

THE NUMERICAL ANALYSIS OF EIGENVALUE PROBLEM SOLUTIONS IN THE MULTIGROUP NEUTRON DIFFUSION THEORY

Zbigniew, I. Woznicki

Institute of Atomic Energy
05-400 Otwock-Swierk, Poland

ABSTRACT

In the paper a general iteration strategy for solving the discrete form of multidimensional neutron diffusion equations is described. Usually the solution method is based on the system of inner and outer iterations. The present-matrix formalism allows us to visualize clearly, how the used matrix splitting influences the structure of the matrix in an eigenvalue problem to be solved as well as the interdependence between inner and outer iterations within global iterations.

To keep a page limit, the present version of the paper consists only with first three of five sections given in the original paper under the same title (which will be published as soon).

1. INTRODUCTION

The neutron diffusion theory is the most widely used method in the analysis of criticality of nuclear reactors. The consideration of criticality is generally referred to as an eigenvalue problem for the multigroup neutron diffusion equations which solution provides the reactivity eigenvalue, i.e., the effective multiplication factor and power profiles in large scale reactors subject to nonuniform fuel loading and depletion [1]. Hence the numerical solution for realistic heterogeneous reactor problems requires detailed neutron diffusion calculations in either two- or three-dimensional geometries.

In the next section the matrix form of multigroup neutron diffusion equations is formulated together with describing the structure of matrices and solution properties. Iterative strategies based on different levels of (global, outer, inner) iterations are presented for single splittings in Section 3. In the original paper the same iterative strategies are discussed for double splittings [10] in Section 4 and results of numerical experiments on some realistic reactor problems for different iterative strategies are given in Section 5.

2. PROBLEM FORMULATION

The time-independent multigroup neutron diffusion equations representing a system of coupled elliptic partial differential equations of the second order can be written, as follows

$$-\nabla D_g(r) \nabla \phi_g(r) + \Sigma_g^r(r) \phi_g(r) - \sum_{g \neq g'} \Sigma_{g'g}^s(r) \phi_{g'}(r) = \frac{1}{\lambda} \chi_g \sum_1^G \nu \Sigma_g^f(r) \phi_g(r) \quad (2.1)$$

$$g = 1, 2, \dots, G$$

where notation is standard [1,4]. The following group-dependent boundary conditions

earlier developments see, for example, References given in [2,5].

The matrix \mathbf{E} is nonsingular and monotone, i.e., its inverse is nonnegative, where each A_g^{-1} is a positive matrix, i.e., $A_g^{-1} > 0$, and the eigenvalue problem (2.3) can be written in the following form

$$\lambda\psi = \mathbf{B}\psi \quad (2.6)$$

where

$$\mathbf{B} = \mathbf{E}^{-1}\mathbf{X}\mathbf{F}^T \geq 0 \quad (2.7)$$

For solving the above eigenvalue problem, much effort have been devoted over the last four decades to the development of efficient iterative methods and implemented in numerous computer codes (see, e.g. References in [4,7]). A large class of methods for determining the eigenvalue of largest modulus λ and the corresponding eigenvector φ_1 is based on the power method [2,8] in which successive estimates for λ_1 and φ_1 are generated by the process

$$\varphi(l+1) = \frac{1}{\lambda(l)}\mathbf{B}\varphi(l) \quad (2.8)$$

and

$$\lambda(l+1) = \lambda(l) \frac{\|\varphi(l+1)\|_p}{\|\varphi(l)\|_p} \quad (2.9)$$

where l is the iteration index and two norms either maximum $\|\cdot\|_\infty$ or Euclidean $\|\cdot\|_2$ are most commonly used. Since the largest (in modulus) eigenvalue λ_1 of the nonnegative matrix \mathbf{B} is positive and simple, the power method is a convergent process for almost randomly chosen nonnegative starting vector $\varphi(0)$, i.e.

$$\lambda(l) \rightarrow \lambda_1, \quad \varphi(l) \rightarrow \varphi_1 \quad \text{as } l \rightarrow \infty$$

The rate of convergence in the power method is governed by the *subdominance ratio* (according to the terminology proposed in [8])

$$\sigma(\mathbf{B}) = |\lambda_2|/|\lambda_1| \quad (2.10)$$

assuming that the eigenvalues λ_i of the matrix \mathbf{B} are ordered in such a way that

$$\lambda_1 > |\lambda_2| \geq |\lambda_3| \geq \dots \quad (2.11)$$

The smaller the subdominance ratio, the faster the convergence. Assuming that for sufficiently large values of l , $\lambda(l)$ is approximately equal to λ_1 , we can equivalently consider the problem

$$\varphi(l+1) = \mathbf{B}(\lambda_1)\varphi(l) \quad (2.12)$$

where

$$\mathbf{B}(\lambda_1) = \frac{1}{\lambda_1} \mathbf{E}^{-1}\mathbf{X}\mathbf{F}^T \quad (2.13)$$

has eigenvalues $\nu_{B,1} = \lambda_1/\lambda_1$ and according to the above ordering, we have

$$\nu_{B,1} = \rho[\mathbf{B}(\lambda_1)] = 1 > |\nu_{B,2}| \geq |\nu_{B,3}| \geq \dots$$

and

$$\sigma(\mathbf{B}) \equiv \sigma[\mathbf{B}(\lambda_1)] = |\nu_{B,2}| \quad (2.14)$$

2.1 REDUCED PROBLEM

Since the rank of the matrix \mathbf{F} is only N , the eigenvalue problem (2.6) with the order of $G \times N$ can be reduced to the variant with the order of N which ite-

rates on the fission source vector [2,4]

$$\psi = F^T \varphi \quad (2.15)$$

Multiplying Eq.(2.6) by F^T and using (2.7) and (2.15), one obtains the reduced problem

$$\lambda \psi = O \psi \quad (2.16)$$

where

$$O = F^T E^{-1} X \geq 0 \quad (2.17)$$

Both matrices $B = (E^{-1}X)(F^T)$ and $O = (F^T)(E^{-1}X)$ have the same rank and their nonzero eigenvalues are identical but this denotes that both eigenvalue problems given by Eqs.(2.6) and (2.16) are mathematically equivalent.

