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A NODAL METHOD FOR FAST REACTOR ANALYSIS

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INTRODUCTION

In the past few years, a number of "nodal" methods for solving the neutron diffusion equations have been developed.[1-6] These methods, originally developed for application to light water reactors, are in general applicable only to few group, x-y geometry neutron diffusion problems.

The application of nodal methods to fast reactor diffusion theory analysis introduces two major complexities. The method must first handle any number of neutron energy groups, with a general scattering bandwidth. In addition, the method must be extendable to hexagonal geometry. To develop a method possessing these characteristics, it is instructive to review some of the existing methods, and examine their applicability.

To the author's knowledge, none of the above referenced methods have been extended to hexagonal geometry, although some work has been done on higher order difference equations.[7,8] It seems likely, however, that a method in which the spatial problem is reduced to a series of one dimensional problems[1,3-6] could be successfully extended to hexagonal geometry. Therefore, this technique will be used in the development of methods for fast reactor analysis.

The nodal methods mentioned above show significant variation in the techniques used in the energy domain. Of the above methods, only Sims'[3] and Lawrence's[5] allow an arbitrary energy group structure. Both Wagner's[1] and Werner's[2] methods require the solution of G x G matrix problems in the generation of coefficient matrices. The method developed by Shober[3,9] and its progeny[4,6] are restricted to at most two neutron energy groups. From studying these methods, it is concluded that a development in which the solution of the one-group diffusion equation is isolated from all other energy groups will lead to a method which allows an arbitrary number of energy groups.

Based on the above research, a program has been initiated at the Argonne National Laboratory to develop a method which is applicable to fast reactor diffusion theory analysis. This method extends the analytical method described in references 3, 4, 6, and 9. This paper will first show the derivation of the relevant equations in two-dimensional x-y geometry. Solution techniques for these equations are discussed, and two-dimensional static results for two test problems are summarized. Future plans for this method are then discussed.

DEVELOPMENT OF EQUATIONS

GLOBAL EQUATIONS

The development begins with the static two-dimensional neutron diffusion equation in x-y geometry. For convenience, an external source is not included.

$$- \frac{\partial}{\partial x} D_g(x,y) \frac{\partial}{\partial x} \phi_g(x,y) - \frac{\partial}{\partial y} D_g(x,y) \frac{\partial}{\partial y} \phi_g(x,y)$$

$$+ \Sigma_{Rg}(x,y)\, \phi_g(x,y) = \frac{\chi_g}{\lambda} \sum_{g'=1}^{G} \nu\Sigma_{fg'}(x,y)\, \phi_{g'}(x,y)$$

$$+ \sum_{\substack{g'=1 \\ g \neq g'}}^{G} \Sigma_{s\, gg'}(x,y)\, \phi_{g'}(x,y) \qquad (1)$$

The terms in Eq. 1 have their conventional meanings. Next, partition the domain of solution into discrete homogeneous mesh intervals, as:

$$R_{i,j} \in \begin{cases} (x_i, x_{i+1}) & , \ i=1,\ldots,I \\ (y_j, y_{j+1}) & , \ j=1,\ldots,J \end{cases}$$

Integrating Eq. 1 over $R_{i,j}$, the following equation is obtained:

$$h_j L_{gx_{i,j}} + h_i L_{gy_{i,j}} + h_i h_j \Sigma_{Rg_{i,j}} \bar{\phi}_{g_{i,j}}$$

$$= \frac{\chi_g}{\lambda} \sum_{g'=1}^{G} h_i h_j \nu\Sigma_{fg'_{i,j}} \bar{\phi}_{g'_{i,j}}$$

$$+ \sum_{\substack{g'=1 \\ g \neq g'}}^{G} h_i h_j \Sigma_{s\, gg'_{i,j}} \bar{\phi}_{g'_{i,j}} \qquad (2)$$

