

SPECTRAL NODAL METHOD FOR ONE-SPEED X,Y-GEOMETRY EIGENVALUE DIFFUSION PROBLEMS

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ABSTRACT

Presented here is a new numerical nodal method for steady-state multidimensional neutron diffusion equation in rectangular geometry. Our method is based on a spectral analysis of the transverse-integrated nodal diffusion equations. These equations are obtained by integrating the diffusion equation in X and Y directions, and then considering flat approximations for the transverse leakage terms. These flat approximations are the only approximations that we consider in this method; as a result the numerical solutions are completely free from truncation errors in slab geometry. We show numerical results to illustrate the method's accuracy for coarse mesh calculations in a heterogeneous medium.

Keywords: diffusion, nodal method, spectral analysis, eigenvalue problems.

1. Introduction. The multigroup diffusion equation is a mathematical model for the neutron balance within the core of a nuclear reactor. Therefore, we write

$$-\nabla D^g \nabla \phi^g + \Sigma_r^g \phi^g - \sum_{g'=1}^{g-1} \Sigma_s^{g' \rightarrow g} \phi^{g'} = \frac{\chi^g}{K_{\text{eff}}} \sum_{g'=1}^g \nu \Sigma_f^{g'} \phi^{g'} \quad , \quad (1)$$

where g represents the energy group ($g = 1 : G$); ϕ^g is the neutron scalar flux, D^g , Σ_r^g , $\Sigma_s^{g' \rightarrow g}$, $\nu \Sigma_f^{g'}$ are the nuclear constants that define the properties of the core, i.e., diffusion coefficient, removal, scattering and fission macroscopic cross sections respectively), χ^g is the fraction of the fission spectrum corresponding to the neutrons with energy in the g 'th group, and k_{eff} is the effective multiplication factor.

The issue here consists on reducing the numerical solution of the eigenvalue problem (1) to a solution of an eigenvalue discrete problem. Traditionally the diffusion problem has been solved numerically using fine-mesh finite difference methods (FD), which have severe limitations regarding accuracy and computational efficiency. In contrast to this, nodal methods have gone in constant development to being used in nuclear reactors global calculations.

In this paper, we describe a nodal method for numerically solving neutron diffusion equation using one - speed X,Y - geometry models. Similarly to the one-dimensional case, the spectral nodal method in X,Y geometry is based on a spectral analysis of the nodal transverse integrated diffusion equations. Therefore, the two-dimensional problem is divided into two "one-dimensional" problems. The resulting systems of ordinary differential equations (ODEs) are then solved analytically inside an arbitrary node of the spatial grid. The only approximation we consider in this method is the flat current along the node edges. Furthermore, the one-dimensional system of algebraic linear equations is formed by considering the continuity of the scalar flux and current along the node interfaces. We expect that the numerical solutions generated by this method is more accurate than those obtained by traditional numerical methods for coarse-mesh calculations.

We used the alternate direction scheme in the inner iterations of each outer iteration, where we used the power method to converge the dominant numerical eigensolution. This special arrangement of the unknowns allows

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increasing the convergence rate and the accuracy of the numerical results. In this paper, we present numerical results to two typical model problems and compare them with simple analytic solutions and conventional fine-mesh calculation

2. Spectral Nodal Method. The one speed neutron diffusion equation in a square domain of dimensions L can be written as

$$\frac{\partial J^X(x, y)}{\partial x} + \frac{\partial J^Y(x, y)}{\partial y} + \Sigma_a(x, y)\phi(x, y) = \frac{1}{K_{eff}} \nu \Sigma_f(x, y)\phi(x, y) \quad (2.1)$$

$$J^X(x, y) = -D(x, y) \frac{\partial \phi(x, y)}{\partial x} \quad (2.2)$$

$$J^Y(x, y) = -D(x, y) \frac{\partial \phi(x, y)}{\partial y} \quad , \quad (2.3)$$

