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**AIRCRAFT
NUCLEAR
PROPULSION
DEPARTMENT**

MASTER

REVISED ITERATION SEQUENCE
IN PROGRAM $F-N$

P.G. FISCHER

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XDC 61-2-131

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P. G. Fischer

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A. J. Rothstein, Supervisor
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ABSTRACT

The present iteration sequence used in the multigroup Program F-N (ANP No. 308) in which one energy lattice sweep, a so-called inner iteration, is performed for each space power distribution sweep, an outer iteration, exhibits a painfully slow convergence rate in the presence of significant "up-scattering" even for the typical ANP reactor where the dominance ratio between fundamental and first harmonic space modes is about five. A revised iteration sequence in which the energy lattice sweep is iterated to a desired convergence before repeating the power iteration is outlined. The revised procedure should significantly reduce the machine time required for this type of problem.

1. INTRODUCTION

Recent application of Program F-N to multithermal group reactor analysis has pointed up the very poor convergence properties of the present iteration sequence in this type of problem. Thus, even in a typical ANP reactor in which the dominance ratio between fundamental and first harmonic space modes is about five and hence for which the usual multigroup analysis (without up-scattering) requires only perhaps eight iterations for 10^{-6} fission eigenvalue convergence ($5^8 \approx 4 \times 10^5$), a 19 thermal group analysis at elevated temperatures where up-scattering terms are significant may easily require more than 100 iterations to converge. This situation may be remedied somewhat by choosing an eigenvalue other than the usual fission production eigenvalue. Unfortunately, such a procedure introduces serious problems of interpretation and, in addition, the alternate eigenvalue choices in the present program will introduce non-physical distortions in the up-scattering terms relative to the down-scattering.

2. THEORY

In order to clarify the convergence problem and the proposed solution we begin by reviewing the iteration sequence used in the present program. The basic eigenvalue equation

$$(L - S)\phi = \frac{1}{\lambda} F\phi, \quad (1)$$

where L is the neutron removal operator,

S is the scatter-transfer operator,

F is the fission-production operator,

is solved by iteration, in the form

$$(L - S_{\text{down}})\phi^{P+1} = \frac{1}{\lambda^P} F\phi^P + S_{\text{up}}\phi^P, \quad (2)$$

where the scattering operator has been split into upper and lower triangular matrices. This procedure is convergent provided the scattering transfer does not itself lead to a critical system, although as pointed out above, the convergence rate is poor for systems where the second term on the right of (2) is important. The eventual

convergence is insured since the inverse of $(L - S_{\text{down}})$ is essentially non-negative as in the usual multigroup problem and both the source terms are non-negative. The dominance ratio, however, is greatly reduced with respect to the equation

$$(L - S)\phi^{P+1} = \frac{1}{\lambda_P} F\phi^P \quad (3)$$

which (2) reduces to when no up-scattering is present. Thus consider the equations

$$(L - S)\phi_0 = \frac{1}{\lambda_0} F\phi_0 , \quad (4)$$

$$(L - S)\phi_1 = \frac{1}{\lambda_1} F\phi_1 , \quad (5)$$

defining the fundamental and first harmonic space modes. Now assuming

$$\phi^P = (\phi_0 + a_P \phi_1) \quad (6)$$

which defines the harmonic content after P iterations, then using (3)

$$\phi^{P+1} = \frac{1}{\lambda_P} (L - S)^{-1} (F\phi_0 + a_P F\phi_1) \quad (7)$$

or

$$\phi^{P+1} = \frac{\lambda_0}{\lambda_P} \phi_0 + a_P \frac{\lambda_1}{\lambda_P} \phi_1 . \quad (8)$$

