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POLYNOMIAL AND SEMI-ANALYTIC NODAL METHODS FOR NONLINEAR ITERATION PROCEDURE

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ABSTRACT

Two-node kernels of the polynomial, semi-analytic and analytic nodal methods are developed for the implementation in the nonlinear iteration procedure. The polynomial and semi-analytic nodal methods are based on the quartic expansion of the transverse-integrated neutron flux and the quadratic leakage approximation. The basic functions of the both methods are chosen from the orthogonality condition. That results in an efficient algorithm for the solution of the two-node nodal equations: the initial system of 8G nodal equations is reduced to G and 2G equations, where G is a number of neutron energy groups. Implementation of the analytic nodal method (ANM) presents an alternative way to a solution of the two-node problem. The surface-averaged current is expressed in the explicit form in terms of the node-averaged flux, the surface-averaged flux and the transverse leakage expansion coefficients. The five matrix functions used in the expression are computed using the Lagrange-Sylvester interpolation polynomial. The surface-averaged flux is calculated from the flux and current continuity conditions. Numerically, the solution of the two-node problem is reduced to a computation of G eigenvalues of the buckling matrix, a calculation of the five matrix functions and a solution of G equations with respect to the surface-averaged flux.

Accuracy and efficiency of the methods and algorithms are compared for the LWR benchmark problems. The semi-analytic and analytic nodal methods demonstrate similar accuracy. In the case of 2 neutron energy groups, the matrix function theory approach to the solution of the two-node problem shows the best efficiency. A saving in the CPU time is about 25 % for the computed problems.

I. INTRODUCTION

K. Smith[1] has proposed the nonlinear iteration procedure as a solution technique for transverse-integrated nodal methods[2]. In this approach, the coarse mesh finite difference (CMFD) method is forced to match the results of the nodal method. Coupling coefficients of the CMFD method are computed from a solution of the nodal equations for two-node problems. Thus, a solution procedure is decoupled into a local solution of the nodal equations for two-node problems and global iterations of the CMFD method. In comparison with traditional nodal solution techniques, the nonlinear iteration procedure results in a reduction of computer memory requirements and computing time.[2] The nodal expansion method (NEM)[3] is the most popular method used in the nonlinear iteration procedure.[4-6] Other methods are the analytic nodal method (ANM)[7] implemented in the STAR code[8] and the semi-analytic method[9] applied in the SIMULATE-3K[10]. A combination of the ANM and NEM has also been recently proposed.[11]

Although progress in nodal methods make possible to perform fast and accurate LWR calculations even on personal computers, the research in this area is rather growing. Digital reactor control systems, on-line core monitoring and training simulators require the calculations in real-time.[2] That is stimulating the efforts in the improvement of efficiency of nodal methods. From the other hand, the polynomial nodal methods, like NEM, are not very accurate for realistic LWR problems, when applied on the spatial mesh with 1 node per assembly.[11] Analytic and semi-analytic methods increase the accuracy with a minimum overhead in computing time.

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Two-node kernels of the polynomial, semi-analytic and analytic nodal methods developed for implementation in the nonlinear iteration procedure are presented in the paper. In the polynomial and semi-analytic nodal methods, the transverse-integrated neutron flux is expanded into the orthogonal set of basic functions. Legendre polynomials are used in the polynomial nodal method (PNM). In the semi-analytic nodal method (SANM), the 3rd and 4th Legendre polynomials are replaced by the modified hyperbolic sine and cosine. In the both methods, 3rd and 4th flux expansion coefficients are expressed in terms of the 1st and 2nd expansion coefficients in the explicit form. That results that the initial system of 8G nodal equations of two-node problem is reduced to a set of G and 2G equations.

A two-node kernel of ANM is presenting an alternative way to a solution of the two-node problem. The approach is based on matrix function theory. Adding two constraints, the transverse-integrated diffusion equation is led to a boundary value problem. The problem is solved analytically and the surface-averaged current is expressed in terms of the node-averaged flux, the surface-averaged flux and the transverse leakage expansion coefficients. The five matrix functions used in this expression are computed using the Lagrange-Sylvester interpolation polynomial. The surface-averaged flux is calculated using the flux and current continuity conditions. The two-node problem solution is reduced to a computation of G eigenvalues of the buckling matrix, a calculation of the five matrix functions and a solution of G equations with respect to the surface-averaged flux.

The paper is organized as follows. In Sec. II and III, we derive the two-node nodal equations for PNM and SANM, respectively. Section IV presented an alternative approach for two-node kernel in an application to ANM. Sec. V. demonstrates the results of LWR benchmark problem calculations. A summary and conclusions are given in Sec. VI.

