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ABSTRACT

NODEX is a multigroup nodal diffusion theory code based on a high order version of the Nodal Expansion Method (NEM) - one of the modern transverse integrated methods. Nodal schemes of this type are formulated by transverse integrating the multi-dimensional diffusion equation within each node volume in order to obtain a set of one-dimensional equations for the node. In the NEM, these equations are solved by expanding the transverse integrated flux in a series of polynomials and then solving for the expansion coefficients. This process has the attractive feature that it allows the energy groups to be solved for one at a time - thus facilitating implementation in a computer code that permits the use of an arbitrary number of energy groups. The cost of this flexibility, however, is an error component due to the truncation of the polynomial expansion. In order to mitigate this difficulty, NODEX uses a fifth order polynomial expansion which has been found to result in negligible truncation errors for typical applications. The use of such a high order expansion requires some care in the development of the algorithm, however, as schemes greater than fourth order can become computationally quite intensive.

The NODEX algorithm somewhat resembles the nonlinear algorithm first suggested by Smith and Wagner and Koebke. This procedure involves source iterations using a low order coarse mesh finite difference (CMFD) method in which the coupling coefficients may be modified so as to force agreement with a higher order method. The nonlinearity arises as the source iterations are periodically interrupted and the coupling coefficients recomputed using the NEM while holding the eigenvalue, node averaged fluxes, and leakages constant. The source iterations are accelerated by using a variant of Wielandt's method that precludes the need for solving for all energy groups simultaneously. Acceleration by this scheme has been found in practice to be essentially as good as when the usual Wielandt scheme is used and all groups are solved for simultaneously.

In addition to the source iterations, the other major portion of the algorithm is the computation of successively improved values of the coupling terms. This is accomplished by solving - for each node interface - the NEM equations for a two-node problem comprised of the nodes on either side of the interface. For a fifth order method there are thus ten unknown expansion coefficients per group for each of these problems. The corresponding ten equations per group that are solved are: one for the net leakage in the longitudinal direction for each of the nodes, one for the continuity of current and heterogeneous flux at the interface, and three weighted residual equations for each node. The transverse and longitudinal leakages, the node averaged fluxes, and the problem eigenvalue are assumed known from the latest source iteration for the purpose of solving for the expansion coefficients. The longitudinal leakage and continuity equations are used to eliminate the first and second order coefficients, thus leaving six equations per group for the higher order coefficients. These degenerate into two GxG matrix systems and one 4Gx4G system which are then solved by Gaussian elimination using a variation of the SAXPY-KJI method with partial pivoting. This method produces quite good solution times on the Cray-XMP. The resulting expansion coefficients are then used to compute an NEM value for the interface group currents, from which coupling terms for that interface may be determined.

NODEX: A High Order NEM-Based Multigroup Nodal Code

T. M. Sutton

I. Introduction

NODEX is a multigroup nodal diffusion theory code for general three-dimensional reactor analysis. The nodal solution procedure used in the code is based on a high order version of the Nodal Expansion Method (NEM)[1]. This transverse integrated nodal method[2] is capable of obtaining extremely accurate solutions to the node-wise homogeneous diffusion equation on a very coarse computational mesh. NODEX uses a nonlinear iteration stategy in which the source iterations are performed using the low order Coarse Mesh Finite Difference (CMFD) method. The coupling coefficients used during this phase of the calculation are periodically recomputed using the NEM in order to cause the CMFD solution to match that of the higher order method. Source acceleration is achieved using a version of Wielandt's method that permits the group-wise computation of the node averaged flux values. Unlike many nodal codes that are limited to a one-and-a-half or two group energy treatment, NODEX has the ability to handle an arbitrary number of energy groups. When combined with an advanced homogenization scheme based on Generalized Equivalence Theory[3] (GET), the code has the potential to solve heterogeneous reactor problems in a small fraction of the time required by a detailed finite difference or finite element calculation.

In Section II of this report the NODEX solution algorithm is described in detail, including a discussion of the source acceleration scheme. Section III presents a method of using NODEX, or any other advanced nodal code, for accurate three-dimensional depletion calculations. Finally, Section IV briefly mentions some of the directions that NODEX development may take.