The fundamental eigenvalue λ_1 and the corresponding eigenvector ψ_1 which represents fission sources can be obtained by means of the power method described previously.

In actual practice Chebyshev polynomials on the flux vector φ_1 or on the fission source ψ_1 are usually used to accelerate the convergence of the power iterations [2,3,4]. The application of Chebyshev polynomials is based on the assumptions that the eigenvalues of B (or O) are real, nonnegative and ordered in such a way that $\lambda_1 > \lambda_2 \geq \lambda_3 \geq \dots \geq \lambda_N \geq 0$, and the corresponding eigenvectors form a basis for the N -dimensional vector space. However, these hypotheses may be not true in some multigroup neutron diffusion problems.

2.2 BASIC PROBLEM

In the considerations given above, it was assumed that the matrix E^{-1} is given explicitly. In the case of one-dimensional problems however, with the absence of upscattering process, i.e., $S^u = 0$, it is often possible to solve the eigenvalue problem (2.6) directly. In two and three dimensions the inversion of E has proven impractical and a special iterative strategy must be used.

Eq.(2.3) together with Eq.(2.4) can be rewritten as

$$A\varphi = S^d \varphi + S^u \varphi + \frac{1}{\lambda} X F^T \varphi \quad (2.18)$$

and introducing the iteration index l , one obtains

$$A\varphi(l+1) = S^d \varphi(l+1) + S^u \varphi(l) + \frac{1}{\lambda(l)} X F^T \varphi(l) \quad (2.19)$$

or equivalently

$$\varphi(l+1) = A^{-1} [S^d \varphi(l+1) + S^u \varphi(l) + \frac{1}{\lambda(l)} X F^T \varphi(l)] \quad (2.20)$$

The fact that S^d is a strictly lower triangular block matrix allows us to use the components of φ obtained in the latest iteration $l+1$. After completing the calculations for the iteration $l+1$, a new value of $\lambda(l+1)$ is estimated according to the formula given by Eq.(2.9). The above equation can be represented in the following form

$$\varphi(l+1) = T(\lambda(l)) \varphi(l) \quad (2.21)$$

where

$$T(\lambda(l)) = [I - A^{-1} S^d]^{-1} A^{-1} [S^u + \frac{1}{\lambda(l)} X F^T] \quad (2.22)$$

As can be seen the entries of $T(\lambda(l))$ change from iteration to iteration in dependence on changes of $\lambda(l)$ and for sufficiently large values of l , $\lambda(l)$ becomes close to λ_1 and

$$T(\lambda(l)) \rightarrow T(\lambda_1) = [I - A^{-1} S^d]^{-1} A^{-1} [S^u + \frac{1}{\lambda_1} X F^T] \geq 0 \quad (2.23)$$

Assuming that the eigenvalues of $T(\lambda_1)$ are ordered, as follows

$$\nu_{T,1} = \rho[T(\lambda_1)] = 1 > |\nu_{T,2}| \geq |\nu_{T,3}| \geq \dots$$

then for sufficiently large values of l the rate of convergence of iteration process (2.20) is governed by the subdominance ratio

$$\sigma\{T(\lambda_1)\} = |\nu_{1,2}| \quad (2.24)$$

It is evident that with the absence upscattering, i.e., when $S^u = 0$,

$$T(\lambda_1) = B(\lambda_1)$$

The iterative process represented by Eq.(2.20) is referred to as "fission source iteration" or alternatively as "outer iteration" however, for its implementation, it is necessary to have the inverses of the submatrices A_g forming the block diagonal structure of A visualized in (2.5). In one-dimensional problems A_g are three diagonal matrices which inverting can be easily done by the well known forward elimination - backward substitution procedure [2]. For two- and three-dimensional problems the matrices A_g have more than three diagonals and moreover its order is much greater than that in one-dimensional case, so that the inversion of A_g becomes impractical or simply impossible respect to round-off errors. In this case an approximate inversion of A_g is usually done iteratively through a series of "inner iterations". The strategies of different levels of iterations are presented in the next section.

3. SINGLE SPLITTING ITERATIVE STRATEGIES

Inhomogeneous solutions appearing in multigroup diffusion problems are referred to the iterative solution of the linear equation system

$$A\phi = c \quad (3.1)$$

which can be expressed in the form

$$M\phi^{(t+1)} = N\phi^{(t)} + c, \quad t \geq 0 \quad (3.2)$$

where $\phi^{(t)}$ denotes the successive iterates and

$$A = M - N \quad (3.3)$$

represents the *single splitting* of the $N \times N$ nonsingular matrix A as the classical splitting of A in the theory of iterative methods. The above iterative scheme is convergent to the unique solution

$$\phi = A^{-1}c \quad (3.4)$$

for each $\phi^{(0)}$ if and only if M is a nonsingular matrix and the corresponding iteration matrix

$$\mathcal{G} = M^{-1}N \quad (3.5)$$

has the spectral radius

$$\rho(\mathcal{G}) = \max |\gamma_i| < 1, \quad 1 \leq i \leq N \quad (3.6)$$

where γ_i are eigenvalues of \mathcal{G} . Eq.(3.2) can be written in the equivalent form

$$\phi^{(t+1)} = \mathcal{G}\phi^{(t)} + M^{-1}c, \quad t \geq 0 \quad (3.7)$$

or in terms of $\phi^{(0)}$

$$\phi^{(t+1)} = \mathcal{G}^{t+1}\phi^{(0)} + \bar{M}_{(t)}^{-1}c, \quad t \geq 0 \quad (3.8)$$

where

$$\bar{M}_{(t)}^{-1} = (I + \mathcal{G} + \mathcal{G}^2 + \dots + \mathcal{G}^t)M^{-1} = \sum_{i=0}^t \mathcal{G}^i M^{-1} \quad (3.9)$$