II. POLYNOMIAL NODAL METHOD

The transverse-integrated neutron diffusion equation is written in the dimensionless form for x-direction as follows

$$-\frac{d^2}{du^2}\Phi_g^k(u)+\sum_{g'=1}^{G}\left(B_k^2\right)_{gg'}\Phi_{g'}^k(u)=-\frac{\left(\Delta x_k\right)^2}{4D_g^k}S_{gx}^k(u), \quad (1)$$

where k is the index of the node $\left[-\Delta x_k/2,\Delta x_k/2\right]\times$; $\left[-\Delta y_k/2,\Delta y_k/2\right]\times\left[-\Delta z_k/2,\Delta z_k/2\right]$; $u=2x/\Delta x_k$; $u\in\left[-1,1\right]$; g is the index of the neutron energy group; $\Phi_g^k(u)$ is the transverse integrated neutron flux;

$$\left(B_k^2\right)_{gg'}=\frac{\left(\Delta x_k\right)^2}{4D_g^k}\left\{\Sigma_{Rg}^k\delta_{gg'}-\frac{\chi_g}{k_{eff}}\nu\Sigma_{fg'}^k-\Sigma_{sg'\to g}^k\right\};$$

$S_{gx}^k(u)=\frac{1}{\Delta y_k}L_{gy}^k(u)+\frac{1}{\Delta z_k}L_{gz}^k(u)$ is the transverse leakage; and the other notations are fairly standard.

The basic functions in the polynomial nodal method (PNM)[12,13] are Legendre polynomials. They are given as:

$$P_0(u)=1;\ P_1(u)=u;\ P_2(u)=\frac{1}{2}(3u^2-1);$$
$$P_3(u)=\frac{1}{2}(5u^3-3u);\ P_4(u)=\frac{1}{8}(35u^4-30u^2+3).$$

The transverse-integrated neutron flux is expanded into the basic functions as

$$\Phi_g^k(u)=\overline{\Phi}_g^k+\sum_{i=1}^{4}a_{gxi}^kP_i(u),$$

where $\overline{\Phi}_g^k$ is the node-averaged neutron flux; and a_{gxi}^k is the *i*-th flux expansion coefficient.

The transverse leakage term is expanded up to the 2nd order as

$$S_{gx}^k(u)=\sum_{i=0}^{2}s_{gxi}^kP_i(u), \quad (2)$$

where s_{gxi}^k is the *i*-th coefficients of the transverse leakage expansion.

The 1st and 2nd expansion coefficients are computed using a quadratic leakage approximation, as it is described in Ref. 2. In this approach, the expansion (2) is required to preserve the node-averaged transverse leakages for the node k and its two neighboring nodes in the x-direction. If the node k is a boundary node, the expansion (2) is required to satisfy the neuron flux boundary condition. Introducing the dimensionless transverse leakage expansion coefficients the equation (1) is written in the form

$$-\frac{d^2}{du^2}\Phi(u)+\sum_{g'=1}^{G}\left(B_k^2\right)_{gg'}\Phi_{g'}^k(u)=-\sum_{i=0}^{2}\tilde{s}_{gxi}^kP_i(u) \quad (3)$$

where $\tilde{s}_{gxi}^k=\frac{\left(\Delta x_k\right)^2}{4D_g^k}s_{gxi}^k$.

The node-averaged flux, eigenvalue and transverse leakage expansion coefficients are assumed to be known from the results of CMFD iterations. The other coefficients of the neutron flux expansion are obtained by considering a two-node problem for each node interface. The two-node problem contains the adjacent nodes k, k+1 with common

interface. In order to obtain 4x2xG coefficients of the neutron flux expansion (4 expansion coefficients x 2 nodes x G neutron energy groups) the following equations are used: 2G neutron balance equations, 2G 1st-order moment-weighting equations, 2G 2nd-order moment-weighting equations, 2G equations of the flux and current continuity at the internal interface between two nodes. They are given as :

Neutron balance (for nodes k and k+1):

$$-\left\{3a^k_{gx2}+10a^k_{gx4}\right\}+\sum_{g'=1}^{G}\left(B^2_k\right)_{gg'}\overline{\Phi}^k_{g'}=-\tilde{s}^k_{gx0}\,; \qquad (4)$$

1st-order moment-weighting equations (for nodes k and k+1):

$$-15\,a^k_{gx3}+\sum_{g'=1}^{G}\left(B^2_k\right)_{gg'}a^k_{g'x1}=-\tilde{s}^k_{gx1}\,; \qquad (5)$$

2nd-order moment-weighting equations (for nodes k and k+1):

$$-35\,a^k_{gx4}+\sum_{g'=1}^{G}\left(B^2_k\right)_{gg'}a^k_{g'x2}=-\tilde{s}^k_{gx2}\,; \qquad (6)$$

Current continuity at the interface of the node k and k+1:

$$\begin{aligned}-d^k_{gx}\left\{a^k_{gx1}+3a^k_{gx2}+6a^k_{gx3}+10a^k_{gx4}\right\}=\\ -d^{k+1}_{gx}\left\{a^{k+1}_{gx1}-3a^{k+1}_{gx2}+6a^{k+1}_{gx3}-10a^{k+1}_{gx4}\right\},\end{aligned} \qquad (7)$$

where $d^k_{gx}=\dfrac{2D^k_g}{\Delta x_k}$ is the dimensionless diffusion coefficient;

Flux continuity at the interface of the nodes k and k+1:

$$\begin{aligned}\overline{\Phi}^k_g+a^k_{gx1}+a^k_{gx2}+a^k_{gx3}+a^k_{gx4}=\\ \overline{\Phi}^{k+1}_g-a^{k+1}_{gx1}+a^{k+1}_{gx2}-a^{k+1}_{gx3}+a^{k+1}_{gx4}\,.\end{aligned} \qquad (8)$$

The obtained equations are decoupled. The even flux expansion coefficients of the node k do not depend on the odd flux expansion coefficients of the node k and any expansion coefficients of the node k+1.

