B.A.R.C.-1268

B.A.R.C.-1268

FEMSYN - A CODE SYSTEM TO SOLVE MULTIGROUP DIFFUSION THEORY EQUATIONS USING A VARIETY OF SOLUTION TECHNIQUES

Part 4 : SYNTHD - The Synthesis Module

by

V. Jagannathan
Theoretical Physics Division

1985

B. A. R. C. - 1268

GOVERNMENT OF INDIA
ATOMIC ENERGY COMMISSION

B. A. R. C. - 1268

FEMSYN - A CODE SYSTEM TO SOLVE MULTIGROUP DIFFUSION THEORY EQUATIONS USING A VARIETY OF SOLUTION TECHNIQUES

Part 4 : SYNTHD - The Synthesis Module

by
V. Jagannathan
Theoretical Physics Division

BHABHA ATOMIC RESEARCH CENTRE
BOMBAY, INDIA
1985

BARC-1268

INIS Subject Category : E2100; F5100

Descriptors

NEUTRON DIFFUSION EQUATION

MULTIGROUP THEORY

F CODES

S CODES

EIGENVALUES

NEUTRON FLUX

REACTOR CORES

FINITE DIFFERENCE METHOD

FINITE ELEMENT METHOD

ABSTRACT

For solving the multigroup diffusion theory equations in 3-D problems in which the material properties are uniform in large segments of axial direction, the synthesis method is known to give fairly accurate results, at very low computational cost. In the code system FEMSYN, we have incorporated the single channel continuous flux synthesis option. One can generate the radial trial functions by either finite difference method (FDM) or finite element method (FEM). The axial mixing functions can also be found by either FDM or FEM. Use of FEM for both radial and axial directions is found to reduce the calculation time considerably. One can determine eigenvalue, 3-D flux and power distributions with FEMSYN. In this report we give a detailed description of the synthesis module SYNTHD.

FEMSYN - A CODE SYSTEM TO SOLVE MULTIGROUP DIFFUSION THEORY EQUATIONS USING A VARIETY OF SOLUTION TECHNIQUES

Part - 4 SYNTHD - The Synthesis Module

by
V. Jagannathan

1. INTRODUCTION

Multigroup diffusion theory equations are solved for obtaining the detailed flux and power distributions in a nuclear reactor. One has to frequently solve the problem in three dimensions also. The use of the most straight forward method, viz the finite difference method (FDM) leads to large number of unknowns for a reasonably good accuracy requirement, especially in case of light water reactors. For the prasent day PWRs with a fuel assembly size of 20X20 cm one must use at least 25 meshes/box in order to guarantee a good accuracy on the final 3-D flux solution. Finite element method (FEM), on the other hand, has been shown by many authors to give very accurate results with the use of a mesh size as large as one mesh per fuel box or even larger[1-2]. However application of FEM to 3-D problems has received a setback[3-4] mainly due to the inherent hurdles associated with the method with regard to the computation, storage and inversion of highly banded sparse matrix of the 3-D problem[5-6]. Now we note that the reactors are generally less heterogeneous in axial direction than in radial plane. During the last two decades single channel flux synthesis (SCFS) method and its several variations[7-9] have been in use for such 3-D problems. The SCFS method takes advantage of the relatively large homogeneous sections of axial direction which allows the 3-D problem to be broken into a set of 2-D trial function generation

followed by an one dimensional calculation for the mixing functions. The main factor blocking the widespread use of synthesis method is the difficulty in choosing appropriate trial function and the lack of theory to estimate error bounds. However from the evidence of the available literature one may safely conclude that a knowledgeable user can exploit the potentiality of the synthesis methods to obtain at a low cost accurate estimates of eigenvalue, reaction rates, rod worths etc. for both thermal and fast reactors. In the synthesis work mentioned above one uses FDM for determining both trial functions and mixing functions. Since FEM has been found to be succeessful in 1-D and 2-D problems, we have developed a SCFS method where both 2-D trial functions and 1-D mixing functions are evaluated by FEM. Thus we have combined the merits of both FEM and SCFS method and evolved a method called finite element synthesis model[10] (FESM) and incorporated it in the FEMSYN code. In this report we give a description of the SYNTHD module of FEMSYN code system.

2. DERIVATION OF EQUATIONS

2.1 Synthesis Approximation

The three dimensional flux $\phi^g(x,y,z)$ for group 'g' is expanded by means of a linear combination of known trial functions[7],

$$\phi^g(x,y,z) = \sum_{k=1}^{K} H_k^g(x,y)\, Z_k^g(z) \qquad (1)$$

or $$\underline{\phi} = \sum_{k=1}^{K} \underline{H}_k(x,y)\, \underline{Z}_k(z)$$

where K is total number oftrial functions in each group, $H_k^g(x,y)$ are known trial functions in radial plane (evaluated by either

FDM or FEM). $Z_k^g(z)$ are unknown mixing functions in axial direction.

$$\underset{=k}{H} - \text{diag.}(H_k^1, H_k^2, \ldots\ldots H_k^G)$$

$$\underset{-k}{Z} - \text{col.}(Z_k^1, Z_k^2, \ldots\ldots Z_k^G)$$

G - Total number of energy groups

Similar expansion is made for the adjoint flux.

$$\varphi^{*g}(x,y,z) = \sum_{k=1}^{K} H_k^{*g}(x,y)\, Z_k^{*g}(z) \qquad (2)$$

or $$\underset{-}{\varphi^*} = \sum_{k=1}^{K} \underset{=k}{H^*}(x,y)\, \underset{-k}{Z^*}(z)$$