where

$$h_i = x_{i+1} - x_i \quad , \quad h_j = y_{j+1} - y_j$$

$$\bar{\phi}_{g_{i,j}} = \frac{\int_{y_j}^{y_{j+1}} \int_{x_i}^{x_{i+1}} \phi_g(x,y)\, dx\, dy}{h_i h_j}$$

$$\Sigma_{Rg_{i,j}} = \Sigma_{Rg}(x,y) \Big|_{\substack{x \in (x_i, x_{i+1}) \\ y \in (y_j, y_{j+1})}}$$

$$L_{gx_{i,j}} = -\frac{1}{h_j} \left\{ D_{g_{i+1,j}} \frac{\partial}{\partial x} \int_{y_j}^{y_{j+1}} \phi_g(x_{i+1}, y)\, dy - D_{g_{i,j}} \frac{\partial}{\partial x} \int_{y_j}^{y_{j+1}} \phi_g(x_i, y)\, dy \right\}$$

$$L_{gy_{i,j}} = -\frac{1}{h_i} \left\{ D_{g_{i,j+1}} \frac{\partial}{\partial y} \int_{x_i}^{x_{i+1}} \phi_g(x, y_{j+1})\, dy - D_{g_{i,j}} \frac{\partial}{\partial y} \int_{x_i}^{x_{i+1}} \phi_g(x, y_j)\, dy \right\}$$

The terms $\nu\Sigma_{fg'_{i,j}}$ and $\Sigma_{s\ gg'_{i,j}}$ are defined in analogy with $\Sigma_{Rg_{i,j}}$.

To solve Eq. 2, relationships must be found between the x and y directed leakages $L_{gx_{i,j}}$, $L_{gy_{i,j}}$ and the average flux $\bar{\phi}_{g_{i,j}}$. In the present method, a more accurate relationship between the fluxes and leakages than is used in finite difference equations is desired. To derive such relationships, the one dimensional diffusion equation is solved analytically. To obtain this equation, integrate Eq. 1 from y_j to y_{j+1}:

$$- D_{g_{i,j}} \frac{\partial^2}{\partial x^2} \phi_{gj}(x) + \Sigma_{Rg_{i,j}} \phi_{gj}(x)$$

$$= \frac{\chi_g}{\lambda} \sum_{g'=1}^{G} \nu\Sigma_{fg'_{i,j}} \phi_{g'j}(x) + \sum_{\substack{g'=1 \\ g\neq g'}}^{G} \Sigma_{s\ gg'_{i,j}} \phi_{g'j}(x)$$

$$+ D_{g_{i,j}} \int_{y_j}^{y_{j+1}} \frac{1}{h_j} \frac{\partial^2}{\partial y^2} \phi_g(x,y)dy \qquad (3)$$

where

$$\phi_{gj}(x) = \frac{1}{h_j} \int_{y_j}^{y_{j+1}} \phi_g(x,y)dy \qquad , x \in (x_i, x_{i+1})$$

Equation 3 resembles a conventional one-dimensional diffusion equation with the exception of an extra term on the right hand side representing the y-direction, or transverse, leakage. To solve this equation analytically, the functional form of the right hand side of Eq. 3 must be known. At this point a fundamental assumption is made that the right hand side may be approximated as a polynomial within each node. For example, consider the use of quadratic polynomials. Define $T_{gx_{i,j}}(w)$ as the total x-directed fission plus scattering plus transverse leakage source within region $R_{i,j}$. Then

$$T_{gx_{i,j}}(w) = T^{f}_{gx_{i,j}} + T^{l}_{gx_{i,j}} \frac{w}{h_i} + T^{q}_{gx_{i,j}} \frac{w^2}{h_i^2} \tag{4}$$

where $w = x - x_i$. From the analytic solution of Eq. 3 the following equation is obtained:

$$L_{gx_{i,j}} = C^{-}_{x_{i,j}} \bar{\phi}_{g_{i-1,j}} + C^{0}_{x_{i,j}} \bar{\phi}_{g_{i,j}} + C^{+}_{x_{i,j}} \bar{\phi}_{g_{i+1,j}}$$

$$+ \sum_{u=f,l,q} \left\{ E^{u,-}_{x_{i,j}} T^{u}_{gx_{i-1,j}} + E^{u,o}_{x_{i,j}} T^{u}_{gx_{i,j}} + E^{u,+}_{x_{i,j}} T^{u}_{gx_{i+1,j}} \right\} \tag{5}$$

Although not explicity indicated, the coefficients C_x and E_x are group dependent. An expression for $L_{gy_{i,j}}$ is obtained from an analogous procedure in the y direction.

