ADJOINT EQUATION OF NODAL GREEN'S FUNCTION METHOD

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Abstract

Adjoint neutronics equation is frequently referenced in perturbation analysis and higher order harmonics calculation. For modern nodal method, there are two types of adjoint equations, that's is the physical adjoint equation and the mathematical adjoint equation. For each type of nodal equations, the definition and solution strategy for forward equation is different, so the definition and solution strategy for adjoint equation is also different. Taking Nodal Green's Function Method (NGFM) as an example, the physical adjoint equation and mathematical equation is totally different, the mathematical adjoint equation is required for physical analysis, and the solution of the mathematical adjoint equation requires special strategy. The numerical result about the solution of the mathematical adjoint equation, the applications of the mathematical adjoint into the perturbation analysis and the higher order harmonics calculation proves the importance and success of definition and solution of the mathematical adjoint equation of NGFM.

Keyword: Physical adjoint equation, Mathematical adjoint equations, Nodal **G**reen's function method, Perturbation theory, Higher order harmonics

1 Purpose of adjoint equation

Normally neutronics equation referenced in ordinary reactor physics calculation is named as forward equation, which described the behavior of neutron distribution. Along the application of forward equation, the respective adjoint neutronics equation, which usually describes the neutron importance distribution, is also widely used in many reactor physics applications, especially for perturbation analysis [1], reactor kinetics[2], higher order harmonics, flux mapping[3], and etc. Because the forward neutronics equations have the types of transport equation, diffusion equation, or the space-continuous analytical equation, finite difference equation, finite element equation and nodal equation, the adjoint equations will also have same kind of classification. This paper will focus on the adjoint equation of modern nodal equation, which is difficult to solve and is seldom adopted. This paper takes Nodal Green's Function Method (NGFM) [4] as an example to illustrate the definition, solution and application of the adjoint equation under nodal method.

The definition, solution, and application of the adjoint equation of transport equation, finite difference diffusion equation is well studied. For nodal diffusion equation, it is pointed out early that there exists physical adjoint and mathematical adjoint equation, and the solution of mathematical adjoint equation is somewhat difficult[5]. Because each type of nodal equation has different form of definition, coefficient matrix and solution strategy, the form

and solution of adjoint equation will also different for each type of nodal equation. From the literature, mainly the mathematical adjoint equation of nodal expansion method (NEM) [6] or higher order NEM [7] is referenced, or the mathematical nodal adjoint equation is approximated by coarse-mesh finite difference equation, the adjoint equation of NGFM is never discussed. And the application of adjoint equation to the higher order harmonics is seldom mentioned for any type of nodal equation. So this paper will deal with the definition, the solution and usage of the adjoint equation of NGFM.

This paper will firstly present the definition and formula of adjoint equation under NGFM, then present the details of the physical adjoint equation and mathematical adjoint equation. After that, the way to adopt the mathematical adjoint equation into the perturbation and higher order harmonics calculation is discussed. In the end, the numerical result about the calculation and application of mathematical adjoint equation under NGFM is presented, followed by final conclusion.

2 Type of adjoint equation under NGFM

2.1 Forward equation for transport, diffusion and finite difference equation

The neutron transport equation is the origin of all other type of neutronics equations. The (*k*-eigenvalue) stationary transport equation can be written as[1]:

$$\Omega \cdot \nabla \Phi(r,E,\Omega) + \Sigma_t(r,E)\Phi(r,E,\Omega) = \frac{1}{k}\int dE' \int d\Omega' [\, f(E)\nu\Sigma_f(r,E') + \Sigma_s(r,E' \to E, \Omega' \to \Omega)]\Phi(r,\Omega',E') \tag{2.1}$$

The diffusion approximation to the transport equation, the multi-group diffusion equation in continuous space, is the foundation of all numerical solvable diffusion equations, including the finite difference equation and nodal equation, has the form in each energy group *g*[8]:

$$-D_g \nabla^2 \phi_g + \Sigma_g^r \phi_g - \sum_{g' \neq g} \Sigma_{g' \to g}^s \phi_{g'} = \lambda \chi_g \sum_{g'} (\nu\Sigma_f)_{g'} \phi_{g'} \tag{2.2}$$

here the items in Eq.2.2 denote the neutron leakage, removal, scattering, and fission product repectively, and $\lambda = 1/k$ is the eigenvalue, ϕ_g denotes the neutron flux, ∇^2 is the Laplace operator which is the main problem for numerical solution and can be written as $\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$ under Cartesian coordinate, others are standard symbols[8].