From Eq.(3.3) it follows that

$$A^{-1} = (I - M^{-1}N)^{-1}M^{-1} = (I - \mathcal{G})^{-1}M^{-1} \quad (3.10)$$

hence

$$\mathbf{M}^{-1} = (\mathbf{I} - \mathcal{G})\mathbf{A}^{-1} \quad (3.11)$$

Substituting Eq.(3.11) into Eq.(3.9), one obtains

$$\bar{\mathbf{M}}_{(t)}^{-1} = (\mathbf{I} - \mathcal{G}^{t+1})\mathbf{A}^{-1} \quad (3.12)$$

Since by the assumption $\rho(\mathcal{G}) < 1$, \mathcal{G}^t approaches the null matrix when $t \rightarrow \infty$ and consequently $\bar{\mathbf{M}}_{(t)}^{-1} \rightarrow \mathbf{A}^{-1}$, and the solution of (3.8) tends to the unique solution defined by Eq.(3.4) with arbitrary $\phi^{(0)}$. In the convergence analysis of iterative methods the (*asymptotic*) rate of convergence

$$R(\mathcal{G}) = -\ln\rho(\mathcal{G}) \quad (3.13)$$

is certainly the simplest practical measure in the rapidity of convergence for a convergent matrix \mathcal{G} and especially useful for comparing the efficiency of different iterative methods [3,8].

The matrix $\bar{\mathbf{M}}_{(t)}^{-1}$ can be considered as approximating \mathbf{A}^{-1} , which in some sense represents a incomplete inverse of \mathbf{A} after t iterations, and therefore $\bar{\mathbf{M}}_{(t)}^{-1}$ is called the *preinversioner of t -degree* of the matrix \mathbf{A} , where $\bar{\mathbf{M}}_{(\infty)}^{-1} = \mathbf{A}^{-1}$, and $\bar{\mathbf{M}}_{(0)}^{-1} = \mathbf{M}^{-1}$ is the preinversioner of *0-degree* of the matrix \mathbf{A} .

Convergence behaviour is usually studied by examining the *error vector* defined by

$$\mathbf{e}^{(t+1)} = \phi - \phi^{(t+1)} \quad (3.14)$$

Specifically for $\phi^{(0)} = 0$, one obtains

$$\mathbf{e}^{(t+1)} = \mathbf{A}^{-1}\mathbf{c} - \bar{\mathbf{M}}_{(t)}^{-1}\mathbf{c}$$

hence by Eq.(3.12)

$$\mathbf{e}^{(t+1)} = \mathcal{G}^{t+1}\mathbf{A}^{-1}\mathbf{c} \quad (3.15)$$

Thus, the solution of Eq.(3.8) obtained after t iterations with $\phi^{(0)} = 0$ corresponds to the solution obtained for the preinversioner $\bar{\mathbf{M}}_{(t)}^{-1}$, and its error vector respect to the unique solution is determined by Eq.(3.15).

3.1 GLOBAL ITERATIONS

Assuming that the splitting of \mathbf{A} is represented by the following matrix form

$$\mathbf{A} = \begin{bmatrix} \mathbf{A}_1 & & & \\ & \mathbf{A}_2 & \mathbf{0} & \\ & & \cdot & \\ \mathbf{0} & & & \cdot \\ & & & & \mathbf{A}_G \end{bmatrix} = \mathbf{M} - \mathbf{N} = \begin{bmatrix} \mathbf{M}_1 & & & \\ & \mathbf{M}_2 & \mathbf{0} & \\ & & \cdot & \\ \mathbf{0} & & & \cdot \\ & & & & \mathbf{M}_G \end{bmatrix} - \begin{bmatrix} \mathbf{N}_1 & & & \\ & \mathbf{N}_2 & \mathbf{0} & \\ & & \cdot & \\ \mathbf{0} & & & \cdot \\ & & & & \mathbf{N}_G \end{bmatrix} \quad (3.16)$$

Eq.(2.18) can be written, as follows

$$\mathbf{M}\varphi = \mathbf{N}\varphi + \mathbf{S}^d\varphi + \mathbf{S}^u\varphi + \frac{1}{\lambda}\mathbf{X}\mathbf{F}^T\varphi \quad (3.17)$$

and introducing the iteration index l , one obtains

$$\mathbf{M}\varphi(l+1) = \mathbf{N}\varphi(l) + \mathbf{S}^d\varphi(l+1) + \mathbf{S}^u\varphi(l) + \frac{1}{\lambda(l)}\mathbf{X}\mathbf{F}^T\varphi(l) \quad (3.18)$$

