New Finite Element Solution Technique
for Neutron Diffusion Equations

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A new, finite element solution technique for neutron diffusion equations has been developed. In this method, calculational accuracy is improved by adding imaginary nodal points, subdividing each triangular element into three quadrilateral subelements, and approximating the spatial variation of neutron flux within each element by three linear planes. In the process of solving the algebraic equations, the additional unknown variables are eliminated so that the number of unknowns remains the same as that in the usual finite element method. This technique has been applied to two types of one-group neutron diffusion equations to test its accuracy. It has been shown that the method yields the same degree of accuracy, in eigenvalues and neutron flux distributions, as the usual finite element method when four times as many elements are used. Under the same degree of accuracy, the computing time of the new method is about 1/4 that of the usual method.

KEYWORDS: neutron diffusion equations, calculational accuracy, computing time, eigenvalue problem, fixed source problem, imaginary subdivision, imaginary nodal point, linear base function, one-group theory, finite element method, analytical solution, numerical solution

I. INTRODUCTION

A finite element method (FEM), developed for use in the field of structural mechanics, is becoming a useful tool in various fields of science because of its applicability to solving differential equations in many different areas. In the field of nuclear engineering, some neutron diffusion and transport calculation codes have been developed based on FEM\(^{(1)}\)\(^{(9)}\). They have been applied to the calculation of neutron flux and power distributions in geometrically complicated systems, since FEM can treat such geometries by dividing them into a finite number of triangular regions (elements).

Solutions obtained by FEM naturally contain calculational errors resulting from the use of a finite number of elements, and therefore, when very accurate calculations are required, it is necessary to use a sufficiently large number of elements. This requires a sizable increase in human labor for input data preparation, as well as in computing time. To improve the calculational accuracy without increasing the number of elements, higher-order base functions were introduced by Silvester\(^{(5)}\). In this method, however, the band width of the coefficient matrix of resulting algebraic equations as well as the number of unknown variables increases, and as a result, computing time is also greatly increased.

In this paper, a new, simple method is described for improving the calculational accuracy of FEM, in which neither the band width nor the number of elements increases, and therefore, the improvement in accuracy is attained in a shorter computing
II. Theory

One method which is often used to improve the calculational accuracy of FEM is to use higher-order base functions. In this method, the spatial variation of neutron flux within an element is approximated by higher-order polynomials. For example, in the case of 2nd-order polynomials being used, the spatial variation of neutron flux $u(x, y)$ within an element is expressed by

$$u(x, y) = a + bx + cy + dx^2 + exy + fy^2,$$

This expression is substituted into the diffusion equation to be solved, the resulting equations are multiplied with appropriate weighting functions and are integrated over the whole volume to obtain a set of simultaneous algebraic equations of $a, b, c$ etc. In this case, a significant increase in computing time is unavoidable, because the number of unknown variables is larger and the band width of the resulting simultaneous equations is wider than in the usual FEM with an equal number of elements.

Another method which is often employed is the use of 'imaginary' nodal points. Here, one nodal point is added at the center of mass of each triangular element and the element is subdivided into three triangular subelements as shown in Fig. 1(a). In this case, the neutron flux value at the center of mass can be expressed by using those at nodal points $i, j$ and $k$ only, and it is possible to eliminate the neutron flux values at the centers of mass so as not to increase the dimensions for the set of final algebraic equations. Thus an increase in accuracy is achieved with little change in the computing time. The drawback of this method is that it must use long-shaped triangles as shown in the figure. This limits the improvement in accuracy.

In this paper, imaginary nodal points are used, but the subdivision of each triangular element is done in a different way to avoid using long-shaped triangular elements. That is, each triangular element is imaginarily subdivided into three quadrilateral sub-

![Fig. 1 Imaginary subdivision of elements](image-url)
elements, as shown in Fig. 1(b), by adding nodal points at the center of mass and midpoints of the boundary. Next, an approximation is made, so as not to increase the number of unknown variables unnecessarily, that the spatial variation within each square element is expressed by a linear plane. This means that the spatial variation of neutron flux within a triangular element is approximated by three linear planes as shown in Fig. 2.