For the finite difference approximation of the diffusion equation, the leakage due to diffusion operator is approximated in each fine mesh by 1-order difference. For example, under 2-dimensional X-Y coordinate, the neutron leakage from mesh (*j*,*i*) due to diffusion term can be written as, after all meshes is numbered as *j*=1,2,…,J in X-coordinate, and *i*=1,2,…,I in Y-coordinate[8]:

$$Mesh\ \ Leakage = \phi_{j,i}(C^x_{j,i,j-1} + C^x_{j+1,i,j} + C^y_{j,i,i-1} + C^y_{j,i+1,i})$$
$$-\phi_{j-1,i}C^x_{j,i,j-1} - \phi_{j+1,i}C^x_{j+1,i,j} - \phi_{j,i-1}C^y_{j,i,i-1} - \phi_{j,i+1}C^y_{j,i+1,i} \quad (2.3)$$

here $\phi_{j,i}$ is the flux in mesh (j,i)， and coefficients

$$C^x_{j,i,j-1} = C^x_{j-1,i,j} = \frac{2\Delta y_i}{\Delta x_j / D_{j,i} + \Delta x_{j-1} / D_{j-1,i}}$$

$$C^y_{j,i,i-1} = C^y_{j,i-1,i} = \frac{2\Delta x_j}{\Delta y_i / D_{j,i} + \Delta y_{i-1} / D_{j,i-1}}$$

And final finite-difference diffusion matrix equation can be written as, after flux in all meshes is represented by a vector ϕ :

$$M\phi + S\phi = \lambda\chi F^T\phi \equiv \lambda B\phi \quad (2.4)$$

Here coefficient matrix *M* corresponding to diffusion leakage (including removal term) is a symmetrical 3-,5-,7-lines diagonal matrix for 1-,2-,3-dimensional Cartesian coordinate respectively. And scattering coefficient matrix ***S***, fission spectrum matrix χ and fission matrix F is simple and well known[8].

The forward equation under modern nodal method can be shown in section 2.3, taking Nodal Green's Function Method(NGFM) as an example.

2.2 Adjoint equations for transport, diffusion, finite difference equation

Corresponding to each type of forward equations mentioned above, there are at least one kind of adjoint equation. For example, the adjoint stationary transport equation corresponding to Eq.2.1 can be written as [1]:

$$\Omega\cdot\nabla\Phi^*(r,E,\Omega) - \Sigma_t(r,E)\Phi^*(r,E,\Omega) = \\ -\int dE'\int d\Omega'[\nu\Sigma_f(r,E)f(E') + \Sigma_s(r,E\to E',\Omega\to\Omega')]\Phi^*(r,\Omega',E') \quad (2.5)$$

The adjoint multi-group diffusion equation corresponding to Eq.2.2 can be written as:

$$-D_g\nabla^2\phi^*_g + \Sigma^r_g\phi^*_g - \sum_{g'\neq g}\Sigma^s_{g\to g'}\phi^*_{g'} = \lambda^*(\nu\Sigma_f)_g\sum_{g'}\chi_{g'}\phi_{g'} \quad (2.6)$$

The adjoint finite-difference diffusion equation corresponding to Eq.2.4 can be obtained by directly transposing all coefficient matrices in Eq.2.4, which can be named as mathematical adjoint equation, as:

$$\mathbf{M}\phi^* + S^T\phi^* = \lambda^* F\chi^T\phi^* \equiv \lambda^*\mathbf{B}^T\phi^* \quad (2.7)$$

Another matrix equation can be deduced from Eq.2.6 by the finite difference discretization method, which can be named as physical adjoint equation. In the case of finite difference diffusion method, the mathematical adjoint equation is identical to the physical adjoint equation, because coefficient matrix M is symmetrical. This is the reason why

mathematical adjoint equation and physical adjoint equation is not distinguished for the finite difference diffusion equation.

But this is not always true. When discontinuity factor (equivalent theory) is applied to finite difference diffusion equation, its mathematical adjoint equation is not identical to the physical adjoint equation. Discontinuity factor theory assumes the flux in adjacent surfaces of two meshes is not same, as $\phi^{x+}_{j-1,i} * g^{x+}_{j-1,i} = \phi^{x-}_{j,i}$, here $\phi^{x+}_{j-1,i}$ denotes the flux in *x*-directional right surface of mesh (*j*-1,*i*), and $\phi^{x-}_{j,i}$ denotes the *x*-directional left surface of mesh (*j*,*i*), $g^{x+}_{j-1,i} = \phi^{x-}_{j,i} \big/ \phi^{x+}_{j-1,i}$ denotes the discontinuity factor in this interface. Then the leakage for mesh (*j*,*i*) can be represented as:

$$\begin{aligned} Mesh\ \ Leakage &= \phi_{j,i}(\tilde{C}^{x}_{j,i,j-1} + g^{x}_{j,i}\tilde{C}^{x}_{j+1,i,j} + \tilde{C}^{y}_{j,i,i-1} + g^{y}_{j,i}\tilde{C}^{y}_{j,i+1,i}) \\ &- \phi_{j-1,i} g^{x}_{j-1,i}\tilde{C}^{x}_{j,i,j-1} - \phi_{j+1,i}\tilde{C}^{x}_{j+1,i,j} - \phi_{j,i-1} g^{y}_{j,i-1}\tilde{C}^{y}_{j,i,i-1} - \phi_{j,i+1}\tilde{C}^{y}_{j,i+1,i} \end{aligned} \qquad (2.8)$$