II. The NODEX Algorithm

The NODEX algorithm is somewhat similar to the nonlinear algorithm originally suggested by Smith[4] and Wagner and Koebke[5]. These schemes employ an outer iterative loop that alternates between a sequence of several source iterations performed using a simple low order method, such as the CMFD method, and a higher order nodal calculation used to compute increasingly more accurate coupling coefficients for use during the next sequence of source iterations. This outermost loop is commonly called the nonlinear iteration as the eigenvalue, node averaged fluxes, and leakages from the latest sequence of source iterations are used in computing the coupling coefficients. In the original nonlinear scheme the coupling adjustment is implemented by applying discontinuity factors to the CMFD equations. NODEX, however, employs an alternative method - also due to Smith - that has proved to be more numerically stable for many applications. This method of formulating CMFD equations with adjustable coupling coefficients will be described next. Following that is a discussion of how the NEM is used to compute the updated values for the coupling coefficients. To end this section, the scheme used to accelerate the source iterations is presented.

Before beginning the development of the NODEX equations, it is necessary to explain the notational system employed (see also Reference 3). To avoid the need to derive separate equations for each of the three directions, a generic coordinate system is introduced with directional variables u, v, and w and their corresponding indices ℓ, m, and n. Each of these directional variables and associated indices may represent any of the three physical directions x, y, or z and their corresponding indices i, j, or k, with the other two variables then representing the other two directions. Hence, $A^u_{\ell+1,m,n}$ represents $A^x_{i+1,j,k}$, $A^y_{i,j+1,k}$, and $A^z_{i,j,k+1}$. Integer subscripts are used to denote quantities defined for node volumes, while half-integer subscripts are used to denote quantities defined on node interfaces.

II.A. The CMFD Formulation

The usual mesh-centered finite difference expression for the u-component of the group g current averaged over the interface between nodes (ℓ,m,n) and $(\ell+1,m,n)$ is given by[4]

$$\bar{J}^{ug}_{\ell+1/2,m,n} = \frac{2}{h^u_\ell / D^g_{\ell,m,n} + h^u_{\ell+1} / D^g_{\ell+1,m,n}} \left[\bar{\phi}^g_{\ell,m,n} - \bar{\phi}^g_{\ell+1,m,n} \right] ; \quad u \in \{x, y, z\} \qquad , (1)$$

where h^u_ℓ is the node spacing and $\bar{\phi}^g_{\ell,m,n}$ is the node averaged flux. Substitution into the nodal balance equation,

$$\sum_{u=x,y,z} \frac{\bar{J}^{ug}_{\ell+1/2,m,n} - \bar{J}^{ug}_{\ell-1/2,m,n}}{h^u_\ell} + \Sigma^g_{r_{\ell,m,n}} \bar{\phi}^g_{\ell,m,n} = \Sigma^{g-1\to g}_{s_{\ell,m,n}} \bar{\phi}^{g-1}_{\ell,m,n} + \sum_{g'} \frac{\chi^g}{\lambda} \nu\Sigma^{g'}_{f_{\ell,m,n}} \bar{\phi}^{g'}_{\ell,m,n} \qquad , (2)$$

results in the standard seven point equations for the node averaged flux. (It is assumed here for simplicity that scattering is to the next lowest group only; the extension to a general downscattering treatment is easily accomplished.)

In NODEX, the expression for the interface current is modified to be

$$\bar{J}^{ug}_{\ell+1/2,m,n} = \frac{2}{h^u_\ell / D^g_{\ell,m,n} + h^u_{\ell+1} / D^g_{\ell+1,m,n}} \left[\bar{\phi}^g_{\ell,m,n} - \bar{\phi}^g_{\ell+1,m,n} + C^{ug}_{\ell+1/2,m,n} \left(\bar{\phi}^g_{\ell,m,n} + \bar{\phi}^g_{\ell+1,m,n} \right) \right] \qquad , (3)$$

where $C^{ug}_{\ell+1/2,m,n}$ is the coupling correction factor that is to be determined from the solution of the NEM equations. Note that there is only one such factor per node interface and energy group in this scheme as opposed to the two factors required by the discontinuity factor-based scheme. Note also that the coupling correction factor is used to multiply the sum of - rather than the difference between - the flux values in the two adjacent nodes. The reason for this is to avoid the numerical difficulty that would arise if the flux difference scheme were used, the flux values in the two nodes were equal (or nearly equal), and the NEM solution yielded a non-zero interface current. Such a situation would lead to an infinite (or extremely large) value for the corresponding coupling factor.

