Application of the hierarchical domain decomposition boundary element method to the simplified P3 equation

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1. Introduction

In recent years, the simplified P3 method (Gelbard, 1960; Larsen et al., 1996; Brantley and Larsen, 2000), or the SP3 method, has attracted much attention in the reactor physics field since this method makes it possible to partly capture the neutron transport effect without a severe increase in computational burden. Various computer programs based on the SP3 method have been developed for thermal reactor applications to date (Tatsumi and Yamamoto, 2003; Beckert and Grundmann, 2007; Baudron and Lautard, 2007; Tada et al., 2008). Generally speaking, the neutron transport effect in fast reactors is larger than that in thermal reactors. Thus, the SP3 method may be considered promising as a fast reactor design calculation tool. Hèbert has developed a finite element-based SP3 method for hexagonal geometries and has incorporated it into the existing diffusion theory code TRIVAC (Hèbert, 2010a). This development may be intended to fast reactor applications of the SP3 method. These computer programs based on the SP3 method employ the finite element method, the nodal method or the finite method for spatial discretization. These spatial discretization methods have been utilized with great success in diffusion theory codes for reactor core calculations.

The boundary element method (BEM) is applied to partial differential equations and has been widely used in the field of engineering. A specific feature of the BEM is that the dimensions of a problem can be reduced by one. For example, a two-dimensional problem can be reduced to a one-dimensional problem. Thus the computational burden, i.e., computer memory storage and computational time, can be greatly reduced. Another advantageous feature of the BEM is that preparation of input data describing problem geometry is easier than in other methods.

The first application of the BEM to the neutron diffusion equation can be found in Koskinen’s seminal work (Koskinen, 1965), in which the neutron diffusion equation is transformed to a corresponding boundary integral equation. Twenty years later, Itagaki applied the BEM to general neutron diffusion problems; namely, criticality, fixed-source and multi-region problems (Itagaki, 1985). This work has been followed by other researchers and several numerical methods based on the BEM have been proposed (Ozgener and Ozgener, 1993; Purwadi et al., 1998; Maiani and Montagnini, 1999; Chiba et al., 2001a,b; Cavder and Ozgener, 2004; Cossa et al., 2010). Among these BEM-based numerical methods, the hierarchical domain decomposition boundary element method (HDD-BEM) (Purwadi et al., 1998; Chiba et al., 2001a,b) was very probably the first to be applied to realistic three-dimensional multi-group problems, since such application took place almost ten years ago (Chiba et al., 2001b). It has also been applied successfully to parallel computers (Tsuji and Chiba, 2000). The HDD-BEM is quite unique. The neutron diffusion equation is first transformed to a set of mode flux equations and these equations are then solved by the BEM. The eigenvalue and inner boundary conditions between neighboring homogeneous regions are estimated iteratively by Newton’s method.

The present study is the first application of the HDD-BEM to the SP3 equation. In the present paper, the application of the HDD-BEM to the SP3 equation will be described, and then it will be verified through a benchmark calculation using a two-dimensional one-group anisotropic-scattering problem.
2. Hierarchical domain decomposition boundary element method for the SP₃ equation

2.1. Mode flux representation for the zero-th and second angular moments of neutron flux

In the conventional HDD-BEM for the multi-region diffusion equation, the original diffusion equation is transformed to a set of mode flux equations for each homogeneous region, as proposed by Koskinen (1965). Derivation of mode flux equations for the multi-region SP₃ equation is straightforward. Here, we consider a one-group SP₃ equation. If the eigenvalue and boundary conditions are given to each region. If the eigenvalue and boundary conditions are given to each

A one-group SP₃ equation can be written as follows:

\[ D \Delta \psi + \left( \sigma - \sigma_0 \right) \psi = 0, \]

where \( D \) is the diffusion coefficient, \( \psi \) is the neutron flux, and \( \sigma \) is the total cross section, \( \sigma_0 \) is the nth Legendre component of scattering cross section, \( \sigma_0 \) is the production cross section, and \( k \) is the eigenvalue, and

\[ D_0 = \frac{1}{3(\sigma - \sigma_0)}, \]

\[ D_2 = \frac{1}{3(\sigma - \sigma_0)}. \]