Here $\tilde{C}^{x}_{j,i,j-1} = \tilde{C}^{x}_{j-1,i,j} = \dfrac{2\Delta y_i}{\Delta x_j / D_{j,i} + g^{x}_{j-1,i}\Delta x_{j-1} / D_{j-1,i}}$

$$\tilde{C}^{y}_{j,i,i-1} = \tilde{C}^{y}_{j,i-1,i} = \frac{2\Delta x_j}{\Delta y_i / D_{j,i} + g^{y}_{j,i-1}\Delta y_{i-1} / D_{j,i-1}}$$

So the final matrix equation for forward finite difference diffusion method can be written as:

$$\tilde{M}\phi + S\phi = \lambda\chi F^T\phi \equiv \lambda B\phi \qquad (2.9)$$

Eq.2.9 has the same form as Eq.2.4, except that coefficient matrix $\tilde{M}$ is an asymmetrical 3-, 5-, 7-lines diagonal matrix. The mathematical adjoint equation is defined as the transpose matrix of Eq.2.9, can be written as:

$$\tilde{M}^T\phi^* + S^T\phi^* = \frac{1}{k^*} F\chi^T\phi^* \equiv \frac{1}{k^*} B^T\phi^* \qquad (2.10)$$

And the physical adjoint equation is deduced from adjoint continuous diffusion equation Eq.2.6 by finite difference method corrected by same discontinuity factor as that for forward equation, and can be written as:

$$\tilde{M}\tilde{\phi}^* + S^T\tilde{\phi}^* = \tilde{\lambda} F\chi^T\tilde{\phi}^* \equiv \tilde{\lambda} B^T\tilde{\phi}^* \qquad (2.11)$$

Here physical adjoint equation Eq.2.11 will be different from the mathematical adjoint equation Eq.2.10, because $\tilde{M}$, the coefficient matrix corresponding to the diffusion operator, is asymmetrical, even with same set of discontinuity factors. The same phenomenon occurs for modern nodal method.

2.3 Forward equation for NGFM

The modern nodal method transfer the 2- or 3-dimensional diffusion equation Eq.2.2 into coupled 1-dimensional equation with the aid of transverse integration[4]. For Nodal Green's Function Method (NGFM), the variables in each direction u(u=x,y,z) and node k include: the moment of partial flux $\phi_{gu}^{k}=(\phi_{gu1}^{k},\phi_{gu2}^{k},\phi_{gu3}^{k})^{T}$, the out-going current in left- and right-surface $J_{gu}^{out,k}=(J_{gu-}^{out,k},J_{gu+}^{out,k})^{T}$ and in-going current $J_{gu}^{in,k}=(J_{gu-}^{in,k},J_{gu+}^{in,k})^{T}$, and some intermediate variables such as the moments of source $Q_{gu}^{k}=(Q_{gu1}^{k},Q_{gu2}^{k},Q_{gu3}^{k})^{T}$, the moment of transverse leakage $L_{gu}^{k}=(L_{gu1}^{k},L_{gu2}^{k},L_{gu3}^{k})^{T}$.

The NGFM calculates the partial flux moment in each group g, each node k and each direction u by:

$$\phi_{gu}^{k}=G_{gu}^{k}(Q_{gu}^{k}-L_{gu}^{k})+D_{gu}^{k}J_{gu}^{in,k} \tag{2.12}$$

But the nodal average flux $\overline{\phi}_{g}^{k}$ must be calculated by neutron balance equation:

$$\overline{\phi}_{g}^{k}=\frac{1}{\Sigma_{g}^{r,k}}\overline{Q}_{g}^{k}-\sum_{v}\frac{1}{2a_{v}^{k}\Sigma_{g}^{r,k}}[J_{gv-}^{out,k}-J_{gv-}^{in,k}+J_{gv+}^{out,k}-J_{gv+}^{in,k}] \tag{2.13}$$