Furthermore, using Eq. (5), the 3rd expansion coefficient is expressed in terms of the 1st coefficient as follows

$$a^k_{gx3}=\frac{1}{15}\left\{\sum_{g'=1}^{G}\left(B^2_k\right)_{gg'}a^k_{g'x1}+\tilde{s}^k_{gx1}\right\}. \qquad (9)$$

Eq. (6) results in the following expression for the 4th expansion coefficient:

$$a^k_{gx4}=\frac{1}{35}\left\{\sum_{g'=1}^{G}\left(B^2_k\right)_{gg'}a^k_{g'x2}+\tilde{s}^k_{gx2}\right\}. \qquad (10)$$

Substituting Eq. (10) into the neutron balance equation (4), we obtain a system of G equations for the 2nd expansion coefficients:

$$\begin{aligned}\sum_{g'=1}^{G}\left\{3\delta_{gg'}+\frac{2}{7}\left(B^2_k\right)_{gg'}\right\}a^k_{g'x2}=\\ \sum_{g'=1}^{G}\left(B^2_k\right)_{gg'}\overline{\Phi}^k_{g'}+\left\{\tilde{s}^k_{gx0}-\frac{2}{7}\tilde{s}^k_{gx2}\right\}.\end{aligned} \qquad (11)$$

Substituting Eq. (9) into the neutron flux and neuron current continuity equations (7)-(8) we obtain 2G equations for the 1st expansion coefficients:

Flux continuity:

$$\begin{aligned}\sum_{g'=1}^{G}\left\{\delta_{gg'}+\frac{1}{15}\left(B^2_{k+1}\right)_{gg'}\right\}a^{k+1}_{g'x1}+\sum_{g'=1}^{G}\left\{\delta_{gg'}+\frac{1}{15}\left(B^2_k\right)_{gg'}\right\}a^k_{g'x1}=\\ \left\{\overline{\Phi}^{k+1}_g+a^{k+1}_{gx2}+a^{k+1}_{gx4}\right\}-\left\{\overline{\Phi}^k_g+a^k_{gx2}+a^k_{gx4}\right\}-\\ \frac{1}{15}\left\{\tilde{s}^{k+1}_{gx1}+\tilde{s}^k_{gx1}\right\}\end{aligned} \qquad (12)$$

Current continuity:

$$\begin{aligned}d^{k+1}_{gx}\left\{\sum_{g'=1}^{G}\left\{\delta_{gg'}+\frac{2}{5}\left(B^2_{k+1}\right)_{gg'}\right\}a^{k+1}_{g'x1}\right\}-\\ d^k_{gx}\left\{\sum_{g'=1}^{G}\left\{\delta_{gg'}+\frac{2}{5}\left(B^2_k\right)_{gg'}\right\}a^k_{g'x1}\right\}=\\ d^{k+1}_{gx}\left\{3a^{k+1}_{gx2}+10a^{k+1}_{gx4}-\frac{2}{5}\tilde{s}^{k+1}_{gx1}\right\}+\\ d^k_{gx}\left\{3a^k_{gx2}+10a^k_{gx4}+\frac{2}{5}\tilde{s}^k_{gx1}\right\}.\end{aligned} \qquad (13)$$

As a result, the initial system of 8G nodal equations is reduced to G equations (11) with respect to the 2nd expansion coefficients of the node k+1 and 2G equations (12)-(13) with respect to the 1st expansion coefficients of the node k+1 and k. The even expansion coefficients for

the node k are known from the solution of the previous two-node problem (k-1, k).

When the neutron flux expansion coefficients are computed, the surface-averaged nodal current $J^{k,\,NOD}_{g,\,x+}$ is calculated from the expression:

$$J^{k,\,NOD}_{g,x+} = -d^{k+1}_{gx}\left\{ a^{k+1}_{gx1} - 3\,a^{k+1}_{gx2} + 6\,a^{k+1}_{gx3} - 10\,a^{k+1}_{gx4} \right\}.$$

An implementation of the nodal coupling into the CMFD method is performed by the same way as in the NESTLE code[14].

It is worth to note, that Legendre polynomials $P_i(u)$ and the NEM basic functions[2] adjusted to the interval [-1,1] satisfy the following relation

$$\begin{pmatrix} P_0^{NEM}(u) \\ P_1^{NEM}(u) \\ P_2^{NEM}(u) \\ P_3^{NEM}(u) \\ P_4^{NEM}(u) \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1/2 & 0 & 0 & 0 \\ 0 & 0 & 1/2 & 0 & 0 \\ 0 & -1/20 & 0 & 1/20 & 0 \\ 0 & 0 & -1/70 & 0 & 1/70 \end{pmatrix} \times \begin{pmatrix} P_0(u) \\ P_1(u) \\ P_2(u) \\ P_3(u) \\ P_4(u) \end{pmatrix}$$

The NEM basic functions span the same subspace as Legendre polynomials. If the moment weighting procedure is used in NEM, both PNM and NEM become equivalent. In our opinion, the nodal equations of the PNM two-node kernel are simpler that that of NEM.