We adopt the variational method[7] to obtain the equations for the mixing functions $\underset{k}{Z}(z)$. Consider the bilinear functional,

$$F(\underset{-}{\varphi^*}, \underset{-}{\varphi}) = \int_V [\underset{-}{\varphi^*}^T (\underset{=}{A}\,\underset{-}{\varphi} - \frac{1}{\lambda}\underset{=}{M}\,\underset{-}{\varphi}) + \nabla\underset{-}{\varphi^*}^T . \underset{=}{D}\nabla\underset{-}{\varphi}]\, dv \qquad (3)$$

$$\underset{-}{\varphi} - \text{col.}(\varphi^1, \varphi^2, \ldots\ldots \varphi^G)$$

$$\underset{-}{\varphi^*} - \text{col.}(\varphi^{*1}, \varphi^{*2}, \ldots\ldots \varphi^{*G})$$

$$\underset{=}{A} - \text{GXG matrix } (\Sigma^{gg'})$$

$$\underset{=}{M} - \text{GXG matrix } (\chi^g \nu\Sigma_f^{g'})$$

$$\underset{=}{D} - \text{diag. } (D^1, D^2, \ldots\ldots D^G)$$

V - total reactor volume

Here $\varphi^g, \varphi^{*g}, D^g, \chi^g, \Sigma_f^g, \Sigma^{gg}$ are respectively the neutron flux, its adjoint, diffusion coefficient, fraction of fission neutrons, fission cross section and total removal cross section appropriate to energy group 'g'. $-\Sigma^{gg'}$ is scattering transfer cross section

from group g' to g. ν is number of neutrons born per fission.

When the functional $F(\varphi^*,\varphi)$ is required to be stationary for arbitrary infinitesimal variations in the adjoint flux, one obtains the multigroup diffusion equations as the Euler-Lagrange equations

$$-\nabla.\underline{D}\,\nabla\varphi + \underline{A}\,\varphi = \frac{1}{\lambda}\underline{M}\,\varphi \qquad (4)$$

subject to the conditions that the current $-\underline{D}\nabla\varphi$ is continuous within volume V and on the surface 'S' bounding the volume V the flux or the current vanishes. For other type of (inhomogeneous) boundary conditions appropriate surface terms could be added subsequently. Thus we follow only a partial variational formulation.

Substituting the expansions (1) and (2) in functional (3) and requiring stationarity of the reduced functional $F(\underline{Z}^*,\underline{Z})$ with respect to $\underline{Z}^*_j$ we would obtain the equations for the mixing functions $\underline{Z}_k$.

$$F(\underline{Z}^*,\underline{Z}) = \int_0^L dz \int_A dxdy \left[\left(\sum_{j=1}^{K} \underline{H}^* Z^*_j \right)^T \left(\left(\underline{A} - \frac{1}{\lambda}\underline{M}\right) \left(\sum_{k=1}^{K} \underline{H}\, Z_k \right) \right) + \nabla\left(\sum_{j=1}^{K} \underline{H}^* Z^*_j \right)^T . \underline{D} \nabla \left(\sum_{k=1}^{K} \underline{H}\, Z_k \right) \right] \qquad (5)$$

L is height of reactor and 'A ' is area of radial plane.

$$\delta Z^{*T}_{-j} \frac{\partial F}{\partial \underline{Z}^*_{-j}} = 0 = \sum_{k=1}^{K} \int_0^L dz\, \delta Z^{*T}_{-j} \left[\int_A dxdy\, \underline{H}^*_{=j} \left(\underline{A} - \frac{1}{\lambda}\underline{M}\right)_{=k} \underline{H}_{-k} + \int_A dxdy\, \nabla_{xy} \underline{H}^*_{=j} . \underline{D} \nabla_{xy} \underline{H}_{=k} \underline{Z}_{-k} - \nabla_z . \left(\int_A dxdy\, \underline{H}^*_{=j} \underline{D}_{=k} \nabla_z \underline{Z}_{-k} \right) \right] \qquad (6)$$

where, $\nabla = \nabla_{xy}\,\vec{m} + \nabla_{z}\,\vec{k}$ with $\vec{m}$ being a unit vector in the radial plane and $\vec{k}$ a unit vector in the axial direction. The surface integral resulting from the divergence term has been assumed to vanish because of the homogeneous boundary conditions stated above.

Defining,

$$A_{=jk} = \int_{Ar} dxdy\; H^{*}_{=j}\; A\; H_{=k} \qquad (7\text{-a})$$

$$M_{=jk} = \int_{Ar} dxdy\; H^{*}_{=j}\; M\; H_{=k} \qquad (7\text{-b})$$

$$DBZ_{===jk} = \int_{Ar} dxdy\; \nabla_{xy} H^{*}_{=j} \cdot D\nabla_{xy} H_{=k} \qquad (7\text{-c})$$

$$D_{=jk} = \int_{Ar} dxdy\; H^{*}_{=j}\; D\; H_{=k} \qquad (7\text{-d})$$

we would obtain the stationarity conditions as

$$\sum_{k=1}^{K} \left[\left(A_{=jk} + DBZ_{===jk} - \frac{1}{\lambda} M_{=jk} \right) Z_{-k}(z) - \nabla.D_{=jk}\, \nabla Z_{-k}(z) \right] = 0 \qquad j=1,2\ldots K \qquad (8)$$

which gives K equations for the mixing functions Z_{-k}.

2.1.1 Evaluation of Radial Integrals

a) Trial functions by FDM

When the trial functions are evaluated by centre mesh finite difference method, the surface integrals of (7-a), (7-b) and (7-d) can be evaluated in a similar manner. They simply reduce to summation over each mesh volume Vi. For instance, A^{hg}_{jk} is found as, (h,g being group indices)

$$A^{hg}_{jk} = \sum_{i=1}^{N} H^{*h}_{j,i}\; \Sigma^{hg}_{i}\; H^{g}_{k,i}\; V_{i} \qquad (9)$$

$H^{g}_{k,i}$ is the value of k^{th} trial function of group g in mesh i, $H^{*h}_{j,i}$ is the value of the adjoint of j^{th} trial function of group h in mesh i, Σ_i^{hg} is the cross section property of mesh i and Vi

is the volume (area) of mesh i. N is total number of meshes in radial plane.