The NODEX form of the CMFD equation is then obtained by substituting Eq. (3) into Eq. (2), yielding

$$-\sum_{u=x,y,z} \frac{2/h_\ell^u}{h_{\ell+1}^u/D_{\ell+1,m,n}^g + h_\ell^u/D_{\ell,m,n}^g}\left(1 - C_{\ell+1/2,m,n}^{ug}\right)\bar{\Phi}_{\ell+1,m,n}^g$$

$$+\left\{\Sigma_{r_{\ell,m,n}}^g + \sum_{u=x,y,z}\left[\frac{2/h_\ell^u}{h_{\ell+1}^u/D_{\ell+1,m,n}^g + h_\ell^u/D_{\ell,m,n}^g}\left(1 + C_{\ell+1/2,m,n}^{ug}\right)\right.\right.$$

$$\left.\left.+\frac{2/h_\ell^u}{h_\ell^u/D_{\ell,m,n}^g + h_{\ell-1}^u/D_{\ell-1,m,n}^g}\left(1 - C_{\ell-1/2,m,n}^{ug}\right)\right]\right\}\bar{\bar{\Phi}}_{\ell,m,n}^g$$

$$-\sum_{u=x,y,z} \frac{2/h_\ell^u}{h_\ell^u/D_{\ell,m,n}^g + h_{\ell-1}^u/D_{\ell-1,m,n}^g}\left(1 + C_{\ell-1/2,m,n}^{ug}\right)\bar{\Phi}_{\ell-1,m,n}^g$$

$$= \Sigma_{s_{\ell,m,n}}^{g-1\to g}\bar{\Phi}_{\ell,m,n}^{g-1} + \sum_{g'}\frac{\chi^g}{\lambda}\nu\Sigma_{f_{\ell,m,n}}^{g'}\bar{\bar{\Phi}}_{\ell,m,n}^{g'} \quad . \quad (4)$$

It is the solution of this seven stripe matrix equation for the nodal fluxes and the eigenvalue that comprises the source iteration loop of the nonlinear algorithm.

II.B. The Coupling Coefficient Calculations

In order for Eq. (4) to converge to an accurate solution, the coupling coefficients must be computed so as to cause the CMFD internodal current values to match those of a high order solution. In NODEX, the high order solution is obtained using the NEM. This method, along with the other transverse integrated nodal methods, is formulated by integrating - for each direction - the three-dimensional diffusion equation within the volume of a node over the two transverse directions. This results in a set of three one-dimensional equations of the form

$$-D_{\ell,m,n}^g\frac{d^2}{du^2}\bar{\Phi}_{\ell,m,n}^{ug}\left(\frac{u-u_\ell}{h_\ell^u}\right) + \Sigma_{r_{\ell,m,n}}^g\bar{\Phi}_{\ell,m,n}^{ug}\left(\frac{u-u_\ell}{h_\ell^u}\right)$$

$$= \Sigma_{s_{\ell,m,n}}^{g-1\to g}\bar{\Phi}_{\ell,m,n}^{ug'}\left(\frac{u-u_\ell}{h_\ell^u}\right) + \sum_{g'}\frac{\chi^g}{\lambda}\nu\Sigma_{f_{\ell,m,n}}^{g'}\bar{\Phi}_{\ell,m,n}^{ug'}\left(\frac{u-u_\ell}{h_\ell^u}\right) + L_{\ell,m,n}^{ug}\left(\frac{u-u_\ell}{h_\ell^u}\right) \quad , \quad (5)$$

where $\bar{\phi}_{\ell,m,n}^{vg}((u-u_\ell)/h_\ell^u)$ is the transverse averaged flux and $L_{\ell,m,n}^{vg}((u-u_\ell)/h_\ell^u)$ is the transverse leakage term defined by

$$L_{\ell,m,n}^{ug} = \frac{D_{\ell,m,n}^g}{h_m^v h_n^w}\left[\int_{w_n-h_n^w/2}^{w_n+h_n^w/2} dw\,\frac{\partial}{\partial v}\Phi_{\ell,m,n}^g\Big|_{v_m-h_m^v/2}^{v_m+h_m^v/2}\right.$$

$$\left.+\int_{v_m-h_m^v/2}^{v_m+h_m^v/2} dv\,\frac{\partial}{\partial w}\Phi_{\ell,m,n}^g\Big|_{w_n-h_n^w/2}^{w_n+h_n^w/2}\right] \quad . \quad (6)$$

The solution of these one-dimensional equations is used to obtain a relationship between the internodal current and the node averaged flux values, with

the method of solution being the key feature that distinguishes one transverse integrated method from another. The particular technique utilized by the NEM involves expanding the transverse integrated flux in a series of polynomials and then solving for the expansion coefficients. The disadvantage of this method is the introduction of an error component due to the necessity of truncating the polynomial expansion. Another of the transverse integrated methods, the Analytic Nodal Method (ANM)[7], does not suffer from this type of error as it solves the one-dimensional equations exactly. Unfortunately, however, it is rather unwieldy in a general multigroup formulation. Thus, in order to obtain the accuracy of the ANM yet retain the multigroup capability, NODEX uses a fifth order polynomial expansion of the form

$$\bar{\Phi}^{ug}_{\ell,m,n}\left(\frac{u-u_\ell}{h^u_\ell}\right) = \bar{\bar{\Phi}}^{g}_{\ell,m,n}\left[1+\sum_{t=1}^{5} a_t{}^{ug}_{\ell,m,n}\, P_t\left(\frac{u-u_\ell}{h^u_\ell}\right)\right] \quad , (7)$$

where P_t is a polynomial of order t. The use of a fifth order expansion has been found to be sufficiently accurate so as to result in negligible truncation errors for typical applications.