This one-group SP₃ equation can be written in a matrix form as follows:

\[ (\nabla^2 + A(k))\psi = 0, \]

where

\[ A(k) = \begin{pmatrix} -\frac{\sigma}{c_0} & \frac{1}{c_0} \nabla \sigma_0 \\ -\frac{\sigma}{c_0} & \frac{1}{c_0} \nabla \sigma_0 \end{pmatrix} - \frac{1}{c_0} \left( \frac{\sigma}{c_0} \right), \]

and \( \psi = (\phi_0, \phi_2) = (\phi_0 + 2\phi_2, \phi_2). \)

The procedure to derive mode flux equations is the same as that for the diffusion equation.

For a homogeneous region \( r \), angular flux moments \( \phi_0 \) and \( \phi_2 \) can be expressed with the “mode flux” \( \phi^j \) as follows:

\[ \phi_0 = \sum_{j=1}^{2} C_{0j} \phi^j, \]

\[ \phi_2 = \sum_{j=1}^{2} C_{2j} \phi^j. \]

The coupling coefficients \( C_{0j} \) and \( C_{2j} \) are determined from the group constants of the region \( r \). The mode flux satisfies the following equation:

\[ (\nabla^2 + B_j^2) \phi^j = 0, \]

where the values \( B_j^2 \) are the roots in the following algebraic equation for \( \nabla^2 \):

\[ \det \left( \nabla^2 + A(k) \right) = 0. \]

As described above, the multi-region SP₃ equation is transformed to a set of mode flux equations for each homogeneous region. If the eigenvalue and boundary conditions are given to each homogeneous region, the mode flux equations can be solved and solutions for \( \phi_0 \) and \( \phi_2 \) for the homogeneous region can be obtained.

2.2. Formulation of boundary integral equation

Here we define the boundary of a homogeneous region \( r \) as \( S_r \), as shown in Fig. 1. Using the weighted residual formulation (Brebbia, 1978), Eq. (9) can be converted to a boundary integral equation as

\[ \tilde{c}_t \phi^j_t(r) = -\int_{S_r} \phi^j_t(r) \phi_r^j(r, r) ds + \int_{S_r} \phi^j_t(r) \phi_r^j(r, r) ds, \]

where \( \phi_r^j \) is a normal derivative of \( \phi^j \), and \( \phi_r^{jn} \) and \( \phi_r^{jn} \) are Green’s function and its normal derivative, respectively. Green’s function \( \phi_r^{jn} \) is given as the fundamental solution of the following equation with a point source \( \delta(r, r) \):

\[ \nabla^2 \phi_r^{jn}(r, r) + B_j^2 \phi_r^{jn}(r, r) + \delta(r, r) = 0. \]

The constant \( \tilde{c}_t \) in Eq. (11) is unity if \( r \) lies inside of the region and \( 1/2 \) if \( r \) lies on a smooth boundary.

In order to discretize the boundary integral Eq. (11), the boundary is divided into \( K \) boundary elements. These boundary elements are denoted as \( S_k \). On each boundary element, we assign nodal points on which values of mode flux and its derivative are determined. The spatial distributions of the mode flux and its derivative on the boundary element are expanded by polynomials by using the values on the nodal points.

Here, we assume that one nodal point is assigned to all the boundary elements. In this case, the mode flux and its derivative are assumed to be constant on each boundary element. Thus the boundary integral Eq. (11) can be written as

\[ \tilde{c}_t \phi^j_t(r_k) = -\sum_{k=1}^{K} \phi^j_t(r_k) \int_{S_k} \phi_r^{jn}(r, r_k) ds + \sum_{k=1}^{K} \phi^j_t(r_k) \int_{S_k} \phi_r^{jn}(r, r_k) ds, \]

where \( r_k \) corresponds to the location of the nodal point on the boundary element \( S_k \). If we set \( r_k \) as \( r_k \) in Eq. (13), we obtain the following \( K \) simultaneous equations:

\[ \tilde{c}_k \phi^j_t(r_k) = -\sum_{k=1}^{K} \phi^j_t(r_k) \int_{S_k} \phi_r^{jn}(r, r_k) ds + \sum_{k=1}^{K} \phi^j_t(r_k) \int_{S_k} \phi_r^{jn}(r, r_k) ds, \quad k = 1, 2, \ldots, K. \]