If the splitting of \mathbf{A} is chosen such that \mathbf{M} is a nonsingular matrix and relatively easy to invert, the above equation can be expressed as

$$\varphi(l+1) = \mathbf{M}^{-1}\{\mathbf{S}^d\varphi(l+1) + \mathbf{N}\varphi(l) + \mathbf{S}^u\varphi(l) + \frac{1}{\lambda(l)}\mathbf{X}\mathbf{F}^T\varphi(l)\} \quad (3.19)$$

or equivalently

$$\varphi(l+1) = \mathbf{V}(\lambda(l))\varphi(l) \quad (3.20)$$

where

$$\mathbf{V}(\lambda(l)) = [\mathbf{I} - \mathbf{M}^{-1}\mathbf{S}^d]^{-1}[\mathbf{V} + \mathbf{M}^{-1}(\mathbf{S}^u + \frac{1}{\lambda(l)}\mathbf{X}\mathbf{F}^T)] \quad (3.21)$$

and the iteration matrix \mathbf{V} , associated with the splitting of \mathbf{A} defined by Eq.(3.16), has the form

$$\mathbf{V} = \mathbf{M}^{-1}\mathbf{N} = \begin{bmatrix} \mathbf{V}_1 & & & \\ & \mathbf{V}_2 & & 0 \\ & & \ddots & \\ 0 & & & \mathbf{V}_G \end{bmatrix} = \begin{bmatrix} \mathbf{M}_1^{-1}\mathbf{N}_1 & & & \\ & \mathbf{M}_2^{-1}\mathbf{N}_2 & & 0 \\ & & \ddots & \\ 0 & & & \mathbf{M}_G^{-1}\mathbf{N}_G \end{bmatrix} \quad (3.22)$$

For sufficiently large values of l , $\lambda(l) \approx \lambda_1$ and

$$\mathbf{V}(\lambda_1) = [\mathbf{I} - \mathbf{M}^{-1}\mathbf{S}^d]^{-1}[\mathbf{V} + \mathbf{M}^{-1}(\mathbf{S}^u + \frac{1}{\lambda_1}\mathbf{X}\mathbf{F}^T)] \quad (3.23)$$

and assuming that the eigenvalues of $\mathbf{V}(\lambda_1)$ are ordered, as follows

$$\nu_{v,1} = \rho[\mathbf{V}(\lambda_1)] = 1 > |\nu_{v,2}| \geq |\nu_{v,3}| \geq \dots$$

the rate of convergence in the iteration process (3.20), representing the *global iteration (l) strategy*, is governed by the subdominance ratio

$$\sigma[\mathbf{V}(\lambda_1)] = |\nu_{v,2}| \quad (3.24)$$

where the index l is referred to global iterations, and the matrix \mathbf{M}^{-1} is the preinverter of zero-order of the matrix \mathbf{A} .

By an analogy to the convergence analysis of iterative methods for solving linear equation systems, one can define the (*asymptotic*) rate of convergence, as follows

$$\dot{\mathbf{R}}(\mathbf{V}) = -\ln\sigma[\mathbf{V}] \quad (3.25)$$

which is useful measure for the rapidity of convergence to the dominant eigenvalue of a given matrix \mathbf{V} in the power method [8]. Since the number of iterations required for obtaining the dominant eigenvalue is roughly inversely proportional to the rate of convergence, the arithmetical effort required for computing the dominant eigenvalue of two different matrices \mathbf{V}_1 and \mathbf{V}_2 , with a given degree of accuracy, by means of the power method can be evaluated by comparing the obtained number of iterations.

The eigenvalue spectrum of $\mathbf{V}(\lambda_1)$ depends on the assumed splitting of the matrix \mathbf{A} . When $\mathbf{A} = \mathbf{M} - \mathbf{N}$ represents a nonnegative splitting of \mathbf{A} [9] (i.e., $\mathbf{M}^{-1} \geq 0$, $\mathbf{M}^{-1}\mathbf{N} \geq 0$ and $\mathbf{N}\mathbf{M}^{-1} \geq 0$) or, its special case, a regular splitting of \mathbf{A} (i.e., $\mathbf{M}^{-1} \geq 0$ and $\mathbf{N} \geq 0$), then $\mathbf{V}(\lambda_1)$ is a nonnegative matrix.

Usually the $N \times N$ submatrices \mathbf{A}_g are defined by the following decomposition

$$\mathbf{A}_g = \mathbf{K}_g - \mathbf{L}_g - \mathbf{U}_g \quad (3.26)$$

where \mathbf{K}_g , \mathbf{L}_g , \mathbf{U}_g are diagonal, strictly lower triangular, and strictly upper triangular matrices, respectively. Moreover these three matrices are nonnegative. Defining the block diagonal matrix \mathbf{A} of Eq.(2.5) in a similar way, i.e.,

$$\mathbf{A} = \mathbf{K} - \mathbf{L} - \mathbf{U} \quad (3.26a)$$

it is evident that the entries of \mathbf{K} , \mathbf{L} and \mathbf{U} are those of \mathbf{K}_g , \mathbf{L}_g and \mathbf{U}_g , for all $g = 1, \dots, G$, respectively. In the majority of numerical problems, iterative schemes are derived from splittings representing the Gauss-Seidel method

[2,3,8] and defined by

$$M_g = K_g - L_g \quad \text{and} \quad N_g = U_g \quad (3.27)$$

or for the block structure

$$M = K - L \quad \text{and} \quad N = U \quad (3.27a)$$

The above equations represent a regular splitting of A (or A_g) and the corresponding iteration matrix \mathcal{L}_1 has the form

$$\mathcal{L}_1 = M^{-1}N = [I - K^{-1}L]^{-1}K^{-1}U \geq 0 \quad (3.28)$$

The SOR method closely related with the Gauss-Seidel method, is represented by the following splitting

$$M_\omega = \frac{1}{\omega}K[I - \omega K^{-1}L] \quad \text{and} \quad N_\omega = \frac{1}{\omega}[\omega U - (\omega-1)K] \quad (3.29)$$

and the associated iteration matrix \mathcal{L}_ω can be written as

$$\mathcal{L}_\omega = M_\omega^{-1}N_\omega = [I - \omega K^{-1}L]^{-1}K^{-1}[\omega U - (\omega-1)I] \quad (3.30)$$

where ω is the relaxation factor. It is evident that for $\omega = 1$, the above equations reduce to Eqs.(3.27a) and (3.28) representing the Gauss-Seidel method.