The leakage matrix DBZ is diagonal. It is found as

$$DBZ^{gg}_{jk} = \int_{Ar\,xy\,j} \nabla H^{*g}_{g\,xy\,j} .D \nabla H^{g}_{g\,xy\,k}\, dxdy$$

$$= \sum_i \int_{Vi\;xy\,j} \nabla H^{*g}_{g\,xy\,j} .D \nabla H^{g}_{g\,xy\,k}\, dxdy$$

$$= \sum_i \left(\left[H^{*g}_{i\;j} .D \nabla H^{g}_{g\,xy\,k} \right]_{\Omega i} - \int_{Vi\;j} \nabla H^{*g}_{xy\;g\,xy\,k} .D \nabla H^{g}_{g\,xy\,k}\, dxdy \right)$$

The first term on r.h.s. vanishes because of continuity of adjoint flux and current and the homogeneous boundary conditions on the external boundary. Therefore,

$$DBZ^{gg}_{jk} = - \sum_{i\;j,i} H^{*g}_{i} \int_{Vi\;xy\;g\,xy\,k} \nabla .D \nabla H^{g}\, dxdy$$

$$= \sum_{i\;j,i} H^{*g}_{i} \int_{Vi\;g\;xy\,k} (-D \nabla H^{g}) \cdot \vec{n}\, ds \qquad \text{(Green's theorem)}$$

$$= \sum_{i\;j,i} H^{*g}_{i} \sum_{m\;g,im\;k,i\;k,m} \bar{D}_{g,im} (H^{g}_{k,i} - H^{g}_{k,m}) * S_{im} \qquad \text{(Refer part 2 of this report)} \qquad (10)$$

Here m is any of the four neighbours of i.

$$\bar{D}_{g,im} = \frac{2}{\left[\frac{hi}{D_{g,i}} + \frac{hm}{D_{g,m}} \right]} \qquad (11)$$

S_{im} is the surface area of the boundary interface between 'i' and 'm'.

b) Trial functions by FEM

The trial functions are represented by a finite element model. Within an element 'e', we write for group 'g' (with the

group subscript 'g' being implicitly assumed)

$$H_k^{(e)} = P_{-e}^T(x,y)\, H_{-k,e} \qquad (12)$$

where $H_{k,e}$ is the vector of discrete nodal flux values for the element 'e' and the vector P_e is a low order Lagrange interpolation polynomial function. It can be defined in terms of the natural coordinates (ξ,η) within the element 'e'. (see Appendix B of part 2 of this report). We assume that the interpolation functions are the same for all trial functions, for all groups and for direct and adjoint fluxes. Substituting the form of H_k and H^*_j from eq.(12) into eqs.(7) one can find that the integrals A_{jk}^{hg}, M_{jk}^{hg} and D_{jk}^{hg} can be evaluated in a manner similar to

$$A_{jk}^{hg} = \sum_e \int_{Ve} dxdy\, H^{*h}_j \sum_{(e)} H^g_k$$

$$= \sum_e \sum_{(e)} (H^{*h}_{-j,e})^T \left(\int_{Ve} P_{-e}\, P_{-e}^T dxdy \right) H^g_{-k,e} \qquad (13)$$

The radial buckling term DBZ_{jk}^{gg} is given by

$$DBZ_{jk}^{gg} = \sum_e D_{(e)}^g (H^{*h}_{-j,e})^T \left(\int_{Ve} \nabla P_{-e} \cdot \nabla P_{-e}^T dxdy \right) H^g_{-k,e} \qquad (14)$$

Ve is the area of the element 'e'. The matrices $\int_{Ve} P_{-e}\, P_{-e}^T dxdy$ and $\int_{Ve} \nabla P_{-e} \cdot \nabla P_{-e}^T dxdy$ are the element submatrices which are described in Appendix B of part 2 of this report. They are independent of the trial function and energy group. It may be observed here that when the trial functions satisfy already the appropriate radial boundary conditions the eq.(14) is sufficient to get the correct radial buckling $\underline{\underline{DBZ}}_{jk}$ and it is not necessary to add any further

surface terms.

The radial integrals are to be evaluated separately for each of the distinct coarse mesh axial zones which have axially homogeneous properties.

2.2 Solution of the 1-D Mixing Functions

a) Mixing functions by FDM

The one dimensional equations for the mixing functions, eq.(8), is finite differenced in the same way like normal diffusion theory equation. In place of D, Σ_a etc. we have surface integrals which can be regarded as weighted average of the absorption, production and diffusion properties of the different axial segments.

One can use fine meshes axially. The finite difference form for the mixing functions equation is obtained by integrating eq.(8) over a fine mesh 'i' with height 'hi'

$$\sum_{k=1}^{K} \left\{ h_i \left(A_{=jk} + DBZ^2_{=jk} - \frac{1}{\lambda} M_{=jk} \right) Z_{-k,i} + \sum_{i'=i-1,i+1} D^{-ii'}_{=jk} \left(Z_{-k,i} - Z_{-k,i'} \right) \right\} = 0 \qquad j=1,2,\ldots K \qquad (15)$$

$$D^{-g,ii'}_{jk} = \frac{2}{\left[\frac{hi}{D^{g,i}_{jk}} + \frac{hm}{D^{g,i'}_{jk}} \right]}$$

The matrix of eq.(15) can be recognised as block tri-diagonal matrix which can be easily inverted by generalised forward elimination and backward substitution. This will be explained in section 3.

b) Mixing Functions by FEM

The z-dependence of the one-d functions $Z_k(z)$ will be represented by piecewise Lagrange polynomials in each axial segment or element considered in the axial direction. For the purpose of introducing the finite element approximation we shall rewrite eq.(8) explictly for group 'g'.

$$\sum_{k=1}^{K}\sum_{g=1}^{G}\left(L^{hg}_{jk}\,Z^{g}_{k}(z) - \nu\Sigma^{hg}_{z,jk}\,\nu Z^{g}_{z,k}(z)\right) = 0 \qquad \begin{matrix} j=1,2\ldots K \\ h=1,2\ldots G \end{matrix} \tag{16}$$

where $L^{hg}_{=jk} = A^{hg}_{=jk} + DBZ^{hg}_{==jk} - \frac{1}{\lambda}M^{hg}_{=jk}$