A set of the boundary integral Eq. (14) can be written in the following matrix equation:

\[ G \phi^j_t = H \phi^j_t. \]

As shown in Eq. (14), we have \( K \) simultaneous linear equations. Thus if \( K \) of \( \phi^j_t(r_k) \) and \( \phi^j_t(r_k) \) are known, others can be obtained.

Fig. 1. Definition of region and boundary elements.
by solving matrix Eq. (15). Generally the mode fluxes or its derivatives on the outer boundaries are known and those on inner boundaries between neighboring two homogeneous regions are unknown. In the HDD-BEM, the inner boundary conditions, i.e., values of mode fluxes, and eigenvalue are initially assumed. Thus the boundary integral equation can be solved for each homogeneous region.

For finer spatial discretization, the mode flux and its derivative can be expanded by the polynomials if two or more nodal points are assigned on a boundary element. On these boundary elements, two of the nodal points are placed on the extremes of the boundary element. If the extreme of the boundary element coincides with a “corner point” where the derivative of the boundary curvature along the boundary changes discontinuously, the concept of the non-conforming elements has to be introduced. On non-conforming elements, nodal points are not placed on the extremes but on a position slightly inside of the extremes. Details of the non-conforming element can be found in Chiba et al. (2001a).

2.3. Modification of eigenvalue and inner boundary conditions by Newton’s method

In the HDD-BEM, the eigenvalue and the inner boundary condition, i.e., mode fluxes on the inner boundaries, are initially assumed, and these are modified through iterations. This procedure for the SP$_3$ equation is the same as that for the diffusion equation.

Consider an inner boundary element $l_p$ between two homogeneous neighboring regions. On this boundary element, two sets of mode fluxes and their derivatives are defined, i.e., those included in one region denoted as $r(l_p^+)$ and those included in another region denoted as $r(l_p^-)$. In the HDD-BEM, mode fluxes on the inner boundary in the region $r(l_p^+)$ are initially assumed. Since all the mode fluxes on inner boundaries are known, boundary integral Eq. (15) can be solved and the derivatives of the mode fluxes can be obtained. If the assumed eigenvalue and inner boundary conditions are correct, the following equation should be preserved since the derivatives of $\phi_0$ and $\phi_2$ on the inner boundaries should be continuous:

$$F' = \left( \begin{array}{c} F_0' \\ F_2' \end{array} \right) = \left( \begin{array}{c} F_0^l \\ F_2^l \end{array} \right) = 0,$$

(16)

where

$$F_0^l = \left( \begin{array}{c} F_{0,0}^l \\ F_{1,0}^l \\ \vdots \\ F_{q-1,0}^l \end{array} \right), \quad F_2^l = \left( \begin{array}{c} F_{0,0}^l \\ F_{1,0}^l \\ \vdots \\ F_{q-1,0}^l \end{array} \right),$$

and

$$F_{0,1}^l = -D_{0} \left[ \sum_{j=1}^{q-1} C_{ij}^{l+} \phi_{j+}^{l+} + \sum_{j=1}^{q-1} C_{ij}^{l-} \phi_{j}^{l+} \right],$$

(18)

$$F_{2,1}^l = -D_{2} \left[ \sum_{j=1}^{q-1} C_{ij}^{l+} \phi_{j+}^{l-} + \sum_{j=1}^{q-1} C_{ij}^{l-} \phi_{j}^{l-} \right].$$