The above equations may be rewritten in a more convenient matrix form. In addition, the following change of variables is made

$$L^{*}_{gx_{i,j}} = \frac{1}{h_i} L_{gx_{i,j}} \tag{6}$$

$$L^{*}_{gy_{i,j}} = \frac{1}{h_j} L_{gy_{i,j}} \tag{7}$$

The following equation is obtained:

$$\left[h_i h_j\right] \left\{ \left[L^{*}_{gx}\right] + \left[L^{*}_{gy}\right] \right\} + \left[h_i h_j \Sigma_{Rg}\right] \left[\bar{\phi}_g\right]$$

$$= \frac{\chi_g}{\lambda} \sum_{g'=1}^{G} \left[h_i h_j \nu\Sigma_{fg'}\right] \left[\bar{\phi}_{g'}\right] + \sum_{\substack{g'=1 \\ g \neq g'}}^{G} \left[h_i h_j \Sigma_{s\ gg'}\right] \left[\bar{\phi}_{g'}\right] \tag{8}$$

where

$[h_i h_j]$ is a diagonal matrix whose entries are $h_i h_j$

$[L^*_{gx}]$ is a column vector whose entries are $L^*_{gx_{i,j}}$.

The other matrices and vectors in Eq. 8 are defined in analogy with the two terms above. The equations for the leakages become:

$$[h_i h_j][L^*_{gx}] = [C_x][\bar{\phi}_g] + \sum_{u=f,1,q} [E^u_x][T^u_{gx}] \tag{9}$$

$$[h_i h_j][L^*_{gy}] = [C_y][\bar{\phi}_g] + \sum_{u=f,1,q} [E^u_y][T^u_{gy}] \tag{10}$$

In summary, the method developed here deals with the solution of average fluxes and leakages. This differs from the methods of Wagner,[1] Sims,[3] and Lawrence,[5] in which the unknowns to be calculated are the average partial currents at each node face. Since this method will be extended to three dimensions and hexagonal geometry, it is felt that the use of partial currents as unknowns would significantly decrease the efficiency of the method in comparison to the one developed here.

NODEWISE PROPERTIES

In the above method, the right hand side of Eq. 3 was replaced by a polynomial representation within each node. One component of this right hand side is the transverse leakage term. The solution of Eqs. 9 and 10 gives the average leakage in each direction for each node. In order to obtain a quadratic representation of the leakage, information from adjacent nodes is used to construct a quadratic function, which is then used only over the current node.[10]

The quadratic expansion of the total source may be written as the flat (or constant) transverse leakage term plus the remainder of the expansion. The remainder is composed of fissioning and scattering sources, plus the higher order leakage approximation. The source may be written as:

$$T_{gx_{i,j}}(w) = -L^{*}_{gy_{i,j}} + T^{f,m}_{gx_{i,j}} + T^{l,m}_{gx_{i,j}} \frac{w}{h_i} + T^{q,m}_{gx_{i,j}} \frac{w^2}{h_i^2} \qquad (11)$$

Substituting Eq. 11 and its counterpart in the y direction into Eqs. 9 and 10 gives:

$$\left[h_i h_j\right]\left[L^{*}_{gx}\right] + \left[E^{f}_{x}\right]\left[L^{*}_{gy}\right] = \left[C_x\right]\left[\bar{\phi}_g\right] + \left[S_{\ell x}\right] \qquad (12)$$

$$\left[h_i h_j\right]\left[L^{*}_{gy}\right] + \left[E^{f}_{y}\right]\left[L^{*}_{gx}\right] = \left[C_y\right]\left[\bar{\phi}_g\right] + \left[S_{\ell y}\right] \qquad (13)$$

$$\left[S_{\ell x}\right] = \sum_{u=f,l,q} \left[E^{u}_{x}\right]\left[T^{u,m}_{gx}\right]$$

$$\left[S_{\ell y}\right] = \sum_{u=f,l,q} \left[E^{u}_{y}\right]\left[T^{u,m}_{gy}\right]$$