The mixing function $Z_k^g(z)$ is approximated as

$$Z^{g}_{k}(z) = \sum_{e=1}^{E} P^{T}_{-e}(z)\,\alpha^{g}_{-k,e} = \sum_{e=1}^{E} P^{T}_{-e}\,J^{\alpha}_{=e}\,\alpha^{g}_{-k} \tag{17}$$

Here P_e is nx1 vector of known Lagrange polynomials where n is number of nodes in element 'e'. E is total number of elements. $\alpha^g_{k,e}$ is nx1 vector giving the values of the unknown mixing functions $Z^g_k(z)$ at the nodes of the element 'e'. α^g_k is Nx1 vector giving the values of $Z^g_k(z)$ function at the N nodes where N is the total number of nodes in axial direction. J_e is a boolean transformation matrix of order nxN, which is used to pick up the element vector $\alpha^g_{k,e}$ from the global vector α^g_k. α^g_k are the new unknowns for finite element discretisation.

We can get the equations for α^g_k by method of weighted residuals. We can use Galerkin weighting. Substituting eq.(17) in eq.(16) and using weight function as $J_e^T P_e$ within element 'e' and integrating over z, we get

$$\sum_{k=1}^{K}\sum_{g=1}^{G}\sum_{e=1}^{E} J^{T}_{=e}\left(L^{hg(e)}_{jk} + D^{hg(e)}_{=e\,jk}\,G^{g}_{=e}\right)J^{\alpha}_{=e-k} = 0 \qquad \begin{matrix} j=1,2\ldots K \\ h=1,2\ldots G \end{matrix} \tag{18}$$

where,

$$\underline{I}_e = \int_{Ve} \underline{P}_{-e}^T \underline{P}_{-e} \, dz$$

$$\underline{G}_e = \int_{Ve} \underline{\nabla P}_{z-e}^T \underline{\nabla P}_{z-e} \, dz \qquad (19)$$

$\underline{I}_e$ and $\underline{G}_e$ are 1-D element submatrices of order n. They are easily evaluated within an axial segment for any Lagrange polynomial of a given degree.

3. METHODS OF SOLUTION

Eqs.(15) or Eqs.(18) represent the set of linear equations for NxKxG unknowns of the mixing coefficient functions, N being number of points in axial direction. When linear polynomial is used in FEM method of solution, the associated matrix will have the same block-tridiagonal structure like that for FDM, though in case of FEM the off-diagonal blocks would comprise of both diffusion and removal terms whereas in case of FDM they are pure diffusion terms. For higher order polynomials, the FE-synthesis matrix would be block-penta (quadratic) or block-hepta (cubic) diagonal matrix. The solution of the FE-synthesis equation is therefore more complicated. FD-synthesis matrix is a sub-set of FE-synthesis matrices and hence we will describe the methods of solution of the latter only.

The multigroup problem has to be solved by the standard inner-outer iteration procedure. Iterative scheme of solution for the inner loop will however require large number of iterations since the associated matrix is highly banded. It is desirable therefore to obtain the solution directly without any iterations.

The equations for the mixing functions of a given group 'g' can be written as

$$\underline{B}^g \underline{\alpha}^g = \underline{f}^g \qquad (20)$$

Here $\underline{B}^g$ is a matrix of order (KxN) computed from the diagonal matrices $\underline{D}_{jk}$, $\underline{DBZ}_{jk}$ and diagonal part of $\underline{A}_{jk}$. $\underline{f}^g$ is a column vector of size (KxN) computed from $\underline{M}_{jk}$ and the off-diagonal terms of $\underline{A}_{jk}$. $\underline{\alpha}^g$ is the column vector of size (KxN) representing the unknown mixing functions of a given group.

For simplicity we will drop the subscript 'g' in the subsequent discussions.

If we assume the vector $\underline{\alpha}$ to be composite of N subvectors each of order K stacked in order of the nodes 1 to N and the matrix $\underline{B}$ also to be partitioned into the corresponding submatrices of order K, we can make a few remarks about the structure of the matrix.

The typical structures of the matrix $\underline{B}$ are shown in figures 1,2 and 3 for the cases of linear, parabolic and cubic polynomial approximations respectively. Three elements have been considered in axial direction for the purpose of illustration.

As was mentioned earlier we get block tri-diagonal, block penta-diagonal and block-hepta diagonal matrices respectively for linear, quadratic and cubic polynomials. The matrices are block symmetric because the element submatrices $\underline{Ge}$ and $\underline{Ie}$ are symmetric. If we use Galerkin weighting method, i.e., if we choose the trial functions $H_j{}^h$ themselves, instead of the adjoint functions $H^*{}_j{}^h$ as weighting functions, the matrix $\underline{B}$ will not only be block symmetric but completely symmetric. In this case the Choleski decomposition method offers the most efficient means of

solution. When we have only block symmetry (i.e. adjoint weighting scheme), we can use band elimination method generalised for block structure. We shall describe application of these two methods in the following.