Combing Eq.2.12 and Eq.2.13, ϕ_{gu1}^{k}, the first order moment of the partial flux in all directions, should be equal to nodal average flux $\overline{\phi}_{g}^{k}$, that's to say, the ϕ_{gu1}^{k} in Eq.2.12 is replaced by $\overline{\phi}_{g}^{k}$ in Eq.2.13, so the final partial flux moment can be rewritten as, by combining as $\phi=\underset{g}{col}(\underset{k}{col}(\underset{u}{col}(\phi_{gu}^{k})))$, matrix $G=\underset{g}{diag}(\underset{k}{diag}(G_{g}^{k}))$:

$$\phi=G\,Q-A\,L+D\,J^{in}+C\,(J^{out}-J^{in}) \tag{2.14}$$

The out-going current can be calculated by: $J^{out}=P\,(Q-L)+R\,J^{in}$ (2.15)

The neutron source is calculated as: $Q=\lambda\chi F^{T}\phi+S\phi$ (2.16)

The continuity condition for current is that the the in-going current in one surface equals to the out-going current in adjacent surface, and this relationship can be written as a matrix equation[6]: $J^{in}=\prod J^{out}$ (2.17)

The transverse leakage can be calculated from the net current in adjacent nodes by 2-order linear approximation: $L=H\,(J^{out}-J^{in})$ (2.18)

So Eq.2.14, 2.15, 2.16, 2.17, 2.18 composite the complete NFGM equation, and can be written as one super matrix equation as:

$$\begin{bmatrix} I & -C & C-D & A & -G \\ 0 & I & -R & P & -P \\ 0 & -\Pi & I & 0 & 0 \\ 0 & -H & H & I & 0 \\ -S & 0 & 0 & 0 & I \end{bmatrix} \begin{pmatrix} \phi \\ J^{out} \\ J^{in} \\ L \\ Q \end{pmatrix} = \lambda \begin{bmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ \chi F^T & 0 & 0 & 0 & 0 \end{bmatrix} \begin{pmatrix} \phi \\ J^{out} \\ J^{in} \\ L \\ Q \end{pmatrix} \tag{2.19}$$

$$\equiv M\psi_n = \lambda B\psi_n$$

Of course Eq.2.19 can be collapsed into the equation explicitly about the flux itself as Eq.2.20, but Eq.2.20 is difficult to be solved:

$$\{\{G + [(CH^{-1} - A)H(I - \Pi) + D\Pi][I + PH - (PH + R)\Pi]^{-1}P\}^{-1} - S\}\phi \equiv E\phi = \lambda\chi F^T\phi \tag{2.20}$$

2.4 Adjoint equation of NGFM

For modern nodal method, for example NGFM, there are two kinds of adjoint equation. One is the physical adjoint equation, which is the result of nodal discretization on the adjoint diffusion equation Eq.2.6, so the final matrix equation will have same structure, same coefficient matrix as forward equation Eq.2.19, except the matrix for scattering and fission is transposed, so equation can be written as:

$$\begin{bmatrix} I & -C & C-D & A & -G \\ 0 & I & -R & P & -P \\ 0 & -\Pi & I & 0 & 0 \\ 0 & -H & H & I & 0 \\ -S^T & 0 & 0 & 0 & I \end{bmatrix} \begin{pmatrix} \tilde{\phi} \\ \tilde{J}^{out} \\ \tilde{J}^{in} \\ \tilde{L} \\ \tilde{Q} \end{pmatrix} = \tilde{\lambda} \begin{bmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ F\chi^T & 0 & 0 & 0 & 0 \end{bmatrix} \begin{pmatrix} \tilde{\phi} \\ \tilde{J}^{out} \\ \tilde{J}^{in} \\ \tilde{L} \\ \tilde{Q} \end{pmatrix} \tag{2.21}$$

$$\equiv \tilde{M}\tilde{\psi} = \tilde{\lambda}\tilde{B}\tilde{\psi}$$

Eq.2.21 is the nodal approximation of adjoint Eq.2.6, represents the neutron importance distribution. As the fine distribution of the neutron flux can be reconstructed from the solution of forward nodal equation Eq.2.19 [9], the fine distribution of neutron importance can also be reconstructed from the solution of physical adjoint equation Eq.2.21 by same techniques. This is the main purpose of the physical adjoint equation of the nodal methods.

At the same time, the mathematical adjoint equation corresponding to Eq.2.19, which is directly matrix transpose of Eq.2.19 can be obtained mathematically as:

$$\begin{bmatrix} I & 0 & 0 & 0 & -S^T \\ -C^T & I & -\Pi^T & -H^T & 0 \\ C^T - D^T & -R^T & I & H^T & 0 \\ A^T & P^T & 0 & I & 0 \\ -G^T & -P^T & 0 & 0 & I \end{bmatrix} \begin{pmatrix} \phi^* \\ J^{out,*} \\ J^{in,*} \\ L^* \\ Q^* \end{pmatrix} = \lambda^* \begin{bmatrix} 0 & 0 & 0 & 0 & F\chi^T \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix} \begin{pmatrix} \phi^* \\ J^{out,*} \\ J^{in,*} \\ L^* \\ Q^* \end{pmatrix} \quad (2.22)$$

$$\equiv M^T \psi^* = \lambda^* B^T \psi^*$$

This mathematical adjoint equation has no explicit physical meaning, and obviously is different from the physical adjoint equation Eq.2.21, although some authors suggest that they can transform the solution of physical adjoint equation into the solution of mathematical adjoint for certain nodal methods[5], because the mathematical adjoint equation is difficult to be solved and physical adjoint equation is easy to be solved. But it is mathematical adjoint equation that is required for perturbation analysis and higher order harmonics calculation as discussed in section 5, because the nodal matrix itself is directly dealt with.