It is recognized that further components of the transverse leakage remain in the source expansion terms. However, it is felt that separating out the flat leakage contribution will remove most of the leakage from these terms, and therefore not interfere with the methods of solution to be discussed later.

To calculate the quadratic expansion of the source on the right hand side of Eq. 3, a quadratic expansion of the group fluxes is made within each node. Thus:

$$\phi_{gj}(w) = a^{f}_{x_{i,j}} + a^{l}_{x_{i,j}} \frac{w}{h_i} + a^{q}_{x_{i,j}} \frac{w^2}{h_i^2} \qquad (14)$$

From this expansion, the fissioning and scattering sources are easily calculated.

The technique used to calculate the flux expansion coefficients above was found to be of prime importance in determining the overall accuracy of the method. It was found that advantage must be taken of the details of the solution inside the node which are known due to the analytic solution. This conclusion is supported by the work of Lawrence.[5] From the analytic solution, an equation of the following form is derived:

$$\phi_{gj}(w) = F^{g}_{1_{i,j}}(w)\,\phi_{gj}(0) + F^{g}_{2_{i,j}}(w)\,J_{gx_{i,j}} + F^{g}_{3_{i,j}}(w)\,T^{f,m}_{gx_{i,j}} + F^{g}_{4_{i,j}}(w)\,T^{l,m}_{gx_{i,j}} + F^{g}_{5_{i,j}}(w)\,T^{q,m}_{gx_{i,j}} \qquad (15)$$

The flux and current at the leftmost node boundary may also be calculated from the analytic solution. A quadratic approximation of Eq. 15 may be found by several techniques. At present, collocation techniques are being used.[11] A quadratic flux approximation is found by collocating Eq. 15 at the three Gaussian points (0.1127, 0.5, 0.8873). Therefore, the quadratic expansion for the flux and leakage components of the right hand side may be calculated.

SOLUTION TECHNIQUES

OUTER ITERATIONS

The static problem is solved by using a fission source iteration accelerated by Chebyshev polynomials.[12] In the present method, components of the fission source from the average fluxes (Eq. 1) and from the flux expansion coefficients (Eq. 3) both exist. It has been found most effective if all of these components are simultaneously accelerated by the Chebyshev polynomials. Thus, at each "outer" iteration, a matrix problem for the fluxes and leakages must be solved.

INNER ITERATION TECHNIQUES

At a particular outer interation, Eq. 2 may be rewritten using the change of variables (Eqs. 6, 7):

$$\left[h_i h_j\right]\left\{\left[L^{*}_{gx}\right] + \left[L^{*}_{gy}\right]\right\} + \left[h_i h_j \Sigma_{Rg}\right]\left[\bar{\phi}_g\right] = \left[S_{\phi g}\right] \qquad (16)$$

Equation 16 is then solved for the average fluxes:

$$\left[\bar{\phi}_g\right] = \left[h_i h_j \Sigma_{Rg}\right]^{-1}\left\{-\left[h_i h_j\right]\left[\left[L^{*}_{gx}\right] + \left[L^{*}_{gy}\right]\right] + \left[S_{\phi g}\right]\right\} \qquad (17)$$