(19)

in which $P$ corresponds to the total number of inner boundary elements in the system, $L_p$ corresponds to the number of nodal points on the boundary element $l_p$, and $F_{0,1}^l$ and $F_{2,1}^l$ correspond to the continuity conditions of the derivatives of $\phi_0$ and $\phi_2$ on the $l$-th nodal point of the boundary element $l_p$. The problem of determining the correct eigenvalue and inner boundary conditions is then reduced to the problem of determining the roots of Eq. (16). While the eigenvalue and the $2 \times 1 = \sum_{p=1}^P L_p$ inner boundary conditions (i.e., $\phi_{0,1}^{l+}, \phi_{1,1}^{l+}$) are unknown, the number of the continuity conditions, expressed by Eq. (15), is $2L$. Thus it is required to add another condition. In the conventional HDD-BEM, the following scaling equation is added:

$$F' = 1 - \sum_{p=1}^P \sum_{j=1}^{L_p} \sum_{l=1}^{2} \phi_{j,l}^{l+} = 0. \quad (20)$$

The roots of Eqs. (16) and (20) are searched iteratively by Newton’s method as follows:

$$F(\phi'_{n}, k^{(n)}) = \left( \begin{array}{c} F_{0,1}^{(n)} \\ F_{2,1}^{(n)} \end{array} \right), \quad \phi'_{n} = \left( \begin{array}{c} \phi_{0,1}^{(n)} \\ \phi_{1,1}^{(n)} \end{array} \right),$$

(21)

$$\phi'_{n+1} = \phi_{n} + \frac{\phi'_{n}}{\phi_{n}} \text{ evaluated at } \phi'_{n}.$$

(22)

where $n$ denotes the number of iterations and the vector $\phi'$ is composed of $\phi_{0,1}^{l+}, \phi_{1,1}^{l+}$. The Jacobian matrix $J^{(n)}$ is defined as

$$J^{(n)} = \left( \begin{array}{cc} J_{\phi_{0,1}^{(n)}} & J_{\phi_{1,1}^{(n)}} \\ 0 & 0 \end{array} \right),$$

(23)

where

$$J_{\phi_{0,1}^{(n)}} = \left( \frac{\partial F_{0,1}^{(n)}}{\partial \phi_{0,1}^{(n)}} \right), \quad J_{\phi_{1,1}^{(n)}} = \left( \frac{\partial F_{2,1}^{(n)}}{\partial \phi_{1,1}^{(n)}} \right), \quad J_{\phi_{0,1}^{(n)}} = \left( \frac{\partial F_{0,1}^{(n)}}{\partial \phi_{0,1}^{(n)}} \right).$$

(24)

The sizes of these Jacobian submatrices $J_{\phi_{0,1}^{(n)}}$, $J_{\phi_{1,1}^{(n)}}$ and $J_{\phi_{0,1}^{(n)}}$ are $(2L \times 2L)$, $(2L \times 1)$ and $(1 \times 2L)$, respectively.

When the total number of nodal points on the inner boundaries is large, it is difficult to solve matrix Eq. (21) directly. Thus in the HDD-BEM, the block Jacobi method is applied to obtain $\delta k$ and Newton’s method is applied to obtain $\delta \phi$ as follows.

At the $m$th iteration of Newton’s method which modifies the value of $\delta k$ to $\delta k^{(m)}$, the values of $\delta \phi'$ on the inner boundaries are modified iteratively by the following procedure using the results of the previous iteration:

$$\delta \phi_{0,1}^{(m)} = \frac{\phi'_{m}}{\phi_{m}} - \left( J_{\phi_{0,1}^{(m)}} \right)^{-1} \left( \sum_{q=1}^{P} J_{\phi_{0,1}^{(m)}} - F_{0,1}^{(m)} \right),$$

(25)

where the superscript $m$ denotes the iteration number of the block Jacobi method. Note that the inversion of the Jacobian sub-matrix $J_{\phi_{0,1}^{(m)}}$ can be done once before the Newton’s method iteration for $\delta k$ since this matrix does not depend on $\phi_{0,1}^{(m)}$.