By doing this, the approximate solution to the neutron diffusion equation is expressed in the following form:

\[ u(x, y) = \sum_{i=1}^{N} u_i \varphi_i(x, y) + \sum_{m=1}^{M} v_m \varphi_m^*(x, y), \]

where \( \varphi_i(x, y) \) is a "roof function" which has its peak at nodal point \( i \) (Fig. 3), and \( M \) and \( N \) are the numbers of nodal points and elements, respectively. In the usual FEM, only the first term on the R.H.S. of Eq. (1) appears. The second term can be thought of as a correction term.

The shape of \( \varphi_m^*(x, y) \) is shown in
Fig. 4. It has its peak at the center of mass of element \( m \) and does not vanish at the element boundaries except at the nodal points \( i, j \) and \( k \). It has the same height of \( 3/4 \) at the midpoints of the element boundaries. This means that the approximate solution, Eq. (1), has a discontinuity at the element boundaries.

It is necessary to determine the \( M+N \) unknown variables \( u_i \) and \( v_m \) of Eq. (1). This procedure is described next.

To begin with, let the neutron diffusion equation for a fixed source problem be expressed by using an operator \( L \) for simplicity.

\[
Lu = S, \quad (2)
\]

where \( L = -\text{div} \ D(x, y) \text{grad} + \sum a(x, y) \).

The function \( S(x, y) \) corresponds to an external neutron source.

Substituting Eq. (1) into Eq. (2) and multiplying the resulting equation by \( \varphi_i(x, y) \), \( N \) relations are obtained.

\[
\langle \varphi_i, Lu \rangle = \langle \varphi_i, S \rangle, \quad (i=1, 2, \ldots, N) \quad (3)
\]

where the symbol \( \langle \ , \ \rangle \) denotes the volume integration. Equation (3) reduces to the following \( N \) algebraic equations:

\[
\sum_{j=1}^{N} a_{ij} u_j + \sum_{m=1}^{M} a'_{im} v_m = b_i, \quad (i=1, 2, \ldots, N), \quad (4)
\]

where \( a_{ij} = \langle \varphi_i, L \varphi_j \rangle \), \( a'_{im} = \langle \varphi_i, L \varphi_m \rangle \), \( b_i = \langle \varphi_i, S \rangle \).

The other \( M \) equations are obtained by similar procedures except that a pyramid-shaped function \( \varphi^0_m(x, y) \) which has its peak at the center of mass of each element (Fig. 5) is used, instead of \( \varphi_i(x, y) \). Each of these \( M \) equations yields a relationship between \( u_i \), \( u_j \), \( u_k \) and \( v_m \) for each element:

\[
c_{mi} u_i + c_{mj} u_j + c_{mk} u_k + c_{mo} v_m = d_m, \quad (6)
\]

where \( c_{mi} = \langle \varphi^0_m, L \varphi_i \rangle \), \( c_{mj} = \langle \varphi^0_m, L \varphi_j \rangle \), \( c_{mk} = \langle \varphi^0_m, L \varphi_k \rangle \), \( d_m = \langle \varphi^0_m, S \rangle \).

Eliminating \( v_m \) in Eq. (4) by using Eq. (6), the following simultaneous algebraic equations are obtained:

\[
\sum_{j=1}^{N} \left( a_{ij} - \sum_m \frac{a'_{im} c_{mj}}{c_{mo}} \right) u_j + b_i = \sum_m \frac{a'_{im} d_m}{c_{mo}}, \quad (i=1, 2, \ldots, N). \quad (7)
\]

The number of unknowns for a set of these equations is the same as that for the equations derived in the usual FEM. The
band width of the coefficient matrix of the equations is also the same in this method as that in the usual FEM. It is expected, therefore, that, in the present FEM, calculational accuracy is improved without a significant increase in computing time.