Of course, another mathematical adjoint equation can also be defined by transposing the Eq.2.20. This type of definition needs less variables, just ϕ, and is equivalent to Eq.2.22 which contains more variables, but the coefficient matrix E and associated E^T in Eq.2.20 is more complex and difficult to be solved numerically. So afterwards discussion will deal with Eq.2.22 directly.

2.5 Solution of the physical adjoint equation under NGFM

Because the physical adjoint equation Eq.2.21 has similar structure as the forward NGFM equation, it can be solved by same strategy adopted by forward NGFM equation, that is, the power iteration strategy which contains the outer iteration and inner iteration. The inner iteration calculates neutron source, transverse leakage, out-going current, in-going current, and flux moment, nodal average flux sequentially in each group in each outer iteration, then outer iteration calculates the fission source from the flux of all groups, and estimate the eigenvalue $\tilde{\lambda}$ in outer iteration *n* by:

$$\tilde{\lambda}^{(n+1)} = \tilde{\lambda}^{(n)} \left\| \tilde{\psi}^{(n)} \right\| \Big/ \left\| \tilde{\psi}^{(n+1)} \right\| = \tilde{\lambda}^{(n)} \left\| \tilde{Q}^{(n)} \right\| \Big/ \left\| \tilde{Q}^{(n+1)} \right\|$$

The only difference between the solution of physical adjoint equation Eq.2.21 and forward equation Eq.2.19 is that the neutron source in each group using following formula instead of Eq.2.16:

$$\tilde{Q} = (\tilde{\lambda} F\chi^T + S^T)\tilde{\phi}$$

Because the solution strategy is same, the solution efficiency of physical adjoint equation can be supposed to be the same as that for the forward equation, and even better if the convergent forward solution act as the initial iteration value for physical adjoint equation, as shown in section 5.2.

3 Solution of mathematical adjoint equation

The forward NGFM equation Eq.2.19 is a very complex matrix equation, the solution of this equation requires special iteration strategy. As the matrix and solution strategy is unique for each type of nodal method, the matrix and solution strategy for the mathematical adjoint equation of each type of nodal method will be unique too. The mathematical adjoint equation Eq.2.22 is more complex, direct and accurate solution of the mathematical adjoint equation of NGFM is never seen in literature, although the solution of nodal expansion method was reported early[6,7]. Following solution strategy for the mathematical adjoint equation Eq.2.22 is proven to be success after implemented into program. The solution also includes the inner iteration and outer iteration process. The inner iteration is carried out in following order in each group in each outer iteration:

1) Update ϕ^*: $$\phi^{*,(i+1)} = S^T Q^{*,(i+1)} + \lambda^* F \chi^T Q^{*,(i)} \tag{3.1}$$

2) update L^*: $$L^{*,(i+1)} = -A^T \phi^{*,(i+1)} - P^T J^{out,*,(i)} \tag{3.2}$$

3) Update $J^{in,*}$ and $J^{out,*}$ as:

$$(I - R^T \Pi^T) J^{in,*,(i+1)} = (R^T C^T + D^T - C^T)\phi^{*,(i+1)} + (R^T - I) H^T L^{*,(i+1)} \tag{3.3}$$

$$J^{out,*,(i+1)} = \Pi^T J^{in,*,(i+1)} + C^T \phi^{*,(i+1)} + H^T L^{*,(i+1)} \tag{3.4}$$

4) Update Q^*: $$Q^{*,(i+1)} = G^T \phi^{*,(i+1)} + P^T J^{out,*,(i+1)} \tag{3.5}$$

And the outer iteration is also illustrated in Eq.3.1, which update fission source from the value $Q^{*,(i)}$ of all group of last outer iteration, but the scattering term depends on the value $Q^{*,(i+1)}$ of same outer iteration.