The eigenvalues of $V(\lambda_1)$ defined by Eq.(3.23) satisfy the equation

$$[I - M^{-1}S^d]^{-1}M^{-1}(N + S^u + \frac{1}{\lambda_1}XF^T)x = \nu x \quad (3.31)$$

or equivalently

$$[N + \nu S^d + S^u + \frac{1}{\lambda_1}XF^T]x = \nu Mx \quad (3.31a)$$

and substituting Eqs.(3.27a) into Eq.(3.31a), one obtains

$$K^{-1}[\nu(L + S^d) + U + S^u + \frac{1}{\lambda_1}XF^T]x = \nu x \quad (3.32)$$

In the case of using Eqs.(3.29) the corresponding equations can be written as

$$V_\omega(\lambda_1)y \equiv [I - M_\omega^{-1}S^d]^{-1}M_\omega^{-1}(N_\omega + S^u + \frac{1}{\lambda_1}XF^T)y = \eta y \quad (3.33)$$

or equivalently

$$[N_\omega + \eta S^d + S^u + \frac{1}{\lambda_1}XF^T]y = \eta M_\omega y \quad (3.33a)$$

and after substituting Eqs.(3.29) into Eq.(3.33a), one obtains

$$K^{-1}[\eta(L + S^d) + U + S^u + \frac{1}{\lambda_1}XF^T]y = \frac{\eta + \omega^{-1}}{\omega}y \quad (3.34)$$

From the above equation, it may be seen an implicate dependence of η on the relaxation factor ω , and as is observed in numerical experiments there is ω_b which minimalizes the subdominance ratio $\sigma[V_\omega(\lambda_1)]$. Moreover the value of ω_b is different from ω_{opt} minimizing the spectral radius of \mathcal{L}_ω in the SOR method. For values of ω such that $1 \leq \omega \leq \omega_b$, $\sigma[V_\omega(\lambda_1)]$ decreases monotonously, and for $\omega_b < \omega \leq \omega_{max} < 2$ a strong increase of $\sigma[V_\omega(\lambda_1)]$ is observed and with ω_{max} the disconvergence of iteration process is occurring. It is interesting to mention that in one of examples of Section 5 given in the original paper only this strategy is most efficient in comparison to others.

3.2 GLOBAL-OUTER ITERATIONS

Denoting the fission source term by

$$f(l) = \frac{1}{\lambda(l)}XF^T\varphi(l) \quad (3.35)$$

Eq.(3.18) can be written as

$$(\mathbf{M} + \mathbf{S}^d)\varphi(l+1) = (\mathbf{N} + \mathbf{S}^u)\varphi(l) + \mathbf{f}(l) \quad (3.36)$$

For fixed $\mathbf{f}(l)$ the cycle of outer iterations $p = 1, 2, \dots, P$ can be performed according to the following scheme

$$(\mathbf{M} + \mathbf{S}^d)\varphi(l+\frac{p}{P}) = (\mathbf{N} + \mathbf{S}^u)\varphi(l+\frac{p-1}{P}) + \mathbf{f}(l) \quad (3.37)$$

or equivalently

$$\varphi(l+\frac{p}{P}) = \mathbf{G}\varphi(l+\frac{p-1}{P}) + [\mathbf{I} - \mathbf{M}^{-1}\mathbf{S}^d]^{-1}\mathbf{M}^{-1}\mathbf{f}(l) \quad (3.38)$$

where

$$\mathbf{G} = [\mathbf{I} - \mathbf{M}^{-1}\mathbf{S}^d]^{-1}\mathbf{M}^{-1}(\mathbf{N} + \mathbf{S}^u) = [\mathbf{I} - \mathbf{M}^{-1}\mathbf{S}^d]^{-1}[\mathbf{V} + \mathbf{M}^{-1}\mathbf{S}^u] \quad (3.39)$$

It is easy to notice that

$$\text{for } p=1, \varphi(l+\frac{1}{P}) = \mathbf{G}\varphi(l) + [\mathbf{I} - \mathbf{M}^{-1}\mathbf{S}^d]^{-1}\mathbf{M}^{-1}\mathbf{f}(l),$$

$$\begin{aligned} \text{for } p=2, \varphi(l+\frac{2}{P}) &= \mathbf{G}\varphi(l+\frac{1}{P}) + [\mathbf{I} - \mathbf{M}^{-1}\mathbf{S}^d]^{-1}\mathbf{M}^{-1}\mathbf{f}(l) \\ &= \mathbf{G}^2\varphi(l) + [\mathbf{I} + \mathbf{G}][\mathbf{I} - \mathbf{M}^{-1}\mathbf{S}^d]^{-1}\mathbf{M}^{-1}\mathbf{f}(l) \end{aligned}$$

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$$\text{for } p=P, \varphi(l+1) = \mathbf{G}^P\varphi(l) + [\mathbf{I} + \mathbf{G} + \mathbf{G}^2 + \dots + \mathbf{G}^{P-1}][\mathbf{I} - \mathbf{M}^{-1}\mathbf{S}^d]^{-1}\mathbf{M}^{-1}\mathbf{f}(l)$$

which can be written in the general form

$$\varphi(l+1) = \bar{\mathbf{V}}(\lambda(l))\varphi(l) \quad (3.40)$$

where

$$\bar{\mathbf{V}}(\lambda(l)) = \mathbf{G}^P + \bar{\mathbf{M}}_{(P-1)}^{-1} \frac{1}{\lambda(l)} \mathbf{X}\mathbf{F}^T \quad (3.41)$$

and

$$\bar{\mathbf{M}}_{(P-1)}^{-1} = \sum_{p=0}^{P-1} \mathbf{G}^p [\mathbf{I} - \mathbf{M}^{-1}\mathbf{S}^d]^{-1} \mathbf{M}^{-1} \quad (3.42)$$

Assuming that for sufficiently large values of l , $\bar{\mathbf{V}}(\lambda(l)) \approx \bar{\mathbf{V}}(\lambda_1)$, and the eigenvalues of $\bar{\mathbf{V}}(\lambda_1)$ are ordered, as follows

$$|\bar{v}_{v,1}| = \rho[\bar{\mathbf{V}}(\lambda_1)] = 1 > |\bar{v}_{v,2}| \geq |\bar{v}_{v,3}| \geq \dots$$

the rate of convergence in the iteration process (3.40), representing the global-outer iteration (l,p) strategy, is governed by the subdominance ratio

$$\sigma[\bar{\mathbf{V}}(\lambda_1)] = |\bar{v}_{v,2}| \quad (3.43)$$

where the index p is referred to outer iterations.