3.1 Choleski Decomposition Method

In this method we ignore, temporarily, the partitions between the submatrices and subvectors, i.e., the distinction between trial function index and global axial node number. The matrix $\underline{B}$ is computed and stored in a compact one-dimensional form, row by row and in each row from first non-zero element upto the diagonal element as shown in Fig.4 (see also part 3 of this report). Since there are no fill-in zeroes in any row, there is no increase in storage requirement. (rather it is less compared to other methods since only symmetric part of even the diagonal blocks needs to be stored). The scheme of storage, called locally variable bandwidth storage scheme (LVB), also reduces the storage requirement. We need to compute, however, one additional vector of size (KxN) which gives the position of the diagonal elements in the one dimensional storage of the matrix $\underline{B}$. The matrix $\underline{B}$ is then decomposed into the product of a lower triangular matrix $\underline{L}$ and its transpose $\underline{L}^T$. The elements of $\underline{L}$ are obtained by using the recursion relations[12],

$$
\begin{aligned}
l_{ii} &= \left[b_{ii} - \sum_{k=1}^{i-1} l_{ik}^2 \right]^{1/2} && 1 \le i \le (KXN) \\
l_{ij} &= \left[b_{ij} - \sum_{k=1}^{j-1} l_{ik}\, l_{jk} \right] / l_{jj} && 1 \le i \le (KXN) \\
& && j < i
\end{aligned}
\qquad (21)
$$

Once we know $\underline{L}$, the unknown vector $\underline{\alpha}$ can be obtained by simple forward elimination and backward substitution, because $\underline{L}$ and $\underline{L}^T$ are triangular matrices. In addition $\underline{L}$ has the same 'outward structure' as the matrix $\underline{B}$ and in fact can be stored in the same memory space that was occupied by $\underline{B}$. The solution procedure involves operations of matrix elements within the variable bandwidth store only.

The subroutines for the Choleski decomposition $\underline{L}\,\underline{L}^T$ and the solution of the vector $\underline{\alpha}$, when the matrix $\underline{B}$ is stored in compact one dimensional storage, are given by Jennings[13] in very concise form. The same routines are usable for our matrix $\underline{B}$, provided the position of the diagonal element in the row '(s-1)xk +r', representing r^{th} trial function of s^{th} node, is properly computed and the matrix $\underline{B}$ is also assembled accordingly. We have not examined the possibility of 'l_{ii}' of eq.(21) becoming imaginary. Despite the fact that the matrix $\underline{B}$ is not necessarily positive definite, we did not encounter such difficulty for the sample problems that were tried.

3.2 Block Band Elimination Method

For a symmetric banded matrix and not a blocked one, it is possible to use the Gauss's elimination method, popularly known as triangularisation method. The elimination operations are carried out within the half band above the main diagonal and hence the method is called diagonal band elimination method[13-14] We will carry out similar operations for the block symmetric banded matrix.

The matrix $\underline{B}$ can be symbolically represented in a block symmetric banded form as shown in Fig.5. In this figure we have shown only the block matrices below the main diagonal. In case of quadratic polynomial the semibandwidth is three and hence there are three (KKK) blocks appearing in any column. We store the matrix $\underline{B}$ column block by column block and in each column block from the diagonal block upto the semi-bandwidth, i.e., $\underline{B}$ is stored as

$$(\underline{b}_{11}, \underline{b}_{12}, \underline{b}_{13} | \underline{b}_{22}, \underline{b}_{23}, \underline{0} | \underline{b}_{33}, \underline{b}_{34}, \underline{b}_{35} | \ldots.)$$

It is seen that a few null matrices are also stored in $\underline{B}$ so as to have constant band-width. Because the problem is one dimensional one can easily avoid these null matrices and use variable bandwidth.

Our first aim is to reduce the matrix $\underline{B}$ to upper triangular form. To achieve null matrices below the first diagonal block we carry out the elimination operation on second and higher order row blocks as,

$$\underline{b}^{(1)}_{ij} = \underline{b}_{ij} - \underline{b}_{i1} \underline{b}^{-1}_{11} \underline{b}_{1j} \qquad i,j>1 \qquad (22)$$

The superscript (1) denotes first reduction operations. This operation will be required to be carried out only within the band i.e. upto third block row, here. We then obtain null matrices below the 2^{nd}, 3^{rd}.... diagonal blocks by successive reduction operations. The n^{th} block row will be reduced (n-1) times. The general equation for the n^{th} reduction of i^{th} block row is written as,

$$\underline{b}^{(n)}_{ij} = \underline{b}^{(n-1)}_{ij} - \underline{b}^{(n-1)}_{ni} (\underline{b}^{(n-1)}_{nn})^{-1} \underline{b}^{(n-1)}_{nj} \qquad i,j> n \qquad (23)$$

Eq.(13) is a simple recursion relation by which the matrix $\underline{B}$ can be reduced into an upper triangular block matrix.

Similar reduction operations are carried out on the column vector which consists of N subvectors of order K.

$$\underline{f}_{-i}^{(1)} = \underline{f}_{-i} - \underline{b}_{=1i} \underline{b}_{=11}^{-1} \underline{f}_{-1} \qquad i > 1$$

$$\underline{f}_{-i}^{(n)} = \underline{f}_{-i}^{(n-1)} - \underline{b}_{=ni}^{(n-1)} \left(\underline{b}_{=nn}^{(n-1)}\right)^{-1} \underline{f}_{-n}^{(n-1)} \qquad i > n \qquad (24)$$

Eqs.(24) represent the forward elimination operation on the vector $\underline{f}$. The solution of the vector $\underline{\alpha}$ is then obtained by backward substitution.

$$\underline{\alpha}_{-N} = \left[\underline{b}_{=NN}^{(N-1)}\right]^{-1} \underline{f}_{-N}^{(N-1)}$$

$$\underline{\alpha}_{-i} = \left[\underline{b}_{=ii}^{(i-1)}\right]^{-1} \left[\underline{f}_{-i}^{(i-1)} - \sum_{j=i+1}^{i+w-1} \underline{b}_{=ij}^{(i-1)} \underline{\alpha}_{-j}\right] \qquad i=N-1,N-2,\ldots 2,1 \qquad (25)$$

W - Semibandwidth

It is seen from eqs.(24) and (25) that for the solution of the vector $\underline{\alpha}$ we require only the decomposed or reduced blocks of the matrix $\underline{B}$. Therefore we normally carry out the decomposition operations of eq.(23) on matrix $\underline{B}$ and store the decomposed matrix in the same memory space of $\underline{B}$ so that when we have different source vectors computed at every outer iteration, we need to carry out only the forward elimination and backward substitution operations on the vector $\underline{f}$.