The outer iteration procedure is repeated till Q^* is convergent. Here eigenvalue λ^* can directly use the eigenvalue obtained in forward equation Eq.2.20, but can also be calculated explicitly through equation Eq.3.6. The value calculated from Eq.3.6 must be equal to the eigenvalue of Eq.2.20, and this fact can act as the criteria for the correctness of solution of the mathematical adjoint equation.

$$\lambda^{*,(i+1)} = \lambda^{*,(i)} \left\| Q^{*,(i)} \right\| \Big/ \left\| Q^{*,(i+1)} \right\| \tag{3.6}$$

The most difficult part of the solution of the mathematical adjoint equation Eq.2.22 is the solution of Eq.3.3 and Eq.3.4, especially the term $H^T L^{*,(i+1)}$, because NGFM adopts 2-order linear approximation of transverse leakage. And the adjoint out-gonging current $J^{out,*}$ and

in-going current $J^{in,*}$ can not be simply mapped as Eq.2.17 in forward equation.

4 The usage of the adjoint equation under NGFM

4.1 Perturbation Analysis

The most important purpose of adjoint equation is for perturbation analysis, which effectively estimates some lumped values caused by some cross section changes. For example, if forward eigenvalue equation of the un-disturbed core (including Eq.2.1, Eq.2.2, Eq.2.4, Eq.2.9, Eq.2.19, Eq.2.20) is uniformed as:

$$M\psi = \lambda B\psi \tag{4.1}$$

After some cross section change, the eigenvalue equation for the disturbed core can be represented as:

$$M'\psi' = \lambda' B'\psi' \tag{4.2}$$

or: $(M+\Delta M)(\psi+\Delta\psi) = (\lambda+\Delta\lambda)(B+\Delta B)(\psi+\Delta\psi)$

so the change of eigenvalue can be approximated by variational method [1,2,5]:

$$\Delta\lambda \approx \frac{<\psi^*,(\Delta M - \lambda\Delta B)\psi>}{<\psi^*,(B+\Delta B)\psi>} \tag{4.3}$$

Here, ψ^* should be the solution of the mathematical adjoint equation, not the physical adjoint equation. In the case of Nodal Green's Function Method, the terms in Eq.4.3 can be calculated as, and the coefficient matrix can be referenced from Eq.2.19:

$$\begin{aligned}<\psi^*,(\Delta M - \lambda\Delta B)\psi> =& <\phi^*,-\Delta C(J^{out}-J^{in}) - \Delta D\cdot J^{in} \\ &+ \Delta A\cdot L - \Delta G\cdot Q> + <J^{out,*},-\Delta R\cdot J^{in} - \Delta P(Q-L)> \\ &+ <Q^*,-(\Delta S+\lambda\Delta F)\phi>\end{aligned} \tag{4.4}$$

$$<\psi^*,(B+\Delta B)\psi> = <Q^*,(F+\Delta F)\phi> \tag{4.5}$$

4.2 Higher order harmonics

Higher order harmonics is the solutions of Eq.4.1 (it can represent Eq.2.1, Eq.2.2, Eq.2.4, Eq.2.9, Eq.2.19 and Eq.2.20) whose eigenvalues k_n is less than the largest one, which can be named as fundamental harmonics and is the only solution that the ordinary reactor physics calculation dealt with.

The method to calculate higher order harmonics depend upon the power iteration method modified by source correction[10]. That means, after the fundamental harmonics ψ_1 is

calculated by ordinary way(power iteration method), and the fundamental mathematical adjoint harmonics ψ_1^* is calculated, the similar power iteration process on forward equation Eq.4.1 carried out again, but in each outer iteration, the iterated variables $\psi_n^{(i)}$ must be corrected in each outer iteration *i* so that no component of lower order harmonics ψ_m exist as:

$$\hat{\psi}_n^{(i)} = \psi_n^{(i)} - \sum_{m=1}^{n-1} \frac{< B^T \psi_m^*, \psi_n^{(i)} >}{< B^T \psi_m^*, \psi_m >} \psi_m$$

This correction can be done if the mathematical adjoint equation ψ_m^* is adopted because

$$< \psi_m^*, B\psi_n > = < B^T \psi_m^*, \psi_n > = C\delta_{nm}$$

In the case of NGFM, only $F^T \hat{\phi}_n^{(i)}$ is required to start the inner iteration, other variables depend on this value, so the source correction formula can be simplified as:

$$F^T \hat{\phi}_n^{(i)} = F^T \phi_n^{(i)} - \sum_{m=1}^{n-1} \frac{< \chi^T Q_m^*, F^T \phi_n^{(i)} >}{< \chi^T Q_m^*, F^T \phi_m >} F^T \phi_m$$

Of course, the higher order adjoint harmonics must be calculated after each order of forward harmonics is calculated, and the adjoint source must also be corrected by a similar way[10].

5 Numerical results

In order to verify the necessity of the mathematical adjoint equation, and the correctness of the solution of the mathematical adjoint, some numerical verification on the perturbation calculation and higher order harmonics calculation is presented.