As can be seen for a convergent matrix \mathbf{G} ,

$$\mathbf{G}^P \rightarrow 0 \quad \text{and} \quad \bar{\mathbf{M}}_{(P-1)}^{-1} \rightarrow \mathbf{E}^{-1} \quad (3.44)$$

when $P \rightarrow \infty$, hence, $\bar{\mathbf{V}}(\lambda_1) \rightarrow \mathbf{B}(\lambda_1)$. Thus the matrix $\bar{\mathbf{M}}_{(P-1)}^{-1}$ can be considered as the preinverter of $(P-1)$ -degree of the matrix \mathbf{E} in global-outer iterations. Since, with $P = 1$, this strategy reduces to the global iteration strategy, hence, $\bar{\mathbf{M}}_{(0)}^{-1}$ can be considered as the preinverter of zero-degree of the matrix \mathbf{E} in the global iteration strategy.

This strategy is used in the EQUIPOISE method for which no proofs have been found to guarantee its convergence [6]. However, the necessary and sufficient condition for the convergence of global-outer iterations is this that \mathbf{G} should be a convergent matrix. Assuming that the nonnegative matrix \mathbf{G} defined by Eq.(3.39) has the eigenvalues τ_1 which satisfy the following equation

$$\mathbf{G}\mathbf{x} = \tau\mathbf{x} \quad (3.45)$$

or

$$(\mathbf{N} + \tau\mathbf{S}^d + \mathbf{S}^u)\mathbf{x} = \tau\mathbf{M}\mathbf{x} \quad (3.46)$$

Using the splitting matrices of Eq.(3.27a), one obtains

$$\mathbf{K}^{-1}[\tau(\mathbf{L} + \mathbf{S}^d) + \mathbf{U} + \mathbf{S}^u]\mathbf{x} = \tau\mathbf{x} \quad (3.47)$$

Since the properties of the matrix $\mathbf{E} = \mathbf{A} + \mathbf{S}^d + \mathbf{S}^u$ imply that the nonnegative matrix

$$\mathbf{B} = \mathbf{K}^{-1}[\mathbf{L} + \mathbf{S}^d + \mathbf{U} + \mathbf{S}^u] \quad (3.48)$$

representing the iteration matrix in the Jacobi method is irreducible and its spectral radius is less than unity [2,3], then the spectral radius of the matrix \mathbf{G} , representing in some sense the iteration matrix in the Gauss-Seidel method, is also less than unity and moreover $\rho(\mathbf{G}) < \rho(\mathbf{B})$.

In the case of the splitting matrices of Eq.(3.29) defining the SOR method, one obtains

$$(\mathbf{N}_\omega + \tau\mathbf{S}^d + \mathbf{S}^u)\mathbf{y} = \xi\mathbf{M}_\omega\mathbf{y} \quad (3.49)$$

or

$$\mathbf{K}^{-1}[\xi(\mathbf{L} + \mathbf{S}^d) + \mathbf{U} + \mathbf{S}^u]\mathbf{y} = \frac{\xi + \omega - 1}{\omega}\mathbf{y} \quad (3.50)$$

The above equation shows an implicate dependence of ξ on the relaxation factor ω . As is well known [3], $|\xi| < 1$ for all $1 < \omega < 2$ and exists ω_{opt} which minimizes the dominant eigenvalue ξ_1 , and in the 2-cyclic consistently ordered case

$$\omega_{opt} = \frac{2}{1 + \sqrt{1 - \tau_1}} \quad (3.51)$$

where τ_1 is the dominant eigenvalue of the matrix \mathbf{G} of Eq.(3.45). In general when both matrices \mathbf{S}^d and \mathbf{S}^u are nonnegative the matrix \mathbf{B} has no properties of 2-cyclic consistently ordering and there is no the precise formula for ω_{opt} . In the case when $\mathbf{S}^u = \mathbf{0}$, the matrix \mathbf{B} is block triangular and its eigenvalues are related only with the entries of diagonal submatrices $\mathbf{L}_g + \mathbf{U}_g$, and each of them is 2-cyclic consistently ordered, so that the formula (3.51) can be used.

As is usually observed in practice, the values of ω minimalizing $\sigma[\bar{\mathbf{V}}(\lambda_1)]$ are closely related to the value of ω_{opt} .

3.3 GLOBAL-INNER ITERATIONS

The block structure of Eq.(3.17) allows us, with a fixed index l , to introduce the following cycle of inner iterations, $t = 1, 2, \dots, T_g$, for each group g

$$\mathbf{M}_g \varphi_g(l + \frac{t}{T_g}) = \mathbf{N}_g \varphi_g(l + \frac{t-1}{T_g}) + \mathbf{c}_g(l) \quad (3.52)$$

where

$$\mathbf{c}_g(l) = \sum_{k=1}^{g-1} \mathbf{S}_{k,g}^d \varphi_k(l+1) + \sum_{k=g+1}^G \mathbf{S}_{k,g}^u \varphi_k(l) + \frac{1}{\lambda(l)} \mathbf{X}_g \sum_{k=1}^G \mathbf{F}_k \varphi_k(l) \quad (3.53)$$