A renormalization then yields

$$a_{P+1} = \frac{\lambda_1}{\lambda_0} a_P , \quad (9)$$

which implies that the harmonic content is reduced by the ratio of the eigenvalues after each iteration. For a typical ANP reactor this ratio is about five, providing a very satisfactory convergence rate. Equation (2) on the other hand yields an entirely different convergence rate. Thus, using (4), (5),

$$\phi^{P+1} = \frac{1}{\lambda_P} (L - S_{\text{down}})^{-1} (F + \lambda_P S_{\text{up}}) (\phi_0 + a_P \phi_1) \quad (10)$$

or

$$\begin{aligned} \phi^{P+1} = & \frac{\lambda_0}{\lambda_P} \phi_0 + (\lambda_P - \lambda_0) (L - S_{\text{down}})^{-1} S_{\text{up}} \phi_0 \\ & + a_P \left[\frac{\lambda_1}{\lambda_P} \phi_1 + (\lambda_P - \lambda_1) (L - S_{\text{down}})^{-1} S_{\text{up}} \phi_1 \right] \end{aligned} \quad (11)$$

so that,

$$a_{P+1} = a_P \left[\frac{\lambda_1 + (1 - \frac{\lambda_1}{\lambda_P}) (L - S_{\text{down}})^{-1} S_{\text{up}}}{\lambda_0 + (1 - \frac{\lambda_0}{\lambda_P}) (L - S_{\text{down}})^{-1} S_{\text{up}}} \right] \quad (12)$$

Since $(L - S_{\text{down}})^{-1} S_{\text{up}} < 1$ for all systems for which scattering transfer itself is non-critical, equation (12) yields a dominance ratio greater than unity, but the actual value is sensitive to the importance of the up-scattering. This is the situation observed in trial multi-thermal group calculations where elevated temperature cases in which the up-scattering is relatively large, converge much slower than, for example, room temperature systems.

The larger dominance ratio of (9) may be restored to the power iterations by requiring flux distributions which, for a given power distribution, satisfy equation (3). Because of the inter-group coupling provided by the presence of both up and down scattering, such flux distributions can be obtained only by resorting to repeated inner iterations or by direct inversion of the multigroup matrix $(L - S)$ at each lattice point[†]. The former procedure is proposed for use in Program F-N. Thus, denoting power iterations by the superscript P and inner iterations by i, equation (2) is written as

$$(L - S_{\text{down}}) \phi^{i+1} = \frac{1}{\lambda_P} F \phi^P + S_{\text{up}} \phi^i, \quad (13)$$

[†]This latter procedure is used in Program ODD (ANP No. 657) where the up-scattering is limited to the last five groups and hence where sufficiently accurate numerical procedures for matrix inversion are available.

and this iteration sequence is repeated until

$$\phi^{i'+1} = \phi^{i'} \equiv \phi^{P+1},$$

and hence,

$$(L - S)\phi^{P+1} = \frac{1}{\lambda_P} F\phi^P.$$

Before considering the possible advantages of this double iteration sequence as compared to the sequence defined by equation (2), consider the convergence properties of the inner iteration.

For simplicity consider two groups coupled by up and down scattering. Equation (3) becomes then,

$$\begin{bmatrix} L_1 & -S_{21} \\ -S_{12} & L_2 \end{bmatrix} \begin{bmatrix} \phi_1 \\ \phi_2 \end{bmatrix} = \frac{1}{\lambda_P} \begin{bmatrix} \mathcal{J}_1^P \\ \mathcal{J}_2^P \end{bmatrix} \quad (14)$$

and a direct matrix inversion yields

$$\begin{bmatrix} \phi_1 \\ \phi_2 \end{bmatrix} = \frac{1}{\lambda_P \left(1 - \frac{S_{12}S_{21}}{L_1L_2} \right)} \begin{bmatrix} \frac{1}{L_1} & \frac{S_{21}}{L_1L_2} \\ \frac{S_{12}}{L_1L_2} & \frac{1}{L_2} \end{bmatrix} \begin{bmatrix} \mathcal{J}_1^P \\ \mathcal{J}_2^P \end{bmatrix} \quad (15)$$

or equivalently

$$\phi_1 = \frac{1}{\lambda_P} \left(\frac{\mathcal{J}_1^P}{L_1} + \frac{S_{21}}{L_2} \frac{\mathcal{J}_2^P}{L_1} \right) / \left(1 - \frac{S_{12}S_{21}}{L_1L_2} \right)$$

$$\phi_2 = \frac{1}{\lambda_P} \left(\frac{\mathcal{J}_2^P}{L_2} + \frac{S_{12}}{L_1} \frac{\mathcal{J}_1^P}{L_2} \right) / \left(1 - \frac{S_{12}S_{21}}{L_1L_2} \right).$$