The block band elimination method is slightly more expensive than Choleski decomposition method, since, in general, it requires more storage and greater computational effort. However, it has wider scope than the latter since one can use arbitrary

weighting functions. Also we have seen that there is some possibility of the diagonal elements 'l_{ii}' of the Choleski decomposed matrix becoming imaginary in which case, the band elimination method should guarantee the solution.

In any case the two methods are more efficient than the iterative method of solution as will be shown in section 4.

3.3 Eigenvalue Calculation

The eigenvalue is calculated by power iteration method.

$$\lambda^n = \lambda^{n-1} \frac{\left| \underline{FS}^n \right|}{\left| \underline{FS}^{n-1} \right|} \qquad (26)$$

where $\underline{FS}^n$ is fission source vector of order (KxN) computed using $\underline{M}_{jk}$ and $\underline{a}^n$.

Two parameter Chebyschev acceleration which is explained in parts 2 and 3 of the present report is applied for the above fission source vector as well. It is found to be very beneficial.

4. COMPARISON OF THE METHODS OF SOLUTION

To demonstrate the efficiency of direct methods of solution we analysed the same 3-D IAEA benchmark problem[15] which was studied in our earlier work[10].

We have incorporated in the module 'SYNTHD' of FEMSYN all the solution methods discussed above and in addition an iterative method of solution is also built-in. The description of this benchmark problem is given in part 1 of the present report.

Two trial functions were considered which correspond to the rod-out and rod-in conditions of the partially inserted control rod. FE method of solution and quadratic polynomials were used for both radial trial functions and axial mixing functions.

Twenty one elements were considered in axial direction. Axially mesh size in core was 20cm and in reflector it was 10cm. Zero incurrent boundary condition was used in all directions. Only Galerkin weighting scheme was adopted.

In Table-I, the eigenvalue, thermal flux peak and CPU time on BESM-6 computer for the three different methods of solution are given. We have also added a column corresponding to the finite difference method of solution for the mixing functions with 9t meshes in axial direction. For all the calculations 100 outer iterations were required to achieve the convergence on eigenvalue of $2x10^{-5}$. It is seen that the different techniques of solving matrix equation for the finite element approximation give identical results and compare very well with the finite difference method of solution with somewhat fine mesh size.

The Choleski method is faster than the band elimination method as expected. The iterative method of solution requires 5.5 times the computational time as that of Choleski method for the sample problem. In fact if one uses iterative method of solution, the finite element method for mixing functions becomes much slower than the finite difference method even though the number of unknowns are reduced.

5. CONCLUSIONS

We have incorporated in the SYNTHD module of the FEMSYN code system FD as well as FE method of solution for the mixing functions. The associated complicated matrix equations have been successfully solved by two direct methods of solution and an iterative method also. It is found that the Choleski decomposition method gives fastest solution while block band

elimination method has wider scope when arbitrary weighting functions are used. The finite difference method requires somewhat more time than the direct methods of the FE method of solution, but is still faster than the iterative method of solution of FE method of solution for mixing functions.

The FE-synthesis model is quite fast and can be advantgeously used in transient problems like control rod drop accident where we can use time-independent trial functions.

Acknowledgements

The author is grateful to Dr. F. Pistella and G.P. Cali of CNEN, Rome, Italy for their encouragement and help in fulfilling part of this work when the author underwent IAEA fellowship training in their research centre during 1977 - 1978. It is a pleasure to acknowledge the encouragement provided by s/Shri K.R.Srinivasan and B.P.Rastogi to carry out this work. The author is thankful to Shri T.K.Sudhir for meticulous typing of this report.

REFERENCES

1. L.O. Deppe and K.F. Hansen, Nucl. Sci. Eng. 54, p.456 (1974).

2. H. Komariya and W.F. Waters, Nucl. Sci. Eng. 64, p.576 (1977).

3. M.R. Wagner, 'Current Trends in Multidimensional Static Reactor Calculations', ANS Topical Mtg. on Comp. Meth. in Nucl. Eng., Charleston, CONF-750413, Part 1, p.I-1, (1975)

4. C.H. Adams, Nucl. Sci. Eng., 64, p.552 (1977).

5. H.P. Franke et.al., Atomkernenergie, 26, p.158 (1975)

6. A. Kavenoky and J.J. Lautard, Nucl. Sci. Eng., 64, p.563 (1977).

7. S. Kaplan, Nucl. Sci. Eng., 13, p.22 (1962).

8. J.B. Yasinsky and S. Kaplan, Nucl. Sci. Eng., 28, p.426 (1967)

9. W.M. Stacey,Jr., 'Variational Flux Synthesis Approximations, Proc. Conf. Numerical Reactor Calculations, IAEA-SM-54/17 p.561 (1972).

10. V. Jagannathan and G.P. Cali, Atomkernenergie,35, p.25 (1980).

11. J.K. Reid ed., 'Large Sparse Sets of Linear Equations', Academic Press, London 1971. (see A. Jennings and A.D. Tuff, 'A Direct Method of Solution of Large Sparse Symmetric Simultaneous Equations', for 'A backing store version of the variable bandwidth method')

12. D.K. Faddeev and V.N. Faddeeva, 'Computational Methods of Linear Algebra', Translated from Russian by R.C. Williams, W.H. Freeman & Co. (1963).

13. A.Jennings,'Matrix Computation for Engineers and Scientists', A Wiley Interscience Publication, John Wiley & Sons (1977).