with the following boundary conditions,

$$J^X(0, y) = -\lambda_l \phi(0, y) \quad (3.1)$$

$$J^X(L, y) = \lambda_r \phi(L, y) \quad (3.2)$$

$$J^Y(x, 0) = -\lambda_b \phi(x, 0) \quad (3.3)$$

$$J^Y(x, L) = \lambda_t \phi(x, L) \quad , \quad (3.4)$$

where J^X, J^Y are the neutron currents in the X and Y directions respectively; ϕ is the neutron scalar flux, $D, \Sigma_a, \nu \Sigma_f$ are the diffusion coefficient and the absorption and fission cross sections respectively; K_{eff} is the effective multiplication factor, and the coefficients $\lambda_{l, r, b, t}$ are the constants defining the boundary conditions in each one of the edges of the square.

Considering that the physical properties are constant within each spatial node Ω_{ij} , the system of diffusion equations (2) appears as

$$\frac{\partial J^X(x, y)}{\partial x} + \frac{\partial J^Y(x, y)}{\partial y} + \Sigma_{a, ij} \phi(x, y) = \frac{1}{K_{eff}} \nu \Sigma_{f, ij} \phi(x, y) \quad (4.1)$$

$$J^X(x, y) = -D_{ij} \frac{\partial \phi(x, y)}{\partial x} \quad (4.2)$$

$$J^Y(x, y) = -D_{ij} \frac{\partial \phi(x, y)}{\partial y} \quad . \quad (4.3)$$

Integrating Eqs. (4) in the X and Y directions separately along the node edges, and bearing in mind that the currents along the node edges can be approximated by their average values, which constitute the only approximations of the model, i.e.,

$$J^X_{i \pm 1/2}(y) \equiv \frac{1}{h} \int_{y_{j-1/2}}^{y_{j+1/2}} J^X_{i \pm 1/2}(y) dy = \tilde{J}_{j \pm 1/2} \quad (5.1)$$

$$J^Y_{j \pm 1/2}(x) \equiv \frac{1}{h} \int_{x_{i-1/2}}^{x_{i+1/2}} J^Y_{j \pm 1/2}(x) dx = \hat{J}_{i \pm 1/2} \quad , \quad (5.2)$$

it is possible to separate the two-dimensional problem in partial derivatives (4) into two ‘‘one-dimensional’’ problems of ODEs, that can be easily solved analytically,

$$\frac{d\hat{J}_i^Y(y)}{dy} + \Sigma_{Tij} \hat{\phi}_i(y) = -\frac{\tilde{J}_{ji+1/2} - \tilde{J}_{ji-1/2}}{h} \quad (6.1)$$

$$\hat{J}_i^Y(y) = -D_{ij} \frac{d\hat{\phi}_i(y)}{dy} \quad (6.2)$$

$$\frac{d\tilde{J}_j(x)}{dx} + \Sigma_{Tij} \tilde{\phi}_j(x) = -\frac{\hat{J}_{ij+1/2} - \hat{J}_{ij-1/2}}{h} \quad (7.1)$$

$$\tilde{J}_j^X(x) = -D_{ij} \frac{d\tilde{\phi}_j(x)}{dx} \quad (7.2)$$

Here $\hat{J}_i^Y, \hat{\phi}_i, \tilde{J}_j^X, \tilde{\phi}_j$ represent the values of the scalar flux and current averaged in each one of the corresponding direction and we have defined

$$\Sigma_{Tij} = \Sigma_{a ij} - \frac{1}{K_{eff}} \nu \Sigma_{f ij} \quad (8)$$

The one-dimensional problems (6) and (7) can be solved by the traditional methods of solution of ordinary differential equations. By solving the Y dependent problem (6), we first determine the analytical solution of the homogeneous problem associated with it. That is,

$$\begin{aligned} \hat{\phi}_i^{hom}(y) &= a(\alpha) \exp\left(\frac{y}{\alpha}\right) \\ \hat{J}_i^{hom}(y) &= b(\alpha) \exp\left(\frac{y}{\alpha}\right) \end{aligned} \quad (9)$$