Substituting Eq. 17 into Eqs. 12 and 13 gives:

$$\left[h_i h_j\right]\left[L^*_{gx}\right] + \left[E^f_x\right]\left[L^*_{gy}\right] + \left[C_x\right]\left[\Sigma_R\right]^{-1}\left\{\left[L^*_{gx}\right] + \left[L^*_{gy}\right]\right\}$$

$$= \left[C_x\right]\left[h_i h_j \Sigma_R\right]^{-1}\left[S_{\phi g}\right] + \left[S_{\ell x}\right] \qquad (18)$$

$$\left[h_i h_j\right]\left[L^*_{gy}\right] + \left[E^f_y\right]\left[L^*_{gx}\right] + \left[C_y\right]\left[\Sigma_R\right]^{-1}\left\{\left[L^*_{gx}\right] + \left[L^*_{gy}\right]\right\}$$

$$= \left[C_y\right]\left[h_i h_j \Sigma_R\right]^{-1}\left[S_{\phi g}\right] + \left[S_{\ell y}\right] \qquad (19)$$

Equations 18 and 19 were initially solved by an accelerated Gauss-Seidel iteration, in which the unknowns $L^*_{gx_{i,j}}$ and $L^*_{gy_{i,j}}$ for each point i,j were solved simultaneously. For the test problems discussed here, this iteration converged to yield an error reduction of 0.04 or less on 2-3 iterations. In one test problem attempted, however, the spectral radius of the Gauss-Seidel iteration matrix was 0.73, and the use of over-relaxation caused the problem to diverge. Due to this failure, the runs made for this paper used no over-relaxation in the inner iterations. The large mesh sizes encountered in most test problems will lead to rapidly convergent iterative methods despite this limitation.

The theory used to calculate the over-relaxation parameter used above is applicable only to symmetric, positive definite matrices.[13] The matrix resulting from the above ordering of leakage unknowns can be shown to be asymmetric, and thus the above theory does not apply. In addition, it has been shown that the eigenvalue spectrum of the Gauss-Seidel iteration matrix contains some complex eigenvalues. For cases in which the spectral radius is large, the overrelaxation may lead to oscillatory behavior. The use of overrelaxation is therefore not indicated in the general case.

After Eqs. 18 and 19 have been solved, Eq. 17 is used to calculate the average fluxes.

RESULTS

ONE DIMENSION

In the beginning stages of the investigation, a one-dimensional version of the method described above was tested. A one-dimensional slice through the two-dimensional IAEA benchmark problem (11-A2 of reference 14) was used as a test problem. It was found that quadratic polynomials obtained from a three-point collocation of Eq. 15 led to a maximum error in assembly power for a 20 cm mesh of 4.0%. This result could be improved by performing a four-point collocation to obtain a cubic polynomial, and then determining that quadratic which most closely matches the cubic in a least squares sense. Using this technique (and therefore retaining only quadratic terms), a maximum assembly power error of 2.1% was obtained. From these results, it was felt that a sufficiently accurate quadratic polynomial could be obtained such that it would not be necessary to retain terms higher than quadratic in the analytic solution.

TWO DIMENSIONAL RESULTS - IAEA BENCHMARK PROBLEM

The IAEA benchmark problem[14] has been solved using the method described above with the quadratic transverse leakage approximation and a quadratic flux expansion as calculated from a three-point collocation. It was found that this method of calculating quadratic fluxes and leakages gave results of acceptable accuracy for this problem. The eigenvalue calculated by the nodal method described here (AN2D) is 1.02969. Table 1 compares the AN2D solution with those of other nodal schemes. For comparison purposes, all execution times are reported for a quarter-core problem and with respect to the IBM 370/195. The execution time for IQSBOX assumes the time quoted in reference 1 to be for an octant. Execution times on the 370/195 are assumed to be 0.7 times the execution time on the CYBER 175.

TWO DIMENSIONAL RESULTS - HETEROGENEOUS CORE LMFBR

To evaluate the accuracy and efficiency of AN2D for fast reactor diffusion theory analysis, a two-dimensional x-y geometry model of a heterogeneous core LMFBR was developed. This problem was designed to be an x-y equivalent of a hexagonal geometry core. The model is composed of a 15 × 15 array of square assemblies, with a uniform length of 15 cm on a side. This length was chosen such that the area of the original hexagon is the same as the area of the square fuel assembly. The cross section set is an eight-group set taken from a metal-fuelled design.