5.1 Perturbation on NGFM

Taking the result of perturbation calculation in ref.7 as the reference, perturbation calculation on same perturbation is done by NGFM method, that is, to disturb the absorption cross section in on one assembly of the IAEA 2D benchmark core [7]. The result is listed in Table.1. It can be seen that the eigenvalue $k' = 1/(\lambda + \Delta\lambda)$ estimated from perturbation analysis is consistent with the value direct solved for the disturbed core, and is consistence with the result in Ref.7, or better for larger perturbation.

Table 1 Perturbation analysis on eigenvalue k

Σ_{a2}	$\Sigma_{a2}+\Delta\Sigma_{a2}$	NGFM				Higher order NEM[7]		
		k' from Eq.4.2	k' from Eq.4.3	Deviation (%)	k' alsely by hysical djoint	Direct k'	k' from perturbation	Divation(%)
0.130	0.1300	1.02960	---	---	---	1.02953	---	---
	0.1255	1.02987	1.02983	0.004	1.02970	1.02980	1.02979	0.001
	0.1210	1.03019	1.03008	0.011	1.02981	1.03011	1.03005	0.006
	0.1165	1.03055	1.03036	0.018	1.02994	1.03047	1.03032	0.015
	0.1075	1.03147	1.03097	0.048	1.03021	1.03139	1.03084	0.053
	0.0985	1.03279	1.03170	0.106	1.03054	1.03271	1.03136	0.131
	0.0940	1.03369	1.03212	0.152	1.03072	1.03361	1.03162	0.193
	0.0895	1.03483	1.03258	0.217	1.03093	1.03475	1.03188	0.277
	0.0850	1.03633	1.03308	0.314	1.03115	1.03624	1.03214	0.400

5.2 Difference between physical adjoint equation and mathematical adjoint equation

Of course, the matrix for physical adjoint equation and mathematical adjoint equation is difference, and the eigenvalue of mathematical adjoint is strictly equal to the eigenvalue of forward equation, and the eigenvalue of physical adjoint equation, which is the nodal approximation of continuous adjoint diffusion equation Eq.2.6, may be slightly different from the eigenvalue of forward equation, although the eigenvalue of Eq.2.6 is strictly equal to eigenvalue of Eq.2.2. For example, for IAEA 2D benchmark problem, the eigenvalue of physical adjoint NGFM equation is 1.02960393, versus the forward eigenvalue and mathematical eigenvalue 1.02959527. For IAEA 3D benchmark problem, the forward and mathematical adjoint eigenvalue is 1.029087, and the physical adjoint eigenvalue is 1.029088.

Another aspect for the difference between physical and mathematical adjoint can be illustrated by the perturbation analysis. Eq.4.2 present the correct and standard formula for the perturbation, and an incorrect implementation which use physical adjoint equation can be compared. That is to replace the mathematical term $\psi^* = (\phi^*, J^{out,*}, J^{in,*}, L^*, Q^*)^T$ used in Eq.4.3 and Eq.4.4 by the physical adjoint equation $\tilde{\psi}^* = (\tilde{\phi}^*, \tilde{J}^{out,*}, \tilde{J}^{in,*}, \tilde{L}^*, \tilde{Q}^*)^T$ as $\tilde{\phi}^* \leftrightarrow Q^*, \tilde{J}^{out,*} \leftrightarrow J^{in,*}, \tilde{J}^{in,*} \leftrightarrow J^{out,*}, \tilde{L}^* \leftrightarrow L^*, \tilde{Q}^* \leftrightarrow \phi^*$. The perturbation result is listed in 6th column of Table.1, it can be seen that the result is far worse than the result by mathematical adjoint equation.

By the way, from the calculation of physical adjoint equation, it can be proven that for same precision, the iteration number and calculation time for forward equation and physical adjoint equation is almost same, taking IAEA 2D benchmark problem as an example, the iteration number and calculation time is about 148 and 0.022 min for forward equation, and 94 and 0.013 min for physical adjoint equation respectively.

5.3 Higher order harmonics of NGFM

Another purpose of mathematical adjoint equation is used in calculation of higher order harmonics. We can list the result from ref.4 in Table 2. This result can prove the correctness of the mathematical adjoint, and can provide some idea about the efficiency of the mathematical adjoint, even for higher order harmonics, that is, the iteration number and calculation time is almost same for the calculation of the forward equation and mathematical adjoint equation for each order.