The general solution, that we obtain for problem (6), is given by

$$\begin{aligned} \hat{\phi}_i(y) &= \sum_{l=1}^2 \psi_l \exp\left(\frac{y}{\alpha_l}\right) - \frac{\tilde{J}_{ji+1/2} - \tilde{J}_{ji-1/2}}{\Sigma_{Tij} h} \\ \hat{J}_i(y) &= -\sum_{l=1}^2 \psi_l \frac{D_{ij}}{\alpha_l} \exp\left(\frac{y}{\alpha_l}\right) \end{aligned} \quad (10)$$

In Eq. (10), the spectral eigenvalue α is given by

$$\alpha_l = (-1)^l \sqrt{\frac{D_{ij}}{\Sigma_{Tij}}} \quad l = 1, 2 \quad (11)$$

Following similar procedure, it is possible to obtain a similar expression to Eq. (10) for the general solution of the X dependent problem (7), which is expressed by

$$\begin{aligned} \tilde{\phi}_j(x) &= \sum_{l=1}^2 \xi_l \exp\left(\frac{x}{\alpha_l}\right) - \frac{\hat{J}_{ij+1/2} - \hat{J}_{ij-1/2}}{\Sigma_{Tij} h} \\ \tilde{J}_j(x) &= -\sum_{l=1}^2 \xi_l \frac{D_{ij}}{\alpha_l} \exp\left(\frac{x}{\alpha_l}\right) \end{aligned} \quad (12)$$

The present spectral nodal method is derived in a way so that the analytical solutions (10) are unconditionally preserved inside the nodes for any values of the constants ψ_l, ξ_l . Moreover, the continuity of the solution is guaranteed along the node interfaces and the boundary conditions are satisfied.

To proceed further, by applying the concept of transverse integration in the node, we obtain

$$\frac{\tilde{J}_{ji+1/2} - \tilde{J}_{ji-1/2}}{h} + \frac{\hat{J}_{ij+1/2} - \hat{J}_{ij-1/2}}{h} + \Sigma_{a ij} \bar{\phi}_{ij} = \frac{1}{K_{eff}} \nu \Sigma_{f ij} \bar{\phi}_{ij} \quad (13.1)$$

$$\bar{J}_{ij}^X = -D_{ij} \frac{\tilde{\phi}_{ji+1/2} - \tilde{\phi}_{ji-1/2}}{h} \quad , \quad (13.2)$$

$$\bar{J}_{ij}^Y = -D_{ij} \frac{\hat{\phi}_{ij+1/2} - \hat{\phi}_{ij-1/2}}{h} \quad . \quad (13.3)$$

Equations (13) form a system of algebraic linear equations in seven unknowns for each node: $\tilde{J}_{ji+1/2}, \hat{J}_{ij+1/2}, \bar{J}_{ij}^X, \bar{J}_{ij}^Y, \bar{\phi}_{ij}, \tilde{\phi}_{ji+1/2}, \hat{\phi}_{ij+1/2}$. Therefore, in order to guarantee uniqueness of the solution, it is necessary to introduce four auxiliary equations that we write as

$$\bar{J}_{ij}^Y = \frac{\beta_{ij}^{(1)}}{2} \left(\hat{J}_{ij+1/2} + \hat{J}_{ij-1/2} \right) \quad , \quad (14.1)$$

$$\bar{J}_{ij}^X = \frac{\beta_{ij}^{(0)}}{2} \left(\tilde{J}_{ji+1/2} + \tilde{J}_{ji-1/2} \right) \quad , \quad (14.2)$$

$$\bar{\phi}_{ij} = \frac{\beta_{ij}^{(2)}}{2} \left(\tilde{\phi}_{ji+1/2} + \tilde{\phi}_{ji-1/2} \right) + \gamma_{ij}^{(2)} \quad , \quad (14.3)$$

$$\bar{\phi}_{ij} = \frac{\beta_{ij}^{(3)}}{2} \left(\hat{\phi}_{ij+1/2} + \hat{\phi}_{ij-1/2} \right) + \gamma_{ij}^{(3)} \quad . \quad (14.4)$$