III. SEMI-ANALYTIC NODAL METHOD

In the semi-analytic nodal method (SANM)[13,15], the 3rd and 4th Legendre polynomials are replaced by hyperbolic sine and cosine. The sine and cosine are modified to preserve an orthogonality of the basic functions and normalized to unity at the right end of the interval [-1,1]. Resulting expressions for the 3rd and 4th basic functions are as follows:

$$P_3(u) = \frac{\mathrm{Sinh}(\alpha^k_{gx}u) - m^k_{gx1}(\sinh)P_1(u)}{\mathrm{Sinh}(\alpha^k_{gx}) - m^k_{gx1}(\sinh)};$$

$$P_4(u) = \frac{\mathrm{Cosh}(\alpha^k_{gx}u) - m^k_{gx0}(\cosh)P_0(u) - m^k_{gx2}(\cosh)P_2(u)}{\mathrm{Cosh}(\alpha^k_{gx}) - m^k_{gx0}(\cosh) - m^k_{gx2}(\cosh)}$$

where $u = 2x/\Delta x_k$, $\alpha^k_{gx} = \sqrt{\frac{\Sigma^k_{Rg}}{D^k_g}}\frac{\Delta x_k}{2}$;

$$m^k_{gx1}(\sinh) = \frac{1}{N_1}\int_{-1}^{1}\sinh(\alpha^k_{gx}u)P_1(u)du;$$

$$m^k_{gxi}(\cosh) = \frac{1}{N_i}\int_{-1}^{1}\cosh(\alpha^k_{gx}u)P_i(u)du, \quad \text{for i=0,2;}$$

$N_i = 2/(2i+1)$, for i=0,1,2.

The SANM equations are obtained in the same way as described in Sect. II. The 3rd expansion coefficient is also expressed in terms of the 1st coefficient as follows:

$$a^k_{gx3} = A^k_{gx}\left\{\sum_{g'=1}^{G}\left(B^2_k\right)_{gg'}\,a^k_{g'x1} + \tilde{s}^k_{gx1}\right\}, \qquad (14)$$

where $A^k_{gx} = \left(\frac{\sinh\left(\alpha^k_{gx}\right) - m^k_{gx1}(\sinh)}{\left(\alpha^k_{gx}\right)^2\, m^k_{gx1}(\sinh)}\right)$.

The 4th expansion coefficient is expressed in terms of the 2nd coefficient:

$$a^k_{gx4} = B^k_{gx}\left\{\sum_{g'=1}^{G}\left(B^2_k\right)_{gg'}\,a^k_{g'x2} + \tilde{s}^k_{gx2}\right\}, \qquad (15)$$

where $B^k_{gx} = \frac{\cosh(\alpha^k_{gx}) - m^k_{gx0}(\cosh) - m^k_{gx2}(\cosh)}{\left(\alpha^k_{gx}\right)^2\, m^k_{gx2}(\cosh)}$.

Substituting Eq. (15) into the neutron balance equation and Eq. (14) into the flux and current continuity equations, we again obtain G and 2G equations, which have to be solved for the two-node problem. They are as follows:

Neutron balance equation:

$$\sum_{g'=1}^{G}\left\{3\delta_{gg'} + E^k_{gx}\left(B^2_k\right)_{gg'}\right\}a^k_{g'x2} = \sum_{g'=1}^{G}\left(B^2_k\right)_{gg'}\overline{\Phi}^k_{g'} + \left\{\tilde{s}^k_{gx0} - E^k_{gx}\,\tilde{s}^k_{gx2}\right\}, \qquad (16)$$

where $E^k_{gx} = \left(\frac{m^k_{gx0}(\cosh)}{m^k_{gx2}(\cosh)} - \frac{3}{\left(\alpha^k_{gx}\right)^2}\right)$;

Flux continuity equation:

$$\sum_{g'=1}^{G}\left\{\delta_{gg'} + A^{k+1}_{gx}\left(B^2_{k+1}\right)_{gg'}\right\}a^{k+1}_{g'x1} + \sum_{g'=1}^{G}\left\{\delta_{gg'} + A^k_{gx}\left(B^2_k\right)_{gg'}\right\}a^k_{g'x1} = \left\{\overline{\Phi}^{k+1}_g + a^{k+1}_{gx2} + a^{k+1}_{gx4}\right\} - \left\{\overline{\Phi}^k_g + a^k_{gx2} + a^k_{gx4}\right\} -$$

$$A_{gx}^{k+1}\ \tilde{s}_{gx1}^{k+1} - A_{gx}^{k}\ \tilde{s}_{gx1}^{k}\ ; \qquad (17)$$