When the iteration process with the block Jacobi method is carried out, the value of $\delta k^{(m)}$ is modified by Newton’s method as

$$\delta k^{(m)} = \delta k^{(m-1)} - \delta k^{(m-1)} - \int_{C} \delta \phi_{0,1}^{(m)} + F_{c},$$

(26)

where $\delta \phi_{0,1}^{(m)}$ is a converged solution of the block Jacobi method at the $m$th Newton’s method iteration.

The above mentioned procedure based on Newton’s method can find all the eigenvalues and eigenvectors of the system as discussed in Purwadi et al. (1996). In order to achieve convergence to the fundamental mode solution, the proper setting of initial estimates for the eigenvalue and eigenvector is necessary.

2.4. Boundary condition treatment

In the SP3 equation, the following Marshak-like boundary conditions are usually used for vacuum boundaries:

\[
\begin{align*}
\frac{1}{3} \phi_0 + D_3 \nabla \phi_0 &= \frac{3}{8} \phi_2, \\
\frac{21}{40} \phi_2 + \frac{27}{35} D_2 \phi_2 &= \frac{3}{40} \phi_0.
\end{align*}
\]

(27)

(28)

These equations are described by the mode fluxes as

\[
\begin{align*}
\frac{1}{3} \sum_{j=1}^{N} C_{0j} \phi_j + D_3 \sum_{j=1}^{N} C_{0j} \nabla \phi_j &= \frac{3}{8} \sum_{j=1}^{N} C_{0j} \phi_j, \\
\frac{21}{40} \sum_{j=1}^{N} C_{2j} \phi_j + \frac{27}{35} D_2 \sum_{j=1}^{N} C_{2j} \phi_j &= \frac{3}{40} \sum_{j=1}^{N} C_{0j} \phi_j.
\end{align*}
\]

(29)

(30)

As shown in Eqs. (29) and (30), fluxes and their derivatives of different modes couple with each other. It is the same as with the vacuum boundary conditions for the diffusion equation. In the previous studies of the HDD-BEM for diffusion equations, the values of boundary fluxes and their derivatives of different modes were assumed to be those at the previous iteration step. In the present study, the same technique is utilized.

2.5. Volume-integrated neutron flux calculation

After convergence, mode fluxes and their derivatives on all the inner boundaries are determined. Thus mode flux at an arbitrary position inside each homogeneous region can be calculated by solving Eq. (13).

On the other hand, volume-integrated neutron flux is easily calculated. For example, volume-integrated \( \phi_0 \) is calculated as

\[
\int_{V_r} \phi_0 \, dr = \int_{V_r} \sum_{j=1}^{N} C_{0j} \phi_j \, dr = \sum_{j=1}^{N} C_{0j} \int_{V_r} \phi_j \, dr
\]

\[
= - \sum_{j=1}^{N} C_{0j} \left( \frac{1}{B_{0j}} \int_{V_r} \nabla^2 \phi_j \, dr - \int_{V_r} B_{0j} \phi_j \, ds \right) = \sum_{j=1}^{N} C_{0j} \int_{S_r} \phi_j \, ds.
\]

(31)

In this derivation, the relation \( \nabla^2 \phi_j + B_{0j}^2 \phi_j = 0 \) is used.

3. Verification

3.1. Calculation procedure and benchmark system

In order to verify the HDD-BEM for the SP3 equation, we developed a computer code, ABEMIE, as one of the solvers in a reactor physics simulation code system CBG (Chiba, 2008). The ABEMIE is written using the C++ computer language and can solve one- or two-group SP3 equations and one- or two-group diffusion equations. This code can treat an arbitrary two-dimensional geometry which is composed of lines. The maximum number of nodal points on a boundary element is four. Thus mode fluxes and their derivatives can be expanded at most by third-order polynomials. When two or more nodal points are assigned to a boundary element, the boundary element is treated as a non-conforming element even if it does not include any corner points. The locations of the nodal points are denoted with a non-dimensional quantity \( \xi \). The positions of the extremes of boundary elements correspond to \( \xi = \pm 1.0 \) and the position of the mid-point corresponds to \( \xi = 0 \).