Before discussing the details of how the NEM equations are solved, it is necessary to specify the form that the transverse leakage term, $L^{ug}_{\ell,m,n}$, is to take. NODEX generally uses the quadratic leakage approximation[1] in which the transverse leakage is represented by

$$L^{ug}_{\ell,m,n}\left(\frac{u-u_\ell}{h^u_\ell}\right) = L^{ug}_{0\,\ell,m,n} + L^{ug}_{1\,\ell,m,n}\frac{u-u_\ell}{h^u_\ell} + L^{ug}_{2\,\ell,m,n}\left(\frac{u-u_\ell}{h^u_\ell}\right)^2 \quad . (8)$$

NODEX also allows the use of the flat and buckling approximations[7], but for simplicity these will not be discussed here. It should be emphasized that the quadratic leakage approximation presented here is not rigorously derivable from the three-dimensional diffusion equation. Its use is justified by many observations that it gives acceptable accuracy, and that errors incurred during the homogenization step are typically much more severe that those attributable to this leakage approximation. The method of determining the quadratic transverse leakage expansion coefficients employed by NODEX is a common one[8] in which Eq. (8) is integrated over $u_{\ell-1} - (h^u_{\ell-1}/2) \le u \le u_{\ell-1} + (h^u_{\ell-1}/2)$, $u_\ell - (h^u_\ell/2) \le u \le u_\ell + (h^u_\ell/2)$, and $u_{\ell+1} - (h^u_{\ell+1}/2) \le u \le u_{\ell+1} + (h^u_{\ell+1}/2)$ in order to obtain three equations for the expansion coefficients in terms of the net transverse leakages from nodes $(\ell-1,m,n)$, (ℓ,m,n), and $(\ell+1,m,n)$, respectively. Solving these equations for the coefficients yields

$$L^{ug}_{1\,\ell,m,n} = \frac{h^u_\ell}{h^u_{\ell-1}+h^u_\ell+h^u_{\ell+1}}\left[\left(\bar{L}^{ug}_{\ell+1,m,n}-\bar{L}^{ug}_{\ell,m,n}\right)\frac{2h^u_{\ell-1}+h^u_\ell}{h^u_\ell+h^u_{\ell+1}} - \left(\bar{L}^{ug}_{\ell-1,m,n}-\bar{L}^{ug}_{\ell,m,n}\right)\frac{h^u_\ell+2h^u_{\ell+1}}{h^u_{\ell-1}+h^u_\ell}\right]$$

$$L^{ug}_{2\,\ell,m,n} = \frac{3(h^u_\ell)^2}{h^u_{\ell-1}+h^u_\ell+h^u_{\ell+1}}\left[\left(\bar{L}^{ug}_{\ell+1,m,n}-\bar{L}^{ug}_{\ell,m,n}\right)\frac{1}{h^u_\ell+h^u_{\ell+1}} + \left(\bar{L}^{ug}_{\ell-1,m,n}-\bar{L}^{ug}_{\ell,m,n}\right)\frac{1}{h^u_{\ell-1}+h^u_\ell}\right]$$

$$L^{ug}_{0\,\ell,m,n} = \bar{L}^{ug}_{\ell,m,n} - \frac{1}{12}L^{ug}_{2\,\ell,m,n} \quad , (9a)$$

where the net transverse leakages are simply given by

$$\bar{L}^{ug}_{\ell,m,n} = \frac{\bar{J}^{vg}_{\ell,m-1/2,n} - \bar{J}^{vg}_{\ell,m+1/2,n}}{h^v_m} + \frac{\bar{J}^{wg}_{\ell,m,n-1/2} - \bar{J}^{wg}_{\ell,m,n+1/2}}{h^w_n} \quad . \quad (9b)$$

Note that even though integrals over three adjacent nodes are used in obtaining the quadratic expansion coefficients, a given quadratic is defined only within the middle node when used in Eq. (5).

