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# AUSTRALIAN ATOMIC ENERGY COMMISSION RESEARCH ESTABLISHMENT LUCAS HEIGHTS

SOLUTION OF THE MULTIGROUP COLLISION PROBABILITY EQUATIONS

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G. DOHERTY

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### SOLUTION OF THE MULTIGROUP COLLISION PROBABILITY EQUATIONS

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#### G. DOHERTY

#### ABSTRACT

A method is presented for the solution of the multigroup collision probability equations arising in reactor physics calculations. The method is a block relaxation scheme, involving the direct solution by inversion of the equations for a single group, and it has the conceptual advantage over the successive over-relaxation method that problems without upscatter, which are of interest in fast reactor design, can be solved without inner iteration.

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#### 1. INTRODUCTION

A general purpose integral transport code is now being developed for the IBM 360/50H. The code as envisaged will be modular, allowing input interfaces with data preparation codes, and output interfaces with editing routines and with whole reactor design programs. At present the routines written will perform multigroup lattice calculations, using isotropic collision probabilities for slab, cylindrical and spherical geometries. Details of the calculation of collision probabilities have been given previously (Doherty 1969) and the method of solution of the flux equations is presented here.

#### 2. THE MULTIGROUP COLLISION PROBABILITY EQUATIONS

The multigroup collision probability equations, which may be regarded as a statement of neutron conservation in the reactor cell, can be written:

$$V_{i} \sum_{gi}^{T} \phi_{gi} = \sup_{j} V_{j} \left[ S_{gj} + \frac{1}{\lambda} \chi_{g} \quad S_{gi}^{m} \phi_{g'j} \nu \sum_{g'j}^{F} + S_{gi}^{m} \sum_{g'gj} \phi_{g'j} \right] P_{gji}$$

where

V<sub>i</sub> = volume of region i,

 $\Sigma_{gi}^{T}$  = total cross section in group g, region i,

 $\phi_{gi}$  = scalar neutron flux in group g, region i,

Sgi = fixed source emission rate in group g, region i,

λ = multiplication factor of the reactor cell,

 $X_{g}$  = proportion of fission neutrons born in group g,

 $\nu \Sigma_{gi}^{F}$  = average number of neutrons per fission times the fission cross section in group g, region i,

 $\Sigma_{g^{\dagger}gi} = \text{group } g^{\dagger} \text{ to group } g \text{ scattering cross section in region } i$ 

and  $P_{gji}$  = probability that a neutron born uniformly in volume and isotropically in direction in group g, region j, will have its next collision in region i.

The left-hand side of each equation is the collision rate in group g, region i, and the right-hand side is the production rate in region j multiplied by the probability that neutrons produced in region j will next collide in region i.

A derivation of this set of equations from the continuous space and energy integral transport equation was given by Pull (1963) who also outlined a method of solution based on successive over-relaxation (PIP) which was subsequently implemented by Clayton (1964). The modular structure of the collision probability program allows a number of different methods for solving the equations to be examined without too much difficulty. Rather than implement a PIP-type code based on successive over-relaxation (SOR) it was felt that some effort should be expended on an alternative scheme so that the computational efficiency of both methods could be gauged. The block relaxation scheme discussed in detail in later sections was chosen because of the success of such schemes in diffusion codes and because of their suitability for fast reactor calculations. Comparison between this method and SOR will be made when sufficient running experience has been accumulated. The next section contains sufficient detail on the SOR method to emphasize the differences between it and the method presented subsequently.

#### 3. THE SOR SCHEME

To discuss methods of solution it is necessary to write the multigroup equations in matrix form. Following Pull (1963) we define a collision rate vector x for a system of k regions and n-groups by the equations:

$$x_{1} = V_{1} \sum_{11}^{T} \phi_{11}$$

$$x_{2} = V_{2} \sum_{12}^{T} \phi_{12}$$

$$-----$$

$$x_{k} = V_{k} \sum_{1k}^{T} \phi_{1k}$$

$$x_{k+1} = V_{1} \sum_{21}^{T} \phi_{21} \text{ etc.}$$

so that x is a vector of length kn whose first k elements are the group 1 collision rates, second k elements are the group 2 collision rates, and so on.