is collecting scattering and fission terms for a given group g . Eq.(3.52) can be written in the equivalent form

$$\varphi_g(l + \frac{t}{T_g}) = \mathbf{M}_g^{-1} \mathbf{N}_g \varphi_g(l + \frac{t-1}{T_g}) + \mathbf{M}_g^{-1} \mathbf{c}_g(l) = \mathbf{V}_g \varphi_g(l + \frac{t-1}{T_g}) + \mathbf{M}_g^{-1} \mathbf{c}_g(l) \quad (3.54)$$

and we have

$$\text{for } t=1, \quad \varphi_g(l + \frac{1}{T_g}) = \mathbf{V}_g \varphi_g(l) + \mathbf{M}_g^{-1} \mathbf{c}_g(l)$$

$$\text{for } t=2, \quad \varphi_g(l + \frac{2}{T_g}) = \mathbf{V}_g \varphi_g(l + \frac{1}{T_g}) + \mathbf{M}_g^{-1} \mathbf{c}_g(l)$$

$$= \mathbf{V}_g^2 \varphi_g(l) + (\mathbf{I} + \mathbf{V}_g) \mathbf{M}_g^{-1} \mathbf{c}_g(l)$$

.....

$$\text{for } t=T_g, \quad \varphi(l+1) = \mathbf{V}_g^{T_g} \varphi(l) + (\mathbf{I} + \mathbf{V}_g + \mathbf{V}_g^2 + \dots + \mathbf{V}_g^{T_g-1}) \mathbf{M}_g^{-1} \mathbf{c}_g(l)$$

which can be written as

$$\varphi_g(l+1) = \tilde{V}_g \varphi_g(l) + \tilde{M}_g^{-1} c_g(l) \quad (3.55)$$

where

$$\tilde{V}_g \equiv V_g^{Tg} = (M_g^{-1} N)^{Tg} \quad (3.56)$$

and

$$\tilde{M}_g^{-1} \equiv \tilde{M}_{g, (Tg-1)}^{-1} = \sum_0^{Tg-1} V_g^t M_g^{-1} \quad (3.57)$$

is the preinversioner of $(Tg-1)$ -degree of the matrix A_g .

Defining

$$\tilde{V} = \begin{bmatrix} \tilde{V}_1 & & & \\ & \tilde{V}_2 & & 0 \\ & & \ddots & \\ & 0 & & \tilde{V}_G \end{bmatrix}, \quad \tilde{M}^{-1} = \begin{bmatrix} \tilde{M}_1^{-1} & & & \\ & \tilde{M}_2^{-1} & & 0 \\ & & \ddots & \\ & 0 & & \tilde{M}_G^{-1} \end{bmatrix} \quad \text{and} \quad c(l) = \begin{bmatrix} c_1(l) \\ c_2(l) \\ \vdots \\ c_G(l) \end{bmatrix} \quad (3.58)$$

the group equations (3.55) can be condensed into one equation

$$\varphi(l+1) = \tilde{V}\varphi(l) + \tilde{M}^{-1}c(l) \quad (3.59)$$

or

$$\varphi(l+1) = \tilde{V}\varphi(l) + \tilde{M}^{-1}[S^d\varphi(l+1) + S^u\varphi(l) + \frac{1}{\lambda(l)}\mathbf{X}\mathbf{F}^T\varphi(l)] \quad (3.60)$$

and hence

$$\varphi(l+1) = \tilde{V}(\lambda(l))\varphi(l) \quad (3.61)$$

where

$$\tilde{V}(\lambda(l)) = [\mathbf{I} - \tilde{M}^{-1}S^d]^{-1}[\tilde{V} + \tilde{M}^{-1}(S^u + \frac{1}{\lambda(l)}\mathbf{X}\mathbf{F}^T)] \quad (3.62)$$

Assuming that for sufficiently large values of l , $\tilde{V}(\lambda(l)) \approx \tilde{V}(\lambda_1)$, and the eigenvalues of $\tilde{V}(\lambda_1)$ are ordered, as follows

$$\tilde{\nu}_{v,1} = \rho[\tilde{V}(\lambda_1)] = 1 > |\tilde{\nu}_{v,2}| \geq |\tilde{\nu}_{v,3}| \geq \dots$$

the rate of convergence in the iteration process (3.61), representing the *global-inner iteration* (l, t) strategy, is governed by the subdominance ratio

$$\sigma[\tilde{V}(\lambda_1)] = |\tilde{\nu}_{v,2}| \quad (3.63)$$

where the index t is referred to inner iterations, and T_g may have different values for each g .

As can be seen for each convergent matrix V_g and with $T_g \rightarrow \infty$ for each $g = 1, 2, \dots, G$,

$$\tilde{V} \rightarrow \mathbf{0} \quad \text{and} \quad \tilde{M}^{-1} \rightarrow \mathbf{A}^{-1} \quad (3.64)$$

and

$$\tilde{V}(\lambda_1) \rightarrow \mathbf{T}(\lambda_1) \quad (3.65)$$

where $\mathbf{T}(\lambda_1)$ is defined by Eq.(2.23). When $T_g = 1$ for each $g = 1, 2, \dots, G$, this strategy reduces to the global iteration strategy, hence, $\tilde{M}_{(0)}^{-1}$ can be considered as the preinversioner of zero-degree of the matrix \mathbf{A} in the global iteration strategy.

This global-inner iteration strategy is known in the literature under the name of outer-inner iteration strategy, where index l is referred to outer iterations and t to inner iterations, and is implemented in the majority of computer codes; see, for example, References given in [4,7].