In cases where the R.H.S. of Eq. (7) vanishes (i.e., eigenvalue problems), an iteration technique must be used to solve the equation. The reason for this is that the coefficient matrix of the resulting eigenvalue equations is implicitly dependent on the eigenvalue. That is, in cases of eigenvalue problems, equations of the following form must be solved instead of Eq. (7):

\[
\frac{1}{\sum_{j=1}^{N} A_{ij}(k_{\text{eff}})} \sum_{j=1}^{N} f_{ij} u_j = \frac{1}{K_{\text{eff}}} \sum_{j=1}^{N} f_{ij} u_j, \quad \text{(8)}
\]

where \( f_{ij} = \langle \psi_i, \nu \sum_{j} \langle x, y \rangle \phi_j \rangle \), \( f'_{im} = \langle \psi_i, \nu \sum_{j} \langle x, y \rangle \phi_m \rangle \), \( f_{m0} = \langle \psi_m, \nu \sum_{j} \langle x, y \rangle \phi_m \rangle \).

The quantities \( K_{\text{eff}} \) and \( \nu \sum_{j} \langle x, y \rangle \) are the eigenvalue (effective multiplication factor) and neutron production cross section, respectively.

Equation (8) can be solved by the iteration scheme expressed as follows:

\[
\sum_{j=1}^{N} A_{ij}(k_{\text{eff}}(N)) u_j = \frac{1}{K_{\text{eff}}(N)} \sum_{j=1}^{N} f_{ij} u_j, \quad \text{(9)}
\]

where \( A_{ij}(k_{\text{eff}}) \) stands for the coefficient of \( u_j \) on the L.H.S. of Eq. (8); and \( K_{\text{eff}}(N) \) is the eigenvalue obtained by the \( N \)-th iteration.

### III. Numerical Examples

The present technique has been applied to two types of simple problems to test its accuracy.

(1) Eigenvalue Problem (bare, square homogeneous reactor)

\[-D \frac{\partial^2 \phi}{\partial \alpha^2} + \sum \phi = k \sum \phi, \quad \text{(10)}\]

where \( D=1.0, \sum =1.0 \).

This equation has been solved under the boundary conditions \( \phi(x, \pm 1.5) = \phi(\pm 1.5, y) = 0 \) by the usual method and the method presented. The square homogeneous region has been divided into 18 and 72 elements as shown in Fig. 6 and the calculated eigenvalues have been compared with the analytical solution.

Table 1 shows a comparison of the

<table>
<thead>
<tr>
<th>Table 1 Comparison of eigenvalues</th>
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<tr>
<td>( \text{Number of elements} )</td>
</tr>
<tr>
<td>-----------------------------------</td>
</tr>
<tr>
<td>18</td>
</tr>
<tr>
<td>72</td>
</tr>
</tbody>
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*Relative error
eigenvalues. It is seen that the relative errors of the method presented are about 1/4 of those of the usual FEM, and that the accuracy is comparable to that of the usual FEM with four times as many elements.

(2) Fixed Source Problem (2-region cylindrical cell)

\[ -DF^2\phi + \Sigma_a \phi + S = 0. \]  

This equation has been solved for the 2-region cylindrical cell with the element division shown in Fig. 7. The one-group constants and neutron source have been assumed to be constant in each region:

\[
\begin{align*}
D(r) &= \begin{cases} 
0.1 & \text{Region 1} \\
0.333 & \text{Region 2}, 
\end{cases} \\
\Sigma_a(r) &= \begin{cases} 
2.6 & \text{Region 1} \\
0.01 & \text{Region 2}, 
\end{cases} \\
S(r) &= \begin{cases} 
0.0 & \text{Region 1} \\
1.0 & \text{Region 2}. 
\end{cases}
\]

Disadvantage factors have been evaluated by the presented and usual FEM’s, and the CITATION code\(^{(4)}\) for reference. Table 2 shows a comparison of the calculated results. In this case also, the deviation of the new method’s result from the reference value is about 1/4 that of the conventional result.