We define also an emission rate vector y with similar partitioning by the equations:

$$y_{1} = \underset{g}{\text{Sum}} V_{1} \sum_{g} i_{11} \phi_{g} i_{1} + z_{1}$$

$$y_{2} = \underset{g}{\text{Sum}} V_{2} \sum_{g} i_{12} \phi_{g} i_{2} + z_{2}$$

$$y_{k} = \underset{g}{\text{Sum}} V_{k} \sum_{g} i_{1k} \phi_{g} i_{k} + z_{k}$$

$$y_{k+1} = \underset{g}{\text{Sum}} V_{1} \sum_{g} i_{21} \phi_{g} i_{1} + z_{k+1} \text{ etc.}$$

The fission production term has been deliberately separated within the emission rate vector and will be lumped together with the fixed source term to form a total source vector z, again with similar partitioning, for which we shall give only the first two equations.

$$z_{1} = V_{1} \left[ S_{11} + \frac{1}{\lambda} X_{1} \sup_{g^{1}} \phi_{g^{1}_{1}} \nu \Sigma_{g^{1}_{1}}^{F} \right]$$

$$z_{2} = V_{2} \left[ S_{12} + \frac{1}{\lambda} X_{1} \sup_{g^{1}} \phi_{g^{1}_{2}} \nu \Sigma_{g^{1}_{2}}^{F} \right]$$

With these definitions the multigroup equations can be written

$$x = Py$$
 $y = Qx + z$ ,

where P is the block diagonal matrix

$$\begin{bmatrix} P_1 & 0 & ---- \\ 0 & P_2 & ---- \\ ---- & 0 & 0 & ---- \\ P_n \end{bmatrix}$$

and  $(P_{\ell})_{ij} = P_{\ell ji}$ .

The matrix Q is square and of the form

$$\begin{bmatrix} D_{11} D_{12} & ---- & D_{1n} \\ D_{21} D_{22} & ---- & D_{2n} \\ ---- & D_{n1} & D_{n2} & ---- & D_{nn} \end{bmatrix}$$

where each of the submatrices Dij is diagonal with the elements

$$(D_{ij}) \varrho \ell = \sum_{ji} \ell / \sum_{j}^{T} \ell V_{\ell}$$

The matrix equations can then be written

$$\begin{pmatrix} I & -P \\ -Q & I \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} 0 \\ z \end{pmatrix}$$

and the matrix

$$\begin{pmatrix} I & -P \\ -Q & I \end{pmatrix}$$

possesses Property A which suggests SOR as a suitable method for solving the matrix equation iteratively. For a definition of Property A and its implications in the use of SOR the reader is referred to Varga (1962), and to Pull (1963) and Clayton (1964) for details of the application of SOR to this particular problem.

In problems where fissionable materials are present in the system the vector z contains in the term

$$\frac{1}{\lambda} \chi_{g} \operatorname{Sum}_{g'} \phi_{g'_{i}} \nu \Sigma_{g'_{i}}^{F_{i}}$$

the eigenvalue  $\lambda$  and a guess at the initial flux distribution. The process of solution is divided into an outer—inner iteration scheme. During an outer iteration the z vector remains unchanged while a number of inner iterations are performed to determine the x and y vectors. When a specified number of inner iterations have been performed, a new estimate of the eigenvalue of the system is made from overall neutron balance in the system, the new eigenvalue and the latest fluxes are used to compute a new source vector z, and another outer iteration begins. If no fissionable material is present, the vector z remains unaltered and the solution process consists only of inner iterations until a specified convergence has been achieved.