Current continuity equation:

$$d_{gx}^{k+1}\left\{\sum_{g'=1}^{G}\left\{\delta_{gg'}+F_{gx}^{k+1}\left(B_{k+1}^{2}\right)_{gg'}\right\}a_{g'x1}^{k+1}\right\}-$$
$$d_{gx}^{k}\left\{\sum_{g'=1}^{G}\left\{\delta_{gg'}+F_{gx}^{k}\left(B_{k}^{2}\right)_{gg'}\right\}a_{g'x1}^{k}\right\}=$$
$$d_{gx}^{k+1}\left\{3a_{gx2}^{k+1}+G_{gx}^{k+1}a_{gx4}^{k+1}-F_{gx}^{k+1}\tilde{s}_{gx1}^{k+1}\right\}+$$
$$d_{gx}^{k}\left\{3a_{gx2}^{k}+G_{gx}^{k}a_{gx4}^{k}+F_{gx}^{k}\tilde{s}_{gx1}^{k}\right\}, \qquad (18)$$

where $F_{gx}^{k}=\dfrac{\alpha_{gx}^{k}\cosh(\alpha_{gx}^{k})-m_{gx1}^{k}(\sinh)}{\left(\alpha_{gx}^{k}\right)^{2}m_{gx1}^{k}(\sinh)}$,

$$G_{gx}^{k}=\frac{\alpha_{gx}^{k}\ \mathrm{Sinh}(\alpha_{gx}^{k})-3\,m_{gx2}^{k}(\cosh)}{\mathrm{Cosh}(\alpha_{gx}^{k})-m_{gx0}^{k}(\cosh)-m_{gx2}^{k}(\cosh)}.$$

When the nodal equations are solved, the surface-averaged nodal current $J_{g,x+}^{k,NOD}$ is computed as

$$J_{g,x+}^{k,NOD}=-d_{gx}^{k+1}\left\{a_{gx1}^{k+1}-3a_{gx2}^{k+1}+H_{gx}^{k+1}a_{gx3}^{k+1}-G_{gx}^{k+1}a_{gx4}^{k+1}\right\},$$

where $H_{gx}^{k+1}=\left[\dfrac{\alpha_{gx}^{k+1}\cosh(\alpha_{gx}^{k+1})-m_{gx1}^{k+1}(\sinh)}{\sinh(\alpha_{gx}^{k+1})-m_{gx1}^{k+1}(\sinh)}\right].$

IV. ANALYTIC NODAL METHOD

An alternative approach to a solution of the two-node problem is presented in application to the analytic nodal method (ANM)[7]. The dimensionless transverse-integrated neutron diffusion equations (3) are written in the matrix form as

$$-\frac{d^{2}}{du^{2}}\vec{\Phi}^{k}(u)+\hat{B}_{k}^{2}\ \vec{\Phi}^{k}(u)=-\sum_{i=0}^{2}\vec{\tilde{s}}_{xi}^{k}\ P_{i}(u) \qquad (19)$$

where $\vec{\Phi}^{k}(u)=\mathrm{col}\{\Phi_{1}^{k}(u),\ldots,\Phi_{G}^{k}(u)\}$,

$\vec{\tilde{s}}_{xi}^{k}=\mathrm{col}\{\tilde{s}_{1xi}^{k},\ldots,\tilde{s}_{Gxi}^{k}\}$.

Imposing two constraints:

$$\frac{1}{2}\int_{-1}^{1}\vec{\Phi}^{k}(u)\,du=\vec{\overline{\Phi}}^{k},\ \text{and}\ \ \vec{\Phi}^{k}(+1)=\vec{\Phi}_{+}^{k}, \qquad (20)$$

where $\vec{\overline{\Phi}}^{k}(u)=\mathrm{col}\{\overline{\Phi}_{1}^{k}(u),\ldots,\overline{\Phi}_{G}^{k}(u)\}$,

we obtain a well-possessed boundary value problem.
The transverse-integrated current vector is defined as

$$\vec{J}_{x}^{k}(u)=-\hat{d}_{x}^{k}\frac{d\vec{\Phi}^{k}(u)}{du},$$

where $\hat{d}_{x}^{k}=\mathrm{diag}\left\{d_{1x}^{k},\ldots,d_{Gx}^{k}\right\}$.
Solving the Eq. (19) with the constraints (20 analytically using the symbolic manipulator Mathematica[16], the transverse-integrated current on the right surface of the node is expressed as follows

$$\vec{J}_{x}^{k}(+1)=-\hat{d}_{x}^{k}\left\{\hat{f}_{1}(\hat{B}_{k}^{2})\vec{\overline{\Phi}}_{k}+\hat{f}_{2}(\hat{B}_{k}^{2})\vec{\Phi}_{+}^{k}+\sum_{i=0}^{2}\hat{f}_{i+3}(\hat{B}_{k}^{2})\vec{\tilde{s}}_{xi}^{k}\right\}, \qquad (22)$$

where $\hat{f}_{1}(\hat{B}_{k}^{2})\div\hat{f}_{5}(\hat{B}_{k}^{2})$ are the matrix functions.