The coefficients $\beta_{ij}^{(0,1,2,3)}$ and $\gamma_{ij}^{(2,3)}$, appearing in the auxiliary equations, are calculated in a way that the general solutions, given by the equations (10) and (12), are preserved unconditionally for any value of the constants ψ_1, ξ_1 .

The system of spectral nodal diffusion equations is obtained when we substitute the auxiliary equations (14) into the balance equations (13). The result is

$$\frac{\tilde{J}_{ji+1/2} - \tilde{J}_{ji-1/2}}{h} + \delta_{ij} \frac{\hat{J}_{ij+1/2} - \hat{J}_{ij-1/2}}{h} + \frac{\sum_{a_{ij}} \beta_{ij}}{2} \left(\tilde{\phi}_{ji+1/2} + \tilde{\phi}_{ji-1/2} \right) = \frac{1}{K_{eff}} v \Sigma_{f_{ij}} \bar{\phi}_{ij} \quad (15.1)$$

$$\delta_{ij} \frac{\tilde{J}_{ji+1/2} - \tilde{J}_{ji-1/2}}{h} + \frac{\hat{J}_{ij+1/2} - \hat{J}_{ij-1/2}}{h} + \frac{\sum_{a_{ij}} \beta_{ij}}{2} \left(\hat{\phi}_{ij+1/2} + \hat{\phi}_{ij-1/2} \right) = \frac{1}{K_{eff}} v \Sigma_{f_{ij}} \bar{\phi}_{ij} \quad (15.2)$$

$$\tilde{J}_{ij+1/2} + \tilde{J}_{ij-1/2} = -\frac{2D_{ij}}{\beta_{ij} h} \left(\tilde{\phi}_{ji+1/2} - \tilde{\phi}_{ji-1/2} \right) \quad (15.3)$$

$$\hat{J}_{ji+1/2} + \hat{J}_{ji-1/2} = -\frac{2D_{ij}}{\beta_{ij} h} \left(\hat{\phi}_{ij+1/2} - \hat{\phi}_{ij-1/2} \right) \quad . \quad (15.4)$$

Here, we have defined

$$\delta_{ij} = \frac{\sum_{a_{ij}} \beta_{ij}}{\sum_{T_{ij}}} (\beta_{ij} - 1) + 1 \quad .$$

The system of spectral nodal diffusion equations (15) can be solved and has a unique solution as it is composed of four equations in four unknowns in each node, i.e., $\tilde{J}_{ji+1/2}, \hat{J}_{ij+1/2}, \tilde{\phi}_{ji+1/2}, \hat{\phi}_{ij+1/2}$.

$$\begin{aligned}
 \tilde{\eta}_1 &= -\frac{h \sum_{a_{1j}} \beta_{1j} \delta_{1j}}{4(\delta_{1j}^2 - 1)} \left(\hat{\phi}_{1j+\frac{1}{2}} + \hat{\phi}_{1j-\frac{1}{2}} \right) \\
 \tilde{\eta}_i &= -\frac{h \sum_{a_{ij}} \beta_{ij} \delta_{ij}}{4(\delta_{ij}^2 - 1)} \left(\hat{\phi}_{ij+\frac{1}{2}} + \hat{\phi}_{ij-\frac{1}{2}} \right) - \frac{h \sum_{a_{i+1j}} \beta_{i+1j} \delta_{i+1j}}{4(\delta_{i+1j}^2 - 1)} \left(\hat{\phi}_{i+1j+\frac{1}{2}} + \hat{\phi}_{i+1j-\frac{1}{2}} \right), \quad i = 2 : I \\
 \tilde{\eta}_I &= -\frac{h \sum_{a_{Ij}} \beta_{Ij} \delta_{Ij}}{4(\delta_{Ij}^2 - 1)} \left(\hat{\phi}_{Ij+\frac{1}{2}} + \hat{\phi}_{Ij-\frac{1}{2}} \right)
 \end{aligned} \tag{17.5}$$

