(l)$ and CJ_g^{k+1} in node k+1;

4) Compute $D\Phi_g^{k+1}$ from DJ_g^{k+1} using Eq.(16);

5) Compute $\phi_g^{k+1,u-}(l)$ from $D\Phi_g^{k+1}$ and $C\Phi_g^{k+1}$;

6) Let $\Phi_g^{k,u+}(l) = \Phi_g^{k+1,u-}(l)$;

7) Compute $D\Phi_g^k$ from $\Phi_g^{k,u+}(l)$ and $C\Phi_g^k$ in node k;

8) Compute DJ_g^k from $D\Phi_g^k$ using Eq.(16);

9) Compute $J_g^{k,u+}(l+1)$ from DJ_g^k and CJ_g^k;

10) If $J_g^{k,u+}(l+1)$ for all energy group have converged, stop the iteration; otherwise, go back to step 2);

In order to speed up convergence of the iteration, we introduce relaxation factor. Let $\tilde{\Phi}_g^{k+1,u-}(l) = \phi_g^{k+1,u-}(l)$,which is obtained from step 3), and we define $\phi_g^{k+1,u-}(l)$ as

$$\Phi_g^{k+1,u-}(l) = \varpi_1 \cdot \tilde{\Phi}_g^{k+1,u-}(l) + (1-\varpi_1) \cdot \Phi_g^{k+1,u-}(l-1) \tag{25}$$

Let $\tilde{J}_g^{k,u+}(l+1) = J_g^{k,u+}(l+1)$,which is obtained from step 5), and we define $J_g^{k,u+}(l+1)$ as

$$J_g^{k,u+}(l+1) = \varpi_2 \cdot \tilde{J}_g^{k,u+}(l+1) + (1-\varpi_2) \cdot J_g^{k,u+}(l) \tag{26}$$

The numerical calculation show that the iteration process converge quickly if the relaxation factors are chosen appropriately. Usually 2 to 3 times is enough for obtaining satisfactory accuracy.

3. BENCHMARK RESULTS

We developed the code POLY based on the method described in this paper. The code POLY has been tested by two light water reactor benchmark problems, namely 2-D LRA boiling water reactor problem [2] and 3-D IAEA benchmark problems [3]. The results are listed in Table II. The errors of assembly-averaged power distribution are given in Figs.2, 3. The results show that POLY and NGFM, which is a code based on nodal green's function method with Neumann boundary condition [6], give comparable accuracy, while POLY is about 5 times faster than NGFM. We also developed the code POLY-2 based on the two nodal nonlinear iterative method, and found that the code POLY is slightly faster than POLY-2 because the most time is spent on CMFD calculation which are the same for both method. However, in our one node method the Red-Black iteration is conducted naturally and easily.

0.924 -0.17 0.35	0.867 -0.17 0.24	0.827 -0.21 0.27	0.853 -0.21 0.25	0.932 -0.24 0.25	0.971 -0.19 0.46	0.847 -0.48 0.60	
1.481 0.09 0.11	1.281 0.02 0.00	1.173 -0.12 0.18	1.221 -0.14 0.17	1.421 -0.01 -0.04	1.679 -0.04 0.21	1.621 -0.15 0.38	1.327 -0.32 0.41
1.661 0.23 -0.58	1.151 0.03 0.15	0.967 -0.01 0.13	1.023 -0.05 0.18	1.339 -0.08 0.23	2.051 0.05 -0.40	2.160 0.03 -0.27	
1.385 0.22 -0.64	0.940 0.11 0.00	0.783 0.08 0.00	0.843 0.02 0.07	1.152 -0.04 0.15	1.852 0.04 -0.44		
0.790 0.08 0.00	0.670 0.24 -0.35	0.618 0.15 -0.19	0.678 0.09 0.15	0.864 0.14 -0.27			
0.512 0.16 0.00	0.490 0.20 -0.22	0.492 0.22 -0.26	0.552 0.20 -0.24				
0.413 0.24 -0.19	0.407 0.22 -0.25	0.424 0.26 -0.19					
0.440 0.30 -0.23	0.340 0.33 -0.43						
0.612 0.47 -0.98	-Reference -NGFM error(%) -POLY error(%)						