The matrix functions $\hat{f}_{1}(\hat{B}_{k}^{2})\div\hat{f}_{5}(\hat{B}_{k}^{2})$ are defined by the following scalar functions:

$$\vec{f}_{ANM}^{\,T}(x)=\{f_{1}(x),\ldots,f_{5}(x)\}=$$
$$\left\{x-\frac{1}{\Gamma^{2}},\ \ \frac{1}{\Gamma},\ \ 1-\frac{1-\Gamma}{\Gamma^{2}x},\ \ \frac{1-\Gamma}{\Gamma x}\ \ \frac{\Gamma(3+x)-3}{\Gamma^{2}x^{2}}\right\}, \qquad (23)$$

where $\Gamma=\dfrac{Tanh(\sqrt{x})}{\sqrt{x}}=\begin{cases}Tanh(\sqrt{|x|})/\sqrt{|x|}, & if\ x>0\\ Tan(\sqrt{|x|})/\sqrt{|x|}, & if\ x<0\end{cases}$.

There are several methods to compute functions of marices (see, for example, Ref. 17). D. Vogel applied the similarity transformation in the multigroup extension of ANM.[18] If the buckling matrix $\hat{B}_{k}^{2}$ has G linearly independent eigenvectors the matrix function can be computed using the Lagrange-Sylvester polynomial defined as follows[19-21]

$$\hat{f}(\hat{A})=\sum_{g=1}^{G}f(\lambda_{g})E_{g}(\hat{A},\lambda_{g}), \qquad (24)$$
$$E_{g}(\hat{A},\lambda_{g})=\prod_{j=1,\ j\neq g}^{G}\left(\hat{A}-\lambda_{j}\hat{I}\right)\Big/\left(\lambda_{g}-\lambda_{j}\right),$$

where $\hat{I}$ is an identity matrix; and $E_{g}(\hat{A},\lambda_{g})$ is a projector into the eigensubspace of $\hat{A}$ corresponding to λ_{g}.

The representation (24) gives a simple method to compute the matrix functions in the case of 2 neutron energy groups.

The only unknown in the expression (22) for the surface-averaged current $\vec{J}_x^k(+1)$ is the surface-averaged flux $\vec{\Phi}_+^k$. To find the surface-averaged flux, the flux and current continuity conditions are used. They are written as follows

$$\vec{\Phi}_+^k = \vec{\Phi}_-^{k+1}$$

and

$$-\hat{d}_x^k \left\{ \hat{f}_1(\hat{B}_k^2)\vec{\bar{\Phi}}_k + \hat{f}_2(\hat{B}_k^2)\vec{\Phi}_+^k + \sum_{i=0}^{2} \hat{f}_{i+3}(\hat{B}_k^2)\vec{\tilde{s}}_{xi}^k \right\} = -\hat{d}_x^{k+1} \times$$

$$\left\{ \hat{f}_1(\hat{B}_{k+1}^2)\vec{\bar{\Phi}}_{k+1} + \hat{f}_2(\hat{B}_{k+1}^2)\vec{\Phi}_-^{k+1} + \sum_{i=0}^{2} (-1)^i \hat{f}_{i+3}(\hat{B}_k^2)\vec{\tilde{s}}_{xi}^{k+1} \right\}$$

where $\vec{\Phi}_\pm^k = \vec{\Phi}^k(\pm 1)$.

The continuity equations are reduced to G equations with respect of the surface-averaged flux $\vec{\Phi}_+^k$. Then, the nodal surface-averaged current is computed using the expression (22).

It is worth to note that the matrix function approach can be applied for the other nodal methods. Without going into details we only remark, that redefining only 5 scalar functions as listed below, we easily transform ANM into PNM/NEM. Identity of the last approach to the conventional one has been proven for PNM numerically also.

$$\vec{f}_{PNM}^T(x) = \left\{ \frac{1}{5}\left(-66 + 2x + \frac{2875}{15+x} - \frac{2744}{21+2x}\right),\ 6 - \frac{75}{15+x},\right.$$
$$\left. \frac{525+x(15+x)}{(15+x)(10.5+x)},\ \frac{5}{15+x},\ \frac{21(5+2x)}{5(15+x)(21+2x)} \right\} \quad (25)$$

$$\vec{f}_{NEM}^T(x) = \left\{ \frac{1}{5}\left(-66 + 2x + \frac{2875}{15+x} - \frac{2744}{21+2x}\right),\ 6 - \frac{75}{15+x},\right.$$
$$\left. \frac{525+x(15+x)}{(15+x)(10.5+x)},\ \frac{2\cdot 5}{15+x},\ \frac{2\cdot 21(5+2x)}{5(15+x)(21+2x)} \right\}$$

Because $\vec{f}_{ANM}^T(x) \to \vec{f}_{PNM}^T(x)$, if $x \to 0$, the PNM functions (25) can be used to remove the singularities of the ANM functions (23) around 0. Such way was used in Ref. 11 for all eigenvalues. An another approach to solve this problem is an application of the Taylor or Pade expansion of the ANM matrix functions as performed in Ref. 21.