The DIF3D finite difference code[12] was run using 1 × 1, 2 × 2, 3 × 3, 4 × 4, and 8 × 8 mesh grids per 15 cm assembly. The results of these DIF3D runs are summarized in Table 2. The reference eigenvalue and power distribution was obtained by extrapolating the 4 × 4 and 8 × 8 results.

DIF3D is seen to give results of less than 3.0% error for a 4 × 4 mesh spacing. However, since this problem originated from one in hexagonal geometry, finite difference calcuations would be performed routinely using six triangles per hex. Therefore, the 3 × 3 DIF3D solution would probably be deemed acceptable, since the eiquivalent of a 4 × 4 mesh does not exist in hexagonal geometry.

The nodal solutions are also summarized in Table 2. The AN2D run using quadratic flux and leakage is shown to be very accurate, having a maximum error in assembly power of 1.4%, and an eigenvalue error of 6×10^{-5}. The nodal method described here gives significantly more accurate results than finite differences for this problem with a significant decrease in execution time.

It was felt in view of the following items that the extreme accuracy of the quadratic flux and leakage nodal solution may not be necessary for this problem. As has already been pointed out, the finite difference result using a 3 × 3 mesh would probably be deemed acceptable, and that solution was shown to be in error by as much as 4.0%. In addition, it is likely that the cross sections and homogenization uncertainties could lead to errors of more than 1.5% in assembly powers. Finally, significant transport effects at core-blanket interfaces lead to errors larger than 4.0% in some blanket assemblies. For these reasons, a less costly version of AN2D was desired. The method described in Table 2 as "quadratic → linear" consists of the quadratic flux and leakage approximations calculated as in the original method, then using a least squares technique to calculate a linear function which most closely matches it. Using this technique increases the errors only slightly, while the execution time is reduced by ∿10%. Therefore, the nodal method described in this paper is shown to give significant improvement in accuracy while requiring about three times less computation time than finite differences for this problem.

SUMMARY

In this paper, a nodal method applicable to fast reactor diffusion theory analysis has been developed. This method has been shown to be accurate and efficient in comparison to highly optimized finite difference techniques. The use of an analytic solution to the diffusion equation as a means of determining accurate coupling relationships between nodes has been shown to be highly accurate and efficient in specific two-group applications,[4,6] as well as in the current multigroup method.

Future prospects for this method include extension to three dimensions and hexagonal geometry. Further thought will be given to the use of Eqs. 9 and 10 as the starting point for the development of somewhat less accurate but more efficient computational techniques. This may be a more theoretically sound platform to start than is used in some higher order difference methods.[7,8] Should the method described here prove to be significantly more efficient than finite differences in three dimensions and hexagonal geometry, it will be considered for inclusion into a three-dimensional version of the kinetics code FX2-TH[17] and the fast reactor fuel cycle system REBUS.[18]

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Table 1. Comparison of AN2D and Other Solutions for the IAEA Benchmark Problem

Method	Execution Time (sec on IBM 370/195)	Maximum Error in Assembly Power (%)
AN2D	0.81	2.0
2DTD-II[4,15]	0.56	1.6
QUANDRY[6]	0.75	<1.0
IQSBOX[1]	1.20	1.4
NGFM[5]	1.26	<1.0
SIMULATE[16] (ROCS)	3.40	7.0

Table 2. Heterogeneous Core Problem Summary

Method	Eigenvalue λ	Execution Time (sec on IBM 370/195)	Maximum Error In Assembly Power (%)
Reference	1.113273		
DIF3D			
1 × 1	1.148243	1.2	25.9
2 × 2	1.121355	6.7	8.6
3 × 3	1.116699	19.2	4.0
4 × 4	1.115129	43.9	2.3
8 × 8	1.113644	264.0	0.5
AN2D			
Quadratic–Quadratic	1.113347	7.3	1.4
Quadratic→Linear	1.112156	6.5	1.6