In NODEX, the coupling terms are computed by using the NEM to solve a local problem for each node interface of the original global reactor problem. Each of these local problems is composed of two nodes; specifically, the ones on either side of the interface. Taking the node averaged fluxes, leakages, and eigenvalue to be known from the previous sequence of source iterations, the local problems are then solved for the NEM values of the group currents at the interface between the two nodes. Then, by rearranging Eq. (3) to get

$$C^{ug}_{\ell+1/2,m,n} = \frac{\pm\left(h^u_\ell / D^g_{\ell,m,n} + h^u_{\ell+1} / D^g_{\ell+1,m,n}\right)\bar{J}^{ug}_{\ell+1/2,m,n} - \bar{\Phi}^g_{\ell,m,n} + \bar{\Phi}^g_{\ell+1,m,n}}{\bar{\Phi}^g_{\ell,m,n} + \bar{\Phi}^g_{\ell+1,m,n}} \quad , \quad (10)$$

these interface currents are used to obtain the improved coupling factors for the next sequence of source iterations.

In deriving the NEM equations for the two-node problems, it is convenient to employ the explicit form of the flux expansion polynomials used by NODEX. They are: $P_1(\xi)=\xi$, $P_2(\xi)=\xi^2-1/12$, $P_3(\xi)=\xi^3-\xi/4$, $P_4(\xi)=\xi^4-3\xi^2/10+1/80$, and $P_5(\xi)=\xi^5-\xi^3/3+\xi/48$. These are chosen[1] such that $P_t(\pm 1/2)=0$ for $t>2$, and also such that consecutive polynomials are orthogonal over the range $[-1/2,1/2]$.

The quantities to be determined are the NEM vaules of the interface currents, but to get them one must first compute the five flux expansion coefficients for each of the two nodes and each of the energy groups. Ten equations per energy group in the expansion coefficients are thus required in order to completely specify the unknowns. Two of these ten equations are obtained by constraining the NEM value of the longitudinal leakage in each node to match that of the global solution. To derive these equations, one applies the flux expansion of Eq. (7) to a transverse average of Fick's Law to obtain

$$\bar{J}^{ug}_{\ell,m,n}\left(\frac{u-u_\ell}{h^u_\ell}\right) = -\frac{D^g_{\ell,m,n}}{h^u_\ell}\bar{\Phi}^g_{\ell,m,n}\sum_{t=1}^{5} a^{ug}_{t\,\ell,m,n}\,P'_t\left(\frac{u-u_\ell}{h^u_\ell}\right) \quad . \quad (11)$$

Evaluation of this expression at each of the two u-directed faces of node (ℓ,m,n) results in

$$\bar{J}^{ug}_{\ell\pm 1/2,m,n} = \bar{J}^{ug}_{\ell,m,n}\left(\pm 1/2\right)$$

$$= -\frac{D^g_{\ell,m,n}}{h^u_\ell}\bar{\Phi}^g_{\ell,m,n}\left[a^{ug}_{1\,\ell,m,n} \pm a^{ug}_{2\,\ell,m,n} + \frac{1}{2}a^{ug}_{3\,\ell,m,n} \pm \frac{1}{5}a^{ug}_{4\,\ell,m,n} + \frac{1}{12}a^{ug}_{5\,\ell,m,n}\right] \quad , \quad (12)$$

so that the longitudinal leakage in the u-direction,

$$Q^{ug}_{\ell,m,n} = \frac{\bar{J}^{ug}_{\ell+1/2,m,n} - \bar{J}^{ug}_{\ell-1/2,m,n}}{h^u_\ell} \quad , \quad (13a)$$

may thus be given in terms of the even order expansion coefficients as

$$Q^{ug}_{\ell,m,n} = -\lambda \frac{D^g_{\ell,m,n}}{(h^u_\ell)^2} \bar{\bar{\Phi}}^g_{\ell,m,n} \left[a_2{}^{ug}_{\ell,m,n} + \frac{1}{5} a_4{}^{ug}_{\ell,m,n} \right] \quad . \quad (13b)$$