V. NUMERICAL RESULTS

The two-node kernels of the polynomial, semi-analytic and analytic nodal methods have been incorporated into computer code SKETCH-N[13,15]. Recalculation of the nodal coupling coefficients is performed after a fixed number of outer iterations. The outer iterations are accelerated by the Chebyshev polynomials. The Wielandt shift is applied to reduce a dominance ratio of the iteration matrix. The Block SSOR method is implemented as an inner iteration technique. The number of inner iterations per outer iteration is fixed and equal to 2 for the presented calculations. The following convergence criteria are applied

$$\frac{\left|k_{eff}^{max} - k_{eff}^{min}\right|}{2} \le \zeta_\lambda \ \text{ and } \ \frac{\max_{k,g}\left|\Phi_g^k(i) - \Phi_g^k(i-1)\right|}{\max_{k,g}\left|\Phi_g^k(i)\right|} \le \zeta_\varphi ,$$

where $k_{eff}^{max} = \max_k \left| \sum_{g=1}^{G} \nu\Sigma_{fg}^k \Phi_g^k(i) \right| \Big/ \left| \sum_{g=1}^{G} \nu\Sigma_{fg}^k \Phi_g^k(i-1) \right|$,

$k_{eff}^{min} = \min_k \left| \sum_{g=1}^{G} \nu\Sigma_{fg}^k \Phi_g^k(i) \right| \Big/ \left| \sum_{g=1}^{G} \nu\Sigma_{fg}^k \Phi_g^k(i-1) \right|$,

i is the outer iteration index, ζ_λ, ζ_φ are 10^{-5} for the presented results.

We have carried out calculations of the classical LWR benchmark problems in order to verify the code and to compare the nodal methods. The problems include the 2D & 3D IAEA PWR problems[22], 2D BIBLIS PWR checker-board-loaded core[23] and initial conditions of the neutron kinetics benchmarks: 3D LMW LWR problem[24], 2D and 3D BWR LRA problems[22]. The results of the calculations are presented in Table I. A comparison of the SKETCH-N results is performed against the reference solutions taken from literature, except for the IAEA-3D problem. For this problem, a reference solution is calculated by the SKETCH-N code using SANM on the fine spatial mesh 34x34x38 (5 cm in X-Y directions and 10 cm in Z direction). The NEM results compiled from different sources are added for a comparison. Small discrepancies in the PNM and NEM results are mostly due to different techniques of the quadratic leakage approximation. The presented results demonstrate that all nodal methods result in acceptable accuracy for the traditional LWR benchmarks. The maximum errors of assembly-averaged power density are less than 2.5% and the errors in eigenvalue are about 10-15 pcm. The accuracy of the semi-analytic and analytic methods is usually better than that of PNM, except for the BIBLIS-2D checker-board-loaded core. The Table I show also a number of nonlinear iterations and a total number of outer iterations. The nonlinear iteration procedure is very efficient, the number of the nodal coupling coefficient updates does not exceed 10 for all computed problems.

A next set of calculations is performed for the realistic PWR NEACRP benchmark[25]. Table II presents the results of Case A1 (Hot Zero Power). A reference solution is

generated using SANM on the fine spatial mesh 34x34x36. A reference critical boron concentration is equal to 561.25 ppm. The Table II contains also the NEM results of Ref. 11. The PNM and NEM results are practically identical, which agree with the theory. The both ANM and SANM give a significant improvement in accuracy of the calculations in comparison with the NEM/PNM for the both spatial meshes (1 and 4 nodes per assembly). SANM and ANM demonstrate the similar accuracy. This is well expected, because if the source term defined as

$$Q_g^k(u) = \frac{\chi_g}{k_{eff}} \sum_{g'=1}^{G} \nu\Sigma_{fg'}^k \Phi_{g'}^k(u) + \sum_{g' \neq g}^{G} \Sigma_{sg' \to g}^k \Phi_{g'}^k(u)$$

is presented by a second order polynomial, the SANM method provides an analytical solution of the transverse-integrated equation (3). The error of such approximation is significantly smaller than the error of the quadratic leakage approximation.

We also compared the CPU time of the two approaches: the traditional way of solving the two-node problem as it is described, for example, in the Sec. II for PNM and the matrix function theory approach applied in the ANM two-node kernel. The ANM two-node kernel requires practically the same computing time as that of PNM. To make the comparison complete, the PNM two-node kernel based on the matrix function theory is also implemented. Comparing the results of the two PNM kernels we conclude that the two-node kernels based on the matrix function theory results in 25 % saving of computing time.

VI. CONCLUSIONS

The two-node kernels of the polynomial, semi-analytic and analytic nodal methods have been developed for the solution of the neutron diffusion equations in X-Y-Z geometry. The polynomial and semi-analytic nodal methods are based on the orthogonal set of the basic functions. The two-node kernels of these methods are implemented using the traditional approach developed originally for NEM. Orthogonality of the basic functions results that the initial system of 8G nodal equations is reduced to G equations for the 2nd expansion coefficient of the node k+1 and 2G equations for the 1st expansion coefficients of the node k and k+1.