The locations of nodal points are \( \xi = 0 \) for constant elements, \( \xi = \pm 0.65 \) for linear elements, \( \xi = \pm 0.85 \) and \( \xi = 0 \) for quadratic elements, and \( \xi = \pm 0.85 \) and \( \xi = \pm 0.3 \) for cubic elements.

The initial estimate for the eigenvalue is 1.0, and a constant value is given to the inner boundary conditions as an initial estimate. In order to accelerate the iteration for estimation of the eigenvalue and inner boundary conditions, the Aitken acceleration method is applied.

As a benchmark system, we choose the three-region hexagonal problem with anisotropic-scattering described in Hèbert (2010b). This benchmark is not representative of real-life problems but is designed to magnify transport and anisotropic effects both inside and on the vacuum boundary of the domain. This benchmark system is depicted in Fig. 2 and the cross section data are shown in Table 1. Please note that calculations using ABEMIE are performed for this one-sixth core model with reflective boundary conditions.

Table 2 summarizes results of the diffusion and SP3 calculations with ABEMIE. For the spatial discretization, constant, linear, quadratic, and cubic boundary elements are employed. \( N_{\text{tot}} \) corresponds to the total number of unknowns in the calculations. In order to compare with \( N_{\text{tot}} \) of the TRIVAC whole-core calculations, \( N_{\text{tot}} \) of the ABEMIE calculations are multiplied by six since ABEMIE calculates a one-sixth core. The \( N_{\text{tot}} \) value of the TRIVAC calculation is cited from Hèbert (2010b).

In the diffusion calculation results, large errors are observed in both the eigenvalue and the assembly-wise neutron fluxes even if cubic boundary elements are employed. This is due to errors in the diffusion theory, and these results are consistent with the former results obtained by Hèbert (2010b). Regarding the SP3 calculation results, it is found that the eigenvalue and the assembly-wise neutron fluxes converge to the reference solutions as finer boundary elements are employed. The quadratic boundary elements are sufficiently accurate to spatially discretize the mode fluxes and their

**Table 2:** Description of the hexagonal-geometry 2D one-group benchmark.
expansions, yields results that are nearly consistent with the reference. By using this coarser option, $N_{\text{tot}}$ is reduced to 20,078, which is yet larger than the $N_{\text{tot}}$ of ABEMIE. This is one of advantages of the BEM-based method over the other spatial discretization methods. Note that the matrix structure also significantly affects the convergence property and the effectiveness of the numerical method. A more detailed comparison between the present HDD-BEM and FEM-based methods is necessary in future.

Figs. 3 and 4 show errors in the assembly-wise neutron fluxes in the diffusion and SP$_3$ calculations, respectively. While the diffusion calculations result in large errors around the core peripheral region, these large errors disappear in the SP$_3$ results.

### 4. Concluding remarks

In the present paper, the HDD-BEM, which has been developed to solve diffusion equations, is applied to the SP$_3$ equation. The HDD-BEM solution for the SP$_3$ equation is provided in the present paper. A computer program, ABEMIE, based on the HDD-BEM has been developed, and a two-dimensional one-group anisotropic-scattering benchmark problem is solved with it to verify the present HDD-BEM for the SP$_3$ equation.

Through numerical benchmarking, it has been shown that the present method results in good agreement with the solution obtained by using the existing SP$_3$ solver based on the finite element method for both eigenvalue and neutron flux distribution with a smaller number of unknowns. This benchmark result suggests that the HDD-BEM can be an efficient solver for the SP$_3$ equation. Extension of the present method to three-dimensional and multi-group problems is the next subject. The extension to three-dimensional problems can be carried out as performed for diffusion problems (Chiba et al., 2001b). The extension to multi-group problems may not be straightforward since the number of modes becomes larger than 2 and some of the buckling values $B_i^n$ can take imaginary values if we apply the present method to multi-group SP$_3$ equations. A remedy for such a problem, however, has already been reported in Cossa et al. (2010). The extension to multi-group problems may be possible using this technique.

Please note that an application of one of the BEM-based methods, the BERM method, to the SP$_3$ equation has just recently been published (Giusti et al., 2010). Comparison of the present method with the BERM method also can be a future subject.

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### References