14. L.J.Segerlind,'Applied Finite Element Analysis',John Wiley & Sons Inc. (1976)

15. B.Micheelson and H.Neltrup,'The 3-D IAEA Benchmark Problem', RISO - M - 1572 (1973).

Table-I Comparison of Different Methods of Solution for 3-D IAEA Benchmark Problem

Code/Model	FEMSYN/Finite Element Synthesis			
Method of solution for mixing functions	Finite Element			Finite Difference
	Choleski	Band elimination	Iteration	Forward Elimination +Backward Substitution
No. of trial functions	2	2	2	2
No. of axial meshes	21	21	21	90
Polynomial order	2	2	2	-
Unknowns per mixing function	43	43	43	90
K-effective	1.0293195	1.0293195	1.0293194	1.0292949
$\varphi^{th}_{max} / \varphi^{th}_{avg}$	2.496	2.496	2.496	2.505
Location (x,y,z)	(30,30,170)	(30,30,170)	(30,30,170)	(30,30,177.5)
CP time for iterations on BESM-6* (sec)	58	85	318	110

* BESM-6 computer is about eight times slower than IBM 370/168 computer

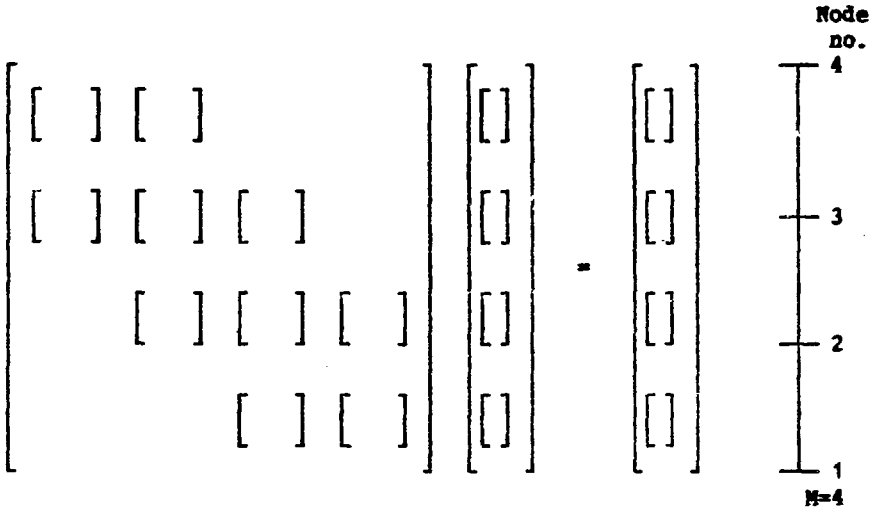


Fig.1 Structure of Matrix B in Case of Linear Polynomial (3 - Elements)

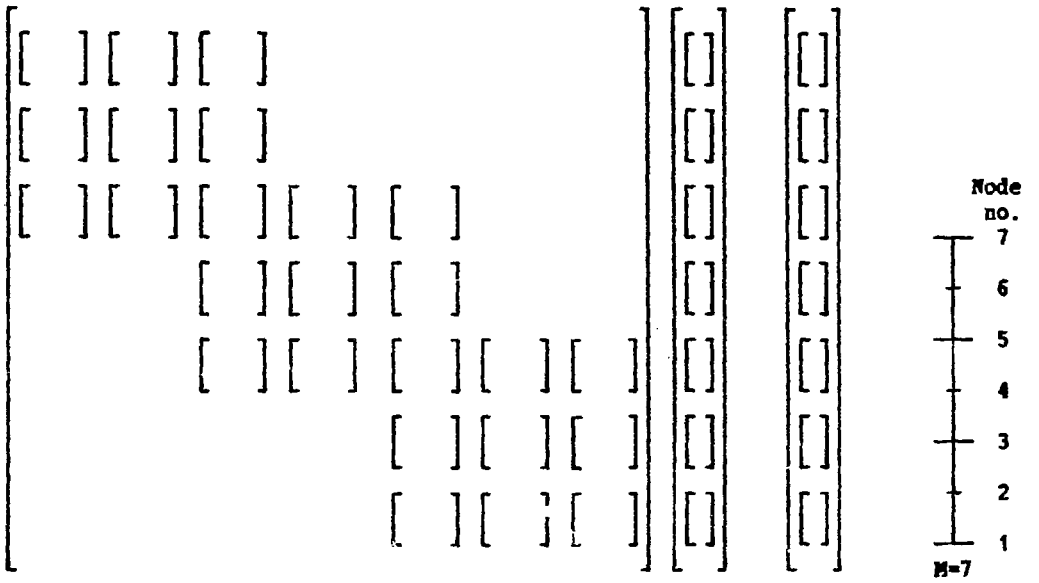


Fig.2 Structure of Matrix B in Case of Quadratic Polynomial (3 - Elements)