There is one of these expressions for each of the two nodes in the local problem. An additional equation may be obtained from the continuity of current condition at the node interface by using Eq. (12) to evaluate the current at the interface in terms of both the node (ℓ,m,n) quantities and the node $(\ell+1,m,n)$ quantities and then equating the two expressions to get

$$\begin{aligned} &- \frac{D^g_{\ell,m,n}}{h^u_\ell} \bar{\bar{\Phi}}^g_{\ell,m,n} \left[a_1{}^{ug}_{\ell,m,n} + a_2{}^{ug}_{\ell,m,n} + \frac{1}{2} a_3{}^{ug}_{\ell,m,n} + \frac{1}{5} a_4{}^{ug}_{\ell,m,n} + \frac{1}{12} a_5{}^{ug}_{\ell,m,n} \right] \\ &= - \frac{D^g_{\ell+1,m,n}}{h^u_{\ell+1}} \bar{\bar{\Phi}}^g_{\ell+1,m,n} \left[a_1{}^{ug}_{\ell+1,m,n} - a_2{}^{ug}_{\ell+1,m,n} + \frac{1}{2} a_3{}^{ug}_{\ell-1,m,n} \right. \\ &\qquad \left. - \frac{1}{5} a_4{}^{ug}_{\ell+1,m,n} + \frac{1}{12} a_5{}^{ug}_{\ell+1,m,n} \right] \end{aligned} \quad . \quad (14)$$

Similarly, the discontinuity condition on the homogeneous flux[3] may be obtained by evaluating Eq. (7) at the node interface

$$\begin{aligned} &\frac{1}{f^{ug+}_{\ell,m,n}} \bar{\bar{\Phi}}^g_{\ell,m,n} \left[1 + \frac{1}{2} a_1{}^{ug}_{\ell,m,n} + \frac{1}{6} a_2{}^{ug}_{\ell,m,n} \right] \\ &= \frac{1}{f^{ug-}_{\ell+1,m,n}} \bar{\bar{\Phi}}^g_{\ell+1,m,n} \left[1 - \frac{1}{2} a_1{}^{ug}_{\ell+1,m,n} + \frac{1}{6} a_2{}^{ug}_{\ell+1,m,n} \right] \end{aligned} \quad , \quad (15)$$

where $f^{ug\pm}_{\ell,m,n}$ is the node (ℓ,m,n) discontinuity factor for the surface at $u_{\ell\pm1/2}$.

The two longitudinal leakage equations along with the conditions on the flux and current at the interface between the two nodes represent only four of the ten expressions needed per energy group. The six additional equations are obtained by applying the weighted residual method to the transverse integrated diffusion equation[1]. Each weighted residual equation is obtained by substituting Eqs. (7) and (8) into Eq. (5), multiplying through by a weighting function, and then integrating over the range [-1/2,1/2]. In NODEX, the three weighting functions P_1, P_2, and P_3 are used, thus resulting in the expressions

$$\sum_{g'} \left[\tau^{g'\to g}_{\ell,m,n} a^{u\,g'}_{1,\ell,m,n} - \left(\frac{1}{10} \tau^{g'\to g}_{\ell,m,n} + \delta_{g,g'}\, 6\, \frac{D^{g'}_{\ell,m,n}}{(h^u_\ell)^2} \right) a^{u\,g'}_{3,\ell,m,n} \right.$$

$$\left. - \left(\frac{1}{420} \tau^{g'\to g}_{\ell,m,n} + \delta_{g,g'} \frac{D^{g'}_{\ell,m,n}}{(h^u_\ell)^2} \right) a^{u\,g'}_{5,\ell,m,n} \right] \bar{\bar{\phi}}^{g'}_{\ell,m,n} = L^{u\,g}_{1,\ell,m,n} \tag{16a}$$

$$\sum_{g'} \left[\tau^{g'\to g}_{\ell,m,n} a^{u\,g'}_{2,\ell,m,n} - \left(\frac{3}{35} \tau^{g'\to g}_{\ell,m,n} + \delta_{g,g'}\, 12\, \frac{D^{g'}_{\ell,m,n}}{(h^u_\ell)^2} \right) a^{u\,g'}_{4,\ell,m,n} \right] \bar{\bar{\phi}}^{g'}_{\ell,m,n} = L^{u\,g}_{2,\ell,m,n} \tag{16b}$$

$$\sum_{g'} \left[\tau^{g'\to g}_{\ell,m,n} a^{u\,g'}_{1,\ell,m,n} - \left(\frac{1}{7} \tau^{g'\to g}_{\ell,m,n} + \delta_{g,g'}\, 6\, \frac{D^{g'}_{\ell,m,n}}{(h^u_\ell)^2} \right) a^{u\,g'}_{3,\ell,m,n} \right.$$

$$\left. - \delta_{g,g'} \frac{1}{7} \frac{D^{g'}_{\ell,m,n}}{(h^u_\ell)^2} a^{u\,g'}_{5,\ell,m,n} \right] \bar{\bar{\phi}}^{g'}_{\ell,m,n} = L^{u\,g}_{1,\ell,m,n} \tag{16c}$$

where

$$\tau^{g'\to g}_{\ell,m,n} = \Sigma^{g'}_{r,\ell,m,n} \delta_{g,g'} - \Sigma^{g'\to g}_{s,\ell,m,n} \delta_{g',g-1} - \frac{\chi^g}{\lambda} \nu \Sigma^{g'}_{f,\ell,m,n} .$$

There is one set of these equations for each of the two nodes, thereby providing the 6·G expressions needed to complete the system.