Usually the SOR method, defined by splitting matrices of (3.29), is used

for accelerating inner iterations and since A_g are 2-cyclic consistently ordered matrices the optimum relaxation factor ω_{opt} , which minimalizes the spectral radius of the associated iteration matrix \mathcal{L}_ω (Eq. (3.30)) can be determined by formula (3.51). For increasing values of T_g in all $g = 1, 2, \dots, G$ the eigenvalue spectrum of $\tilde{V}(\lambda(l))$ tends to the eigenvalue spectrum of $T(\lambda(l))$.

3.4 GLOBAL-OUTER-INNER ITERATIONS

The matrix $\tilde{V}(\lambda(l))$ of Eq. (3.62) representing the cycle of inner iterations in all groups, $g = 1, 2, \dots, G$, can be expressed, as follows

$$\tilde{V}(\lambda(l)) = \tilde{G} + [I - \tilde{M}^{-1}S^d]^{-1}\tilde{M}^{-1}\frac{1}{\lambda(l)}\mathbf{X}\mathbf{F}^T \quad (3.66)$$

where

$$\tilde{G} = [I - \tilde{M}^{-1}S^d]^{-1}[\tilde{V} + \tilde{M}^{-1}S^u] \quad (3.67)$$

As is known from Sec. 3.3, when $T_g \rightarrow \infty$ for all $g = 1, 2, \dots, G$,

$$\tilde{V} \rightarrow 0, \quad \tilde{M}^{-1} \rightarrow A^{-1} \quad \text{and} \quad \tilde{V}(\lambda(l)) \rightarrow T(\lambda(l))$$

With the above form of $\tilde{V}(\lambda(l))$ the global iteration scheme can be written as

$$\varphi(l+1) = \tilde{G}\varphi(l) + [I - \tilde{M}^{-1}S^d]^{-1}\tilde{M}^{-1}\frac{1}{\lambda(l)}\mathbf{X}\mathbf{F}^T\varphi(l)$$

Now introducing the scheme for outer iterations represented by index $p=1, \dots, P$, and using the relation of (3.35), one obtains

$$\begin{aligned} \varphi(l+\frac{p}{P}) &= \tilde{G}\varphi(l+\frac{p-1}{P}) + [I - \tilde{M}^{-1}S^d]^{-1}\tilde{M}^{-1}\mathbf{f}(l) = \\ &= \tilde{G}^p\varphi(l) + [I + \tilde{G} + \tilde{G}^2 + \dots + \tilde{G}^{p-1}][I - \tilde{M}^{-1}S^d]^{-1}\tilde{M}^{-1}\mathbf{f}(l) \end{aligned}$$

and for $p = P$

$$\varphi(l+1) = \tilde{\tilde{V}}(\lambda(l))\varphi(l) \quad (3.68)$$

where

$$\tilde{\tilde{V}}(\lambda(l)) = \tilde{G}^P + \tilde{M}_{(P-1)}^{-1}\frac{1}{\lambda(l)}\mathbf{X}\mathbf{F}^T \quad (3.69)$$

and

$$\tilde{M}_{(P-1)}^{-1} = \sum_{p=0}^{P-1} \tilde{G}^p [I - \tilde{M}^{-1}S^d]^{-1}\tilde{M}^{-1} \quad (3.70)$$

Assuming that for sufficiently large values of l , $\tilde{\tilde{V}}(\lambda(l)) \approx \tilde{\tilde{V}}(\lambda_1)$, and the eigenvalues of $\tilde{\tilde{V}}(\lambda_1)$ are ordered, as follows

$$\tilde{\nu}_{v,1} = \rho[\tilde{\tilde{V}}(\lambda_1)] = 1 > |\tilde{\nu}_{v,2}| \geq |\tilde{\nu}_{v,3}| \geq \dots$$

the rate of convergence in the iteration process (3.68), representing the general form of *global-outer-inner iteration* (l, p, t) *strategy*, is governed by the subdominance ratio

$$\sigma[\tilde{\tilde{V}}(\lambda_1)] = |\tilde{\nu}_{v,2}| \quad (3.71)$$

The matrix $\tilde{M}_{(P-1)}^{-1}$ is the preinverter of $(P-1)$ -degree of the matrix \mathbf{E} .

In inner iterations the values of φ are updated within groups with fixed both scattering and fission terms. On the level of outer iterations the values of φ are computed with updating the down-scattering term in a given outer iteration and the up-scattering term is modified between successive outer iterations. After completing the cycle of outer iterations, which is equivalent to one global iteration, the fission term, $\psi(l+1) = \mathbf{F}^T\varphi(l+1)$ (also called the fission source), is recalculated.

It is evident that the strategies described in Sections 3.1, 3.2 and 3.3 are special cases of the global-outer-inner iteration strategy obtained with assuming $P = 1$ and/or $T_g = 1$ for all $g = 1, 2, \dots, G$. Of course, when $P \rightarrow \infty$

$$\tilde{M}_{(P-1)}^{-1} \rightarrow \mathbf{E}$$

As can be seen the structure of the matrix $\tilde{V}(\lambda_1)$ is strictly related with the choice of the splitting matrices \mathbf{M} and \mathbf{N} , and the values of P and T_9 determining the numbers of outer and inner iterations respectively, and each of them influences the subdominance ratio $\sigma[\tilde{V}(\lambda_1)]$. However, their implicit interdependence makes serious difficulties for theoretical investigations of behaviour of the subdominance ratio in dependence on changes of \mathbf{M} , \mathbf{N} , P and T_9 . Hence, it is clear why an empirical approach, for evaluating iteration parameters in different strategies, is used in actual practice. Iteration strategy parameters are usually assumed as dependent on the type of reactor problem.

However, as can be concluded from experience [11,12,13] and the analysis of numerical results presented in Section 5 given in the original paper, the proper choice of splitting matrices \mathbf{M} and \mathbf{N} ($\mathbf{N} = \mathbf{M} - \mathbf{A}$) has a dominant influence on the efficiency of the solution of neutron diffusion theory problems.

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