Table 2 λ-modes of IAEA 2D core by NGFM and by finite difference method

Order	By NGFM					By finite-difference method				
	k_n	N_f +	T_f +	N_a +	T_a +	k_n	N_f +	T_f +	N_a +	T_a +
1	1.02960	122	0.2	129	0.2	1.02943	232	3.4	185	2.2
2	1.00254	341	0.5	328	0.5	1.00173	1363	27.5	999	14.2
3	0.99161	154	0.2	108	0.2	0.99092	209	4.8	147	2.7
4	0.93920	215	0.3	160	0.3	0.93793	451	11.5	327	6.8
5	0.91399	507	1.0	712	1.2	0.91351	1413	38.5	1206	24.4
6	0.90179	114	0.2	79	0.2	0.90046	968	31.5	602	15.8
7	0.89082	469	1.1	1000	1.8	0.88907	439	15.8	383	15.8
8	0.82769	1000	1.8	1000	2.0	0.82547	1990	67.5	1990	58.0
9	0.82566	540	1.0	282	0.6	0.82454	829	32.6	706	24.7
10	0.81736	239	0.5	173	0.4	0.81373	514	21.2	286	10.5
11	0.79847	168	0.3	174	0.4	0.79584	228	10.1	222	8.8
12	0.76077	661	1.2	496	1.1	0.75829	919	47.9	924	38.3
13	0.75514	452	1.0	419	0.9	0.75119	423	20.5	354	16.0
14	0.72927	255	0.6	190	0.5	0.72528	359	18.7	377	17.8
15	0.71196	790	1.5	518	1.4	0.70837	615	33.1	571	29.0
16	0.69886	220	0.5	157	0.4	0.69300	450	25.9	261	13.9

+Note: N_f: Number of forward iterations; T_f: Computation time for forward solution (unit: minutes); N_a: Number of (mathematical) adjoint iterations; T_a: Computation time for adjoint solution (unit: minutes).

6 Conclusion

Adjoint equation is a fundamental tool for many reactor physics analysis applications such as the perturbation analysis, calculation of higher order harmonics, flux mapping and etc. For continuous or finite difference form of neutronics equations, their adjoint equations are well studied and applied widely. But for modern nodal method, there exist some specialties and difficulties for the definition, solution and application of adjoint equation.

Modern nodal diffusion equations, for example NGFM, are very efficient in calculation time and memory usage, but the equations itself are more complicated, and the diffusion

operator in nodal form is asymmetrical. There are two type of adjoint equation for nodal equation, one is physical adjoint equation which describes the neutron importance distribution, another is mathematical adjoint equation which is the direct matrix transpose equation of the forward nodal equations but has no physical meaning, they are totally different. By contraries, the mathematical adjoint equation is same as the physical adjoint equation in the case of finite-different diffusion equations.

The physical adjoint NGFM equation is based on the adjoint continuous equation, which is the transpose of forward continuous diffusion equation in energy group, by converting the diffusion operator to matrix form just through same method for the forward nodal equation. So the solved distribution from physical adjoint equation has the physical meaning of the nodal approximation of neutron importance distribution, just as the solution of forward equation represents the nodal approximation of continuous neutron distribution. Because the physical adjoint equation has the similar structure as forward equation, except the transpose of the energy group on scattering and fission operator, it can be solved numerically by almost the same code used in the forward nodal equation solution.

On the other side, the mathematical adjoint equation is the direct transpose of the forward NGFM equation, and have no physical meaning at all. Because the forward equation adopt the transverse integration technique to decouple multiple-dimension solution into multiple single-dimensional solution, the neutron flux and neutron current in different nodes is implicitly related by the intermediate variables of transverse leakage. This relationship is very complicated, and the transpose matrix of the NGFM nodal equation is more complicated, is difficult to be described and be solved.

In order to strictly solve the mathematical NGFM equation, the first step is to describe the forward NGFM equation as a single matrix equation. The second step is to transpose the forward equation, and induces the iteration strategy. This iteration strategy consists of the inner iteration in each group and outer iteration to update the adjoint fission source. The inner iteration begins with the update of adjoint neutron, then updates the adjoint leakage, then updates the adjoint in-going current, finally updates the adjoint out-going current. By the way, the eigenvalue of the physical adjoint equation may not equal to the eigenvalue of forward equation, although they are very close.

The most important usage of adjoint equation is for perturbation theory. The correct way to implement the perturbation theory in NGFM requires the mathematical adjoint equation. Another important usage for mathematical adjoint equation is to calculate the higher order harmonics of neutronics eigenvalue equation. In order to calculate the higher order harmonics by NFGM, the eigenvalue equation must be solved order by order, and mathematical adjoint equation must be solved in order to eliminate the lower order harmonics from the result distribution in the iteration process.

The numerical result on the solution and application of adjoint equation of NFGM can prove that: the physical adjoint equation and mathematical adjoint equation of NGFM are different, the mathematical adjoint equation can be strictly solved by special iteration strategy, the physical adjoint equation has physical meaning, but it is the mathematical adjoint equation that is useful for perturbation analysis and calculation of higher order harmonics.

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