Similarly we can obtain a system of algebraic equations associated to the Y direction for any layer $i = 1 : I$. The system associated to each one of the directions presents tridiagonal and well-conditioned matrices that are solved by gaussian elimination with backward substitution. For convergence of the dominant eigenvalue, we use the classic power method and accelerate it using the Chebyshev's polynomials.

The steps used in the algorithm follow. With initial guesses for K_{eff} and for the node average scalar fluxes, we solve the system to the X direction (16) for each one of the layers j , and then the system associated to the Y direction is solved for each one of the layer I , until a prescribed convergence criterion for these inner iterations is achieved. For each outer iteration, the node average scalar fluxes are calculated using Eq. (14.3) or (14.4), to estimate the source and the eigenvalue K_{eff} for the next iteration. To illustrate the accuracy of the offered method, we present numerical experiments in the following section.

3. Numerical Results. The results obtained by comparing the node average scalar flux as generated by the present spectral nodal method and the numerical values obtained from the analytic solution are shown in Table 1, for a homogeneous test problem in a square region with zero scalar flux boundary conditions.

Table 1. Numerical results obtained by comparing the spectral nodal solution with the analytic solution, considering the node average scalar flux.

Nodes / h	ErrorAveFlux (%)	ErrorMaxFlux (%)
8 / 22.5 cm	0.014512	0.025168
10 / 18 cm	0.013324	0.024874
20 / 9 cm	0.012873	0.023581
50 / 3.6 cm	0.014214	0.025315

In Table1, Nodes / h represents the number of spatial nodes in each one of the directions and h is the uniform width of the spatial nodes. Moreover, ErrorAveFlux is the mean value of the relative errors of the node average scalar fluxes, and ErrorMaxFlux is the maximum of the relative error in the whole region. We remark that for all node widths used in these numerical experiments, the errors in the node average scalar flux are less than 0.03% for the maximum error, and less than 0.02% for the mean error. The results showed very good agreement with the analytic solution.

At this point we compare the numerical results generated for the homogeneous test problem with those generated for the same test problem with the conventional fine-mesh diffusion program of fine mesh diffusion finite difference code. We used a spatial grid composed of 100 nodes in each direction, i.e., $h = 1.8$ cm. The reference value for the dominant eigenvalue is 1.018097. A summary of the numerical results is presented in Table 2.

Table 2. Numerical results obtained by comparing the spectral nodal solution with the analytic solution, considering the effective multiplication factor and the node average scalar flux.

Nodes / h	K_{eff}	Error K_{eff}	ErrorAveFlux	ErrorMaxFlux
8/22.5 cm	1.0184327	0.0321	-	-
10/18 cm	1.0180306	0.0200	0.005208	0.009702
20/9 cm	1.0181330	0.0035	0.004120	0.007671
50/3.6 cm	1.0180820	0.0014	0.005208	0.009701

In Table 2, K_{eff} is the dominant eigenvalue generated by the offered spectral nodal method and $\text{Error}K_{\text{eff}}$ is the absolute error with respect to the reference value. As we see, the numerical deviations of the K_{eff} and the scalar flux are within reasonable limits. Table 3 displays the numerical results generated for K_{eff} by the present spectral nodal method, the classic finite difference method, and the one obtained analytically.

Table 3. Comparison between the values of K_{eff} generated by various methods.