Fig. 2 Normalized power distribution and errors of calculation for the 2-D LRA benchmark problem

					0.597 1.02 1.51	-Reference -NGFM error(%) -POLY error(%)	
				0.476 0.04 0.84	0.700 0.37 0.43	0.611 1.34 0.98	
			1.178 -0.15 -0.25	0.972 -0.19 -0.21	0.923 0.20 0.43	0.866 0.73 0.92	
		1.368 -0.35 -0.29	1.311 -0.21 -0.38	1.181 -0.21 -0.34	1.089 -0.04 0.28	1.000 -0.07 0.90	0.711 0.76 1.41
	1.397 -0.57 -0.57	1.432 -0.49 -0.49	1.291 -0.42 -0.39	1.072 -0.38 -0.37	1.055 -0.16 0.19	0.976 -0.06 0.72	0.757 0.20 1.32
0.729 0.11 0.01	1.281 -0.77 -0.86	1.422 -0.66 -0.84	1.193 -0.58 -0.75	0.610 0.15 0.33	0.953 -0.20 -0.21	0.959 -0.02 0.42	0.777 0.03 1.29

Fig. 3 Normalized power distribution and errors of calculation for the 3-D IAEA benchmark problem

Table II. Benchmark results between POLY and NGFM

	2D-IAEA			3D-IAEA		
	Reference	NGFM	POLY	Reference	NGFM	POLY
Keff	0.99637	0.99646	0.99640	1.02903	1.02905	1.02905
CPU(s)		5.88	1.23		136.53	19.22
ε_{max} (%)[a]		0.48	0.98		1.34	1.51

[a] ε_{max} =maximum error in assembly-averaged power

We noted that some authors [6,7,8] had studied some one-node methods which are quite advanced, and can be used in MOX fuel core calculations. these methods are quite revelatory to us though they are different from our method,

CONCLUSIONS

An alternate method of the nonlinear iterative method is developed for solving the 3-D multi-group nodal diffusion equations. In this method, the calculation includes two parts: to solve the CMFD equations to get nodal averaged fluxes and to solve the transverse integrated equations to get nodal interface currents. Unlike the conventional nonlinear iterative method, the computation of the interface currents in our method is performed in every single node, instead of in every two adjacent node simultaneously. Numerical results show that this new method has the potential to accurately solve multidimensional problems with less computing time compared with Nodal Green Function Method.

REFERENCES

1. Smith K S, “Nodal Method Storage Reduction by Nonlinear Iteration”, *Trans. Am. Nucl.* Sci. 44,

265 (1983)

2. Lawrence R D, “Progress in Nodal Methods for the Solution of the Neutron Diffusion and Transport Equations”, *Prog. Nucl. Energy* ,17(3):271-301 (1986)
3. Lee R R. Benchmark 11. ANL-7416 Supplement 2, June 1977
4. Lawrence R D, Dorning J J, “A Nodal Green’s Function Method for Multidimensional Neutron Diffusion Calculations”, *Nucl, Sci. Eng,* 76:218-231 (1980)
5. Hu Yongming, Zhao Xianfeng, “Advanced nodal green’s function method with Neumann boundary condition”, *Journal of Tsinghua University,* Vol 38, No 4 (1998)
6. Y.A.Chao. “A Theoretical Analysis of the CMFD Representation in Advanced Nodal Methods”, [Conference Paper] ANS. Madrid, Spain.
7. Ho Cheol Shin, Yong Hee Kim, Yong Bae Kim. “One-node coarse-mesh finite difference algorithm for fine-mesh difference operator”. [Conference Paper] ANS. Transactions of the American Nuclear Society, vol.81, 1999, pp150-1. USA
8. C.H.Lee, Downar TJ. “Nonlinear formulation for multigroup simplified P_3”, [Conference Paper] ANS, Transactions of the American Nuclear Society, vol.83, 2000, pp.297-9. USA