(3) Fixed Source Problem

(2-region square cell)

Equation (10) has been solved here for the 2-region square cell shown in Fig. 8. The same one-group constants and neutron source as above have been used. Figures 9(a)~(c) show comparison of neutron flux distributions obtained by the presented and usual methods along the 0°, 45° and 22.5° lines, respectively. Figures 9(a) and (b) show that, along the 0° and 45° lines, the neutron flux distribution by the method presented is in a good agreement with that by the usual FEM with four times the number of elements. Figure 9(c) shows a discontinuity of neutron flux, in the absorber region, which is caused by the approximation that neutron flux within each element is expressed by three linear planes.
Fig. 9 (a)~(c) Comparison of neutron flux distribution along 0°, 45° and 22.5° lines as shown in Fig. 2. However, as can be seen from the figure, the average flux in each element is improved as compared with that obtained by the usual FEM with 13 elements, as well as the global distribution. It has thus been confirmed that neutron flux distribution is also improved in the method presented.
(4) Comparison of Computing Time

The same eigenvalue problem as in Sec. (1) has been solved using different numbers of elements, by the presented and usual methods for a comparison of the computing time. The results are summarized in Table 3.

Table 3 Comparison of computing times

<table>
<thead>
<tr>
<th>Method presented</th>
<th>Usual FEM</th>
</tr>
</thead>
<tbody>
<tr>
<td>Number of elements</td>
<td>Computing time (s)</td>
</tr>
<tr>
<td>8</td>
<td>0.2</td>
</tr>
<tr>
<td>32</td>
<td>3</td>
</tr>
<tr>
<td>128</td>
<td>37</td>
</tr>
</tbody>
</table>

† IBM 370/158
‡‡ The arrows indicate that the left and right cases are of the same degree of accuracy.

It is found from this table that, for the calculations with the same number of elements, the method presented requires about three times as much computing time as the usual one. It is also found, however, that the computing time required for the presented FEM calculations is about 1/4 that required by the conventional method for the same degree of accuracy, because the latter requires about four times as many elements as the former.

IV. DISCUSSION

(1) Success of the present technique depends on the fact that, in neutron diffusion problems, neutrons are absorbed and/or produced in most domain of the system treated. In cases where both absorption cross section $\Sigma_a$ and production cross section $\nu\Sigma_f$ vanish (thermal diffusion problems), the method presented can no longer be used to improve the calculational accuracy because $a'_{\text{rel}}$ equals zero in Eq. (4). The use of the function $\phi(x, y)$ physically corresponds to taking the buckling of neutron flux within each triangular element into consideration. And in thermal diffusion problems, the buckling is almost always zero. The reader should be careful in this respect. In eigenvalue problems, this matter does not occur.

(2) In the method presented, discontinuity in neutron flux always appears at element boundaries. However, the average neutron flux in each element is improved and so is the global distribution. This means that base functions should not necessarily be chosen so that neutron flux is continuous at element boundaries. Rather, such base functions often cannot reproduce well steep spatial variations. The essence of the method presented is that base functions are chosen, at the cost of discontinuity appearing, so that steep spatial variations can be reproduced well.

V. SUMMARY

A new, finite element solution technique for neutron diffusion equations has been presented. In this method, imaginary nodal points are added at the center of mass of each triangular element and at the midpoints of its sides. Then, each element is subdivided into three quadrilateral subelements, and the spatial variation of neutron flux within the element is approximated by three linear planes. Since the additional unknown variables are eliminated in the process of solving the resulting algebraic equations, the
number of unknowns does not differ from that of the usual FEM with an equal number of elements. Thus the calculational accuracy is improved within a shorter computing time in this method than in the usual straightforward techniques using higher-order polynomials or increasing the number of elements. The presented technique has been applied to simple, one-group neutron diffusion equations to test its accuracy. And it has been shown that it yields almost the same accuracy as the usual FEM with four times the number of elements. Under the same accuracy, the computing time is about 1/4 that of the usual FEM.

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