Since for systems of interest,

$$\frac{S_{12}}{L_1} < 1, \quad \frac{S_{21}}{L_2} < 1, \quad (16)$$

the series expansion

$$\left(1 - \frac{S_{12}S_{21}}{L_1L_2}\right)^{-1} = 1 + \frac{S_{12}S_{21}}{L_1L_2} + \left(\frac{S_{12}S_{21}}{L_1L_2}\right)^2 + \dots, \quad (17)$$

is absolutely convergent. It can now be shown quite easily that the inner iteration procedure outlined above corresponds exactly to this series expansion and hence is also absolutely convergent. Thus, defining

$$\phi_1^{i+1} = \frac{1}{L_1} \left(\frac{\mathcal{J}_1^P}{\lambda_P} + S_{21}\phi_2^i \right) \quad (18)$$

and

$$\phi_2^{i+1} = \frac{1}{L_2} \left(\frac{\mathcal{J}_2^P}{\lambda_P} + S_{12}\phi_1^{i+1} \right) \quad (19)$$

which correspond to equation (13), where

$$\phi_2^1 = 0,$$

gives, for example,

$$\begin{aligned} \phi_1^2 &= \frac{1}{L_1} \left(\frac{\mathcal{J}_1^P}{\lambda_P} + \frac{S_{21}}{L_2} \frac{\mathcal{J}_2^P}{\lambda_P} + \frac{S_{21}}{L_2} \frac{S_{12}}{L_1} \frac{\mathcal{J}_1^P}{\lambda_P} \right) \\ \phi_2^2 &= \frac{1}{L_2} \left(\frac{\mathcal{J}_2^P}{\lambda_P} + \frac{S_{12}}{L_1} \frac{\mathcal{J}_1^P}{\lambda_P} + \frac{S_{12}S_{21}}{L_1L_2} \frac{\mathcal{J}_2^P}{\lambda_P} + \frac{S_{12}S_{21}S_{12}}{L_1L_2L_1} \frac{\mathcal{J}_1^P}{\lambda_P} \right) \end{aligned}$$

and these are the required expansions of equation (15). Extending the inter-group coupling to more groups simply complicates the algebra.

Thus, the three group system has the characteristic denominator

$$\left(1 - \frac{S_{12}S_{21}}{L_1L_2} - \frac{S_{13}S_{31}}{L_1L_3} - \frac{S_{23}S_{32}}{L_2L_3} - \frac{S_{12}S_{23}S_{31}}{L_1L_2L_3} - \frac{S_{13}S_{32}S_{21}}{L_1L_2L_3}\right)$$

and the series expansion again corresponds to the proposed iteration sequence.

3. DISCUSSION

Intuitively, the proposed iteration sequence since it produces a flux distribution which satisfies (3) for each group before the

recomputation of the fission production source avoids introducing extraaneous and non-physical contributions which only delay the reduction of an arbitrary source guess to the fundamental space mode source.

Mathematically, the inner iterations converge at a rate determined by the largest scatter-transfer probability, S_{jk}/L_j , while the outer iterations depend on λ_1/λ_0 . The total number of outer plus inner iterations required for convergence will be less than the product of the numbers required for convergence of each mode separately starting from an arbitrary distribution since the inner iterations are initiated from an "almost correct" guess after the first power iteration. The present procedure yields a distribution satisfying (3) only at complete convergence while the revised scheme provides this property at the completion of each power iteration. This should produce a significant reduction in machine time for problems where up-scattering is important.

4. PROGRAM MODIFICATIONS

In order to accomplish the desired iteration sequence, the following program modifications will be necessary:

- (a) specification of the number of groups involving up-scattering and hence for which inner iterations are required;
- (b) specification of the maximum number of inner iterations per outer iteration;
- (c) specification of a convergence criteria for the inner iterations.

The inner iteration convergence can be most easily judged in terms of an integrated quantity equivalent to the usual eigenvalue convergence. A suitable integral for this purpose might be simply the total flux in the groups involving the up-scattering.