K_{eff} calculated analytically	K_{eff} (finite difference)	Error K_{eff} (finite difference)	K_{eff} (spectral nodal)	Error K_{eff} (spectral nodal)
1.018032	1.018097	0.0065	1.018031	0.0001

In the heterogeneous test problem, we model a square region of dimensions L , with zero scalar flux boundary conditions, composed by four areas of different composition as we illustrate in Figure 1.

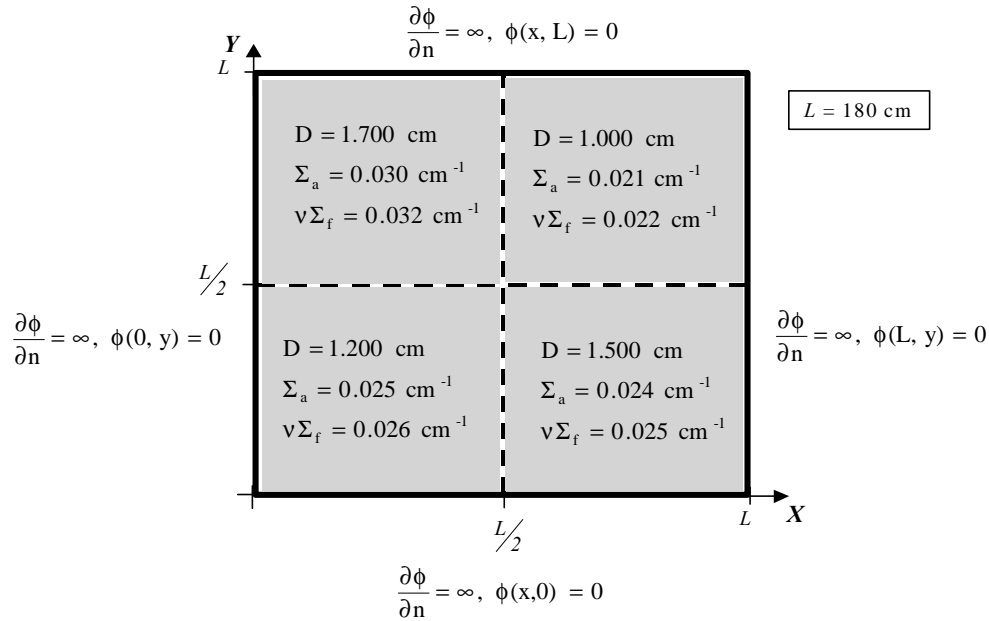


Figure 1. Heterogeneous Test Problem.

We compare the numerical solution generated by the offered spectral nodal method and the conventional finite difference method. The reference solution was obtained under the same conditions of the homogeneous test problem. The reference value of K_{eff} is 1.018473. A summary of the comparison of the results of K_{eff} and neutron scalar flux distribution is shown in Table 4.

Table 4. Heterogeneous Test Problem.

Nodes/h	K_{eff}	Error K_{eff} (%)	ErrorAveFlux (%)	ErrorMaxFlux (%)
8/22.5 cm	1.018906	0.043	-	-
10/18 cm	1.018746	0.027	0.071429	0.300927
20/9 cm	1.018526	0.005	0.045390	0.142208
50/3.6 cm	1.018451	0.002	0.131275	0.386338

From Table 4, we conclude that the present spectral nodal method calculates the effective multiplication factor and neutron flux distribution with good accuracy for heterogeneous test problems. For the case of the eigenvalue, the error turned out to be less than 0.1%. For the neutron flux distribution, the errors are less than 0.1% for the mean error and less than 0.4% for the maximum error.

4. Concluding Remarks. The spectral nodal method for one-speed X,Y-geometry diffusion eigenvalue problems generates accurate numerical results for the neutron flux and the effective multiplication factor with good efficiency in coarse-mesh calculations. As future work, we suggest to extend the present spectral nodal method to two energy group diffusion model to account for the energy change in scattering and fission events.

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