At this point, all 10·G unknowns could be computed by the numerical solution of the 10·G simultaneous equations just derived. A more efficient algorithm may be obtained, however, by taking advantage of the fact that each of the non-weighted residual equations (Eqs. (13b), (14), and (15)) contain expansion coefficients for but a single group. By solving these equations for the two lowest order coefficients in each of the two nodes and substituting the results into Eqs. (16a-c) yields a system of 6·G equations for the 6·G higher order expansion coefficients. A further simplification may be achieved by noting that the use of Eq. (13b) to eliminate the second order coefficient in Eq. (16b) produces a system of equations for just the fourth order coefficients in a single node. These two systems - each consisting of G equations - are solved numerically. With the fourth order coefficients thus known, the system of 6·G equations reduces to a system of 4·G equations for the third and fifth order coefficients.

The solution of each of the local problems for the coupling factors, $C^{u\,g}_{\ell+1/2,m,n}$, is thus achieved in the following manner. First, the CMFD values of the surface averaged current are obtained for each node interface using Eq. (3). The values of the node averaged fluxes used for these calculations are taken from the latest sequence of source iterations, and the coupling factor values are those of the previous nonlinear iteration. Next, these surface averaged currents are used to compute the longitudinal leakage and the transverse leakage expansion coefficients according to Eqs. (9a), (9b), and (13a). At this point, one has everything needed to compute the coefficients and right-hand-side terms of the G simultaneous equations for the fourth order flux expansion coefficients in each of the two nodes in the local prob-

lem. By solving these equations numerically, one may then use the results to compute the coefficients and right-hand-side terms of the system of equations for the third and fifth order coefficients. This system is also solved numerically. Next, with the high order flux expansion coefficients now known, the first and second order coefficients are determined from Eqs (13b), (14), and (15). Updated NEM values for the group currents at the interface between the two nodes of the local problem are then obtained using Eq. (12), and finally the updated coupling factors computed using Eq. (10). This process is repeated for each interface in the nodal model.

For the algorithm just described to be effective, an efficient routine for solving the simultaneous equations for the flux expansion coefficients is essential. This is particularly true if the number of energy groups is large, as the number of unknowns increases with the square of the number of groups. NODEX uses a routine based on the SAXPY-KJI variant' of Gaussian elimination with partial pivoting. This seems to be the most effective method for application on the CRAY-XMP.

When the CMFD coupling terms have been computed for every interface in the model, another sequence of source iterations is begun. These proceed until some source iteration convergence criterion is met, at which time the coupling terms are once again recomputed. The nonlinear algorithm is considered converged when two consecutive sequences of source iterations yield the same solution to within some overall convergence criterion. It is important that this overall convergence criterion be somewhat looser than that used to for the source iterations, else the overall criteria may never be satisfied.

II.C. Acceleration of the Source Iterations

The source iterations in NODEX are performed using the inverse power method[10]. The convergence rate of this method is determined by the dominance ratio $|\lambda_1/\lambda_0|$ - the ratio of the first harmonic eigenvalue to the fundamental eigenvalue. This quantity is always between zero and unity, with convergence being slower the closer the value is to unity. Wielandt's method[10] is a means of accelerating the convergence by altering the problem so as to reduce the dominance ratio while leaving the eigenvector unchanged. This is achieved by subtracting

$$\frac{\chi^g}{\lambda'} \sum_{g'} \nu \Sigma_{f_{\ell,m,n}}^{g'} \bar{\Phi}_{\ell,m,n}^{g'}$$

from both sides of the seven point equations for the node averaged flux, where λ' is an estimate of the eigenvalue. Since the same quantity is subtracted from both sides, the eigenvector is identical to that of the original problem. The dominance ratio for the altered problem, however, is now given by $|(1/\lambda_0-1/\lambda')/(1/\lambda_1-1/\lambda')|$. If $\lambda' > (\lambda_1+\lambda_0)/2$, then the dominance ratio will be smaller than it was in the unaltered problem thus increasing the convergence rate.