The two-node kernel of ANM is implemented using an alternative technique based on the matrix function theory. The transverse-integrated equations with two constraints are solved analytically. The analytic solution is used to express the surface-averaged current in terms of the node-averaged flux, surface-averaged flux and the transverse leakage expansion coefficients. Five matrix functions used in this expression are computed using the Lagrange-Sylvester interpolation polynomial. The surface-averaged flux is calculated from the flux and current continuity conditions. Numerically, the two-node problem is led to a computation of G eigenvalues of the buckling matrix, a calculation of the five matrix functions and a solution of G equations for the surface- averaged flux.

The two-node kernels of the nodal methods have been incorporated into the code SKETCH-N. LWR benchmark problem calculations have been performed in order to compare the nodal methods and numerical algorithms. The numerical results have demonstrated good accuracy of the all nodal methods for the classical LWR benchmarks. The maximum errors of assembly-averaged power density are less than 2.5 % and the errors in eigenvalue are about 10-15 pcm. An additional comparison has been done for the realistic PWR NEACRP benchmark problem. The analytic methods demonstrate a clear advantage in accuracy in the comparison with NEM/PNM. SANM show the same accuracy as ANM. The numerical results of the 2 group problems demonstrate an advantage of the matrix function approach in the comparison with the traditional way of the two-node problem solution. A saving in computing time is about 25%.

A development of the SANM two-node kernel based on the matrix function theory and the comparison of the methods for multi-group problems are subjects of ongoing efforts.

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Table I. Numerical Results of the Traditional LWR Benchmark Problems.

Problem, Mesh	Nodal Method	E_{max}/E_{av}, %	Position of E_{max} (X,Y)	K_{eff}	Reference k_{eff}	Δk_{eff}, pcm	No. Iterations: Nonlinear/Outers
IAEA-2D 9x9	NEM[26]	-2.05/-	(6,5)	1.0295	1.0296	-	-/32
	PNM	-1.8/0.7	(6,6)	1.02950	1.029585[23]	-8	9/28
	SANM	0.5/0.2	(6,5)	1.02956		-3	
	ANM	1.1/0.3	(5,7)	1.02962		+3	
BIBLIS-2D 9x9	NEM[27]	1.25/0.49	-	1.02528	1.02512	-	-
	PNM	-1.2/0.4	(1,8)	1.02521	1.025110[23]	+10	10/30
	SANM	1.8/0.5	(6,6)	1.02526		+15	
	ANM	2.2/0.7	(6,6)	1.02532		+21	
BWR-2D 11x11	NEM[28]	1.36/0.26	(1,1)	0.996329	0.99636[28]	-	-/22
	PNM	1.9/0.6	(1,1)	0.99626		-10	8/28
	SANM	0.5/0.2	(1,1)	0.99635		-1	
	ANM	0.2/0.1	(9,6)	0.99641		+5	
IAEA-3D 17x17	NEM[26]	-1.62/-	(6,6)	1.0290	1.0290	-	-/24
	PNM	-1.8/0.7	(6,6)	1.02899	1.029074*	-8	8/38
	SANM	0.4/0.2	(6,5)	1.02905		-2	
	ANM	1.1/0.3	(7,5)	1.02912		+4	
BWR-3D 12x12x14	NEM[28]	1.17/0.22	(1,1)	0.996361	0.996368[28]	-	7/21
	PNM	1.4/0.4	(1,1)	0.99633		-4	7/37
	SANM	0.4/0.1	(1,1)	0.99637		0	
	ANM	0.5/0.1	(8,8)	0.99643		+6	
LMW 6x6x10	NEM[26]	-1.2/-	(5,4)	0.99958	0.99966[26]	-	-/19
	PNM	-1.3/0.4	(5,4)	0.99958		-8	7/26
	SANM	0.4/0.1	(4,4)	0.99971		+5	
	ANM	0.5/0.2	(4,4)	0.99977		+11	

* Reference solution is computed by the SKETCH-N code with SANM on spatial mesh 34x34x36 (5 cm in X-Y directions and 10 cm in Z direction).

Table II. Numerical Results for NEACRP PWR REA Benchmark Problem (Case A1). Critical boron concentration is 561.25 ppm. A reference solution is calculated by SKETCH-N Code with SANM on the mesh 34x34x38, Reference k_{eff} is 1.000005.

Mesh	Nodal Method	E_{max}/E_{av}, %	Position of E_{max} (X,Y)	Δk_{eff}, pcm	No. of Iterations Nonlinear/Outers	CPU Time, s
9x9x18 (1 nodes / FA)	NEM[11]	9.07/-	-	83	-	-
	PNM	9.3/3.7	(6,5)	78	9/41	0.64/0.56*
	SANM	4.1/1.7	(6,5)	37		0.78
	ANM	4.4/1.9	(6,5)	38		0.66
17x17x36 (4 nodes/FA)	NEM[11]	1.96/-	-	14	-	-
	PNM	2.0/0.7	(6,5)	15	8/41	2.2/1.9*
	SANM	0.4/0.1	(6,5)	3		2.7
	ANM	0.4/0.1	(6,5)	3		2.2

* CPU time of the PNM based on the matrix function formulation.