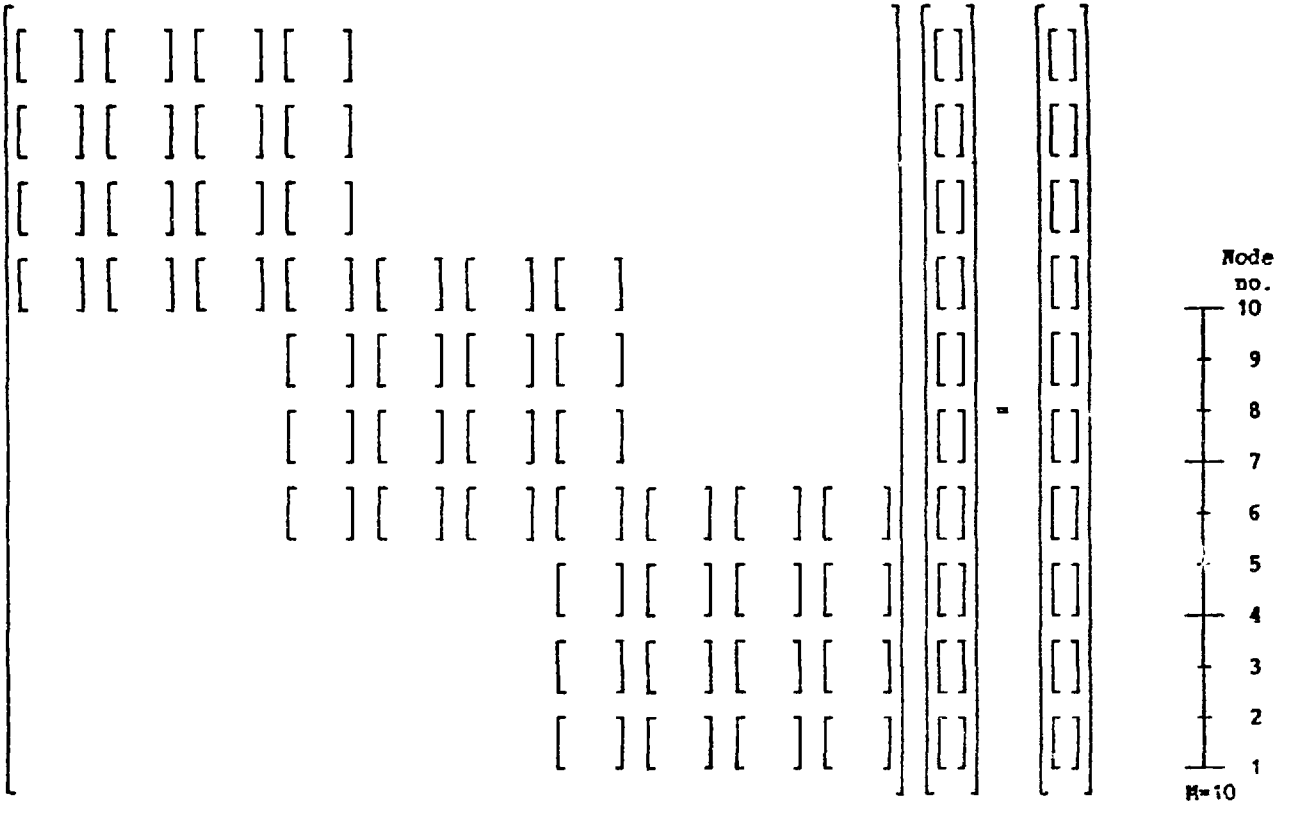
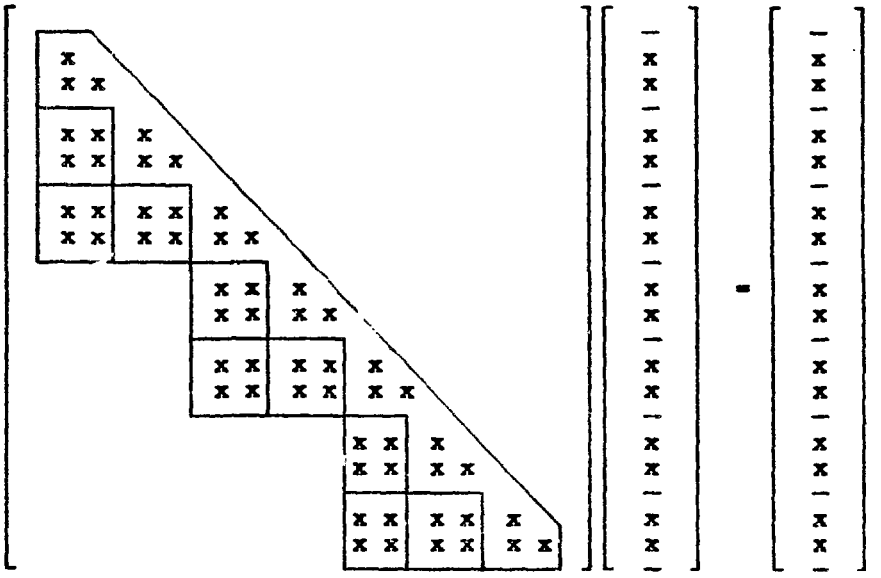


Fig.3 Structure of Matrix B in Case of Cubic Polynomial (3 - Elements)



No. of trial functions K=2
No. of nodes M=7
Polynomial order =2

Fig.4 Storage of Matrix B in Case of Choleski Decomposition Method

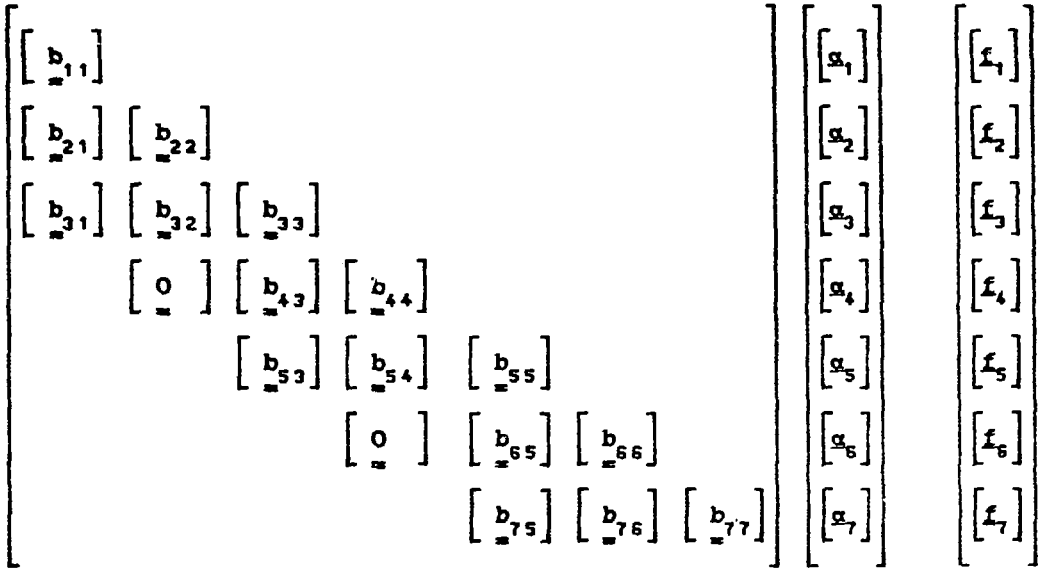


Fig.5 Storage of Matrix B in Case of Block Band Elimination Method

Published by Head, Library & Information Services, BARC, Bombay 400 085, India.