The disadvantage of this method is that it introduces a coupling to the higher energy groups on the left-hand side of the seven point equations, thus preventing the group-wise solution of the equations that is normally possible if there is no upscattering. To address this problem, Wielandt's method is

modified[11] for use in NODEX by changing the quantity that is subtracted from both sides of the seven point equations to

$$\frac{\chi^g}{\lambda}\left[\sum_{g'}\nu\Sigma_{f_{\ell,m,n}}^{g'}\frac{\bar{\phi}_{\ell,m,n}^{g'}}{\bar{\phi}_{\ell,m,n}^{g}}\right]$$

The ratios $\bar{\phi}_{\ell,m,n}^{g'}/\bar{\phi}_{\ell,m,n}^{g}$ are computed based on the results of the latest source iteration and then treated as constants for use in the next source iteration, thereby regaining the group-wise solution capability. As the source iterations converge, this modified method approaches the original Wielandt method.

Wielandt's method is most effective if the estimated eigenvalue, λ', is close to the true eigenvalue of the matrix equation. Since the true eigenvalue is not generally known in advance, however, a means of estimating it during the course of the problem solution is required. Some caution must be exercised during this process as Wielandt's method will cause convergence toward whatever harmonic solution has an eigenvalue nearest to the estimate. A sufficient condition for assuring that convergence is to the fundamental mode is to always choose the estimated eigenvalue such that it is greater than the fundamental eigenvalue. The formula used by NODEX to compute an estimated eigenvalue for use in iteration t+1,

$$\lambda'^{(t+1)} = \lambda^{(t)} + 100\left|\lambda^{(t)} - \lambda^{(t-1)}\right| \quad , \quad (18)$$

is an attempt to achieve this condition while still providing rapid convergence. This method of source acceleration has proved to be both reliable and extremely easy to implement.

III. Depletion Using NODEX

NODEX is a general purpose nodal code that can be utilized in a wide variety of ways. Recently, a NODEX-based procedure has been developed by the author that provides a highly accurate three-dimensional depletion capability. In contrast to conventional methods[3] that rely on single or extended assembly homogenization schemes, the current NODEX procedure obtains node averaged cross sections and discontinuity factors from heterogeneous planar calculations of one or more radial slices through the three-dimensional model. The advantage of this type of homogenization procedure is that it completely avoids the need for developing special schemes for nodes that are not adequately handled by a single or extended assembly homogenization method. The disadvantage, of course, is that the planar slice calculations are generally much more computationally intensive than are single or extended assembly calculations. If, however, the only sufficiently accurate alternative is a heterogeneous three-dimensional calculation, then nodal calculations using data from this planar homogenization procedure are clearly preferred.

The three-dimensional nodal model used for the depletion calculations is constructed with the same radial nodal definition as is used in the planar homogenization calculations. The node spacing in the z-direction is chosen such as to allow any axial heterogeneities to be modeled (e.g., BWR shutdown

zones[12]), and also small enough to yield sufficient accuracy. At beginning-of-life (BOL) in a xenon-free condition, the method of assigning the appropriate planar homogenization parameters to the three-dimensional nodal mesh is straightforward. One simply performs a separate planar calculation for each unique axially uniform region of the reactor; then applies the resulting homogenization parameters for each two-dimensional node to the corresponding radial location of each axial slice in the three-dimensional model comprising that region. Unity discontinuity factors are used for node surfaces perpendicular to the z-direction.

The situation becomes much more complicated for depletion calculations. In this case, the heterogeneous planes corresponding to each of the regions that are axially uniform at BOL are depleted at a prescribed power level. The fraction of fuel remaining in each two-dimensional node at each of the planar depletion timesteps is tabulated along with the homogenization parameters for that node. Each node in the three-dimensional model is then depleted by first computing the fraction of fuel remaining in the node following a timestep based on the node averaged flux, the node averaged fission cross section, and the duration of the timestep. One then refers to the tabulation of homogenization parameters versus fraction of fuel remaining obtained from the planar depletion calculation appropriate to the axial slice containing the node. By performing a linear or quadratic interpolation based on the fraction of fuel remaining in the node in the three-dimensional model, one thus determines the homogenization parameters to be used for that node for the next flux calculation. The homogenized macroscopic node averaged cross sections obtained in this way do not contain a contribution due to xenon. This is handled separately on a microscopic cross section basis.

The effect of temperature feedback on the three-dimensional power distribution is treated by performing each of the planar depletion calculations at more than one temperature. This allows the homogenization parameters to be tabulated versus temperature, thus permitting interpolation on this quantity as well as on the fraction of the fuel remaining on a node-by-node basis.

IV. Summary

NODEX has proved to be a very useful reactor analysis tool when used as described in Section III. Many additional applications of and enhancements to the code will undoubtedly be developed in the future.

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