#### 4. AN ALTERNATIVE APPROACH FOR FIXED SOURCE PROBLEMS

Consider for a moment a fixed source problem. With the SOR scheme we start with an initial guess x' of the collision rate vector x and use the equation

$$y^1 = Q x^1 + z$$

to give us a starting value y' of the vector y.

The iteration scheme of SOR can be written

$$x^{n+1} = wPy^n + (1 - w) x^n$$
  
 $y^{n+1} = wQx^{n+1} + wz + (1 - w) y^n$ 

where w is the over-relaxation parameter and x n+1 and x n are the n+1th and nth iterates respectively.

After one iteration has been completed

$$x^2 = wPy^1 + (1 - w) x^1$$
  
 $y^2 = wQx^2 + wz + (1 - w) y^1$ .

All the values of x<sup>2</sup> were computed from the old vectors x<sup>1</sup> and y<sup>1</sup>. For this reason the SOR method is unable to take advantage of a class of problems important in fast reactor design, namely purely downscattering problems. The difficulty experienced in applying the SOR approach to this problem is analogous to the problem involved in using the Jacobi iteration scheme for lower triangular matrices. A simple 3 x 3 matrix will serve to illustrate the problem.

$$x_1 = b_1$$

$$a_{21} x_1 + x_2 = b_2$$

$$a_{31} x_1 + a_{32} x_2 + x_3 = b_3$$

Using the Jacobi scheme this becomes

$$x_1^{n+1} = b_1$$
  
 $x_2^{n+1} = b_2 - a_{21} x_1^n$   
 $x_3^{n+1} = b_3 - a_{31} x_1^n - a_{32} x_2^n$ 

Starting from an initial guess x1 three iterations must be performed before the correct answers are obtained. However if instead the Gauss-Seidel scheme

$$x_1^{n+1} = b_1$$

$$x_2^{n+1} = b_2 - a_{21} x_1^{n+1}$$

$$x_3^{n+1} = b_3 - a_{31} x_1^{n+1} - a_{32} x_2^{n+1}$$

had been employed, then the correct result would have been obtained without iteration.

It is evident that a calculation scheme analogous to Gauss-Seidel can be designed for the downscattering problem in particular, and such a scheme could provide a more efficient alternative to SOR on a wider range of problems. If we return to the original equations:

$$V_{i} \sum_{gi}^{T} \phi_{gi} = \sup_{j} V_{j} \left[ S_{gj} + \frac{1}{\lambda} X_{g} S_{um} \phi_{g'j} \nu \sum_{g'j}^{F} + S_{um} \sum_{g'gj} \phi_{g'j} \right] P_{gji}$$

and consider the equations for a particular group (dropping the index g) we obtain k equations of the form:

$$\begin{array}{rcl} V_i \; \boldsymbol{\Sigma}_i^T \; \boldsymbol{\phi}_i &=& \operatorname{Sum} \; V_j \; [T_j \; + \; \boldsymbol{\Sigma}_j^S \; \boldsymbol{\phi}_j \;] \; P_{jji} \quad , \\ \\ \mathbf{W}_i \; \boldsymbol{\Sigma}_i^T \; \boldsymbol{\phi}_i &=& \operatorname{Sum} \; V_j \; [T_j \; + \; \boldsymbol{\Sigma}_j^S \; \boldsymbol{\phi}_j \;] \; P_{jji} \quad , \\ \\ \mathbf{W}_j \; &=& \operatorname{Sum} \; \boldsymbol{\Sigma}_{gj} \; + \; \frac{1}{\lambda} \; \; \boldsymbol{\chi}_g \; \operatorname{Sum} \; \boldsymbol{\phi}_{g^lj} \; \boldsymbol{\nu} \; \boldsymbol{\Sigma}_{g^lj}^F \; + \; \operatorname{Sum} \; \; \boldsymbol{\Sigma}_{g^lgj} \; \boldsymbol{\phi}_{g^lj} \\ \\ \mathbf{\Sigma}_j^S \; &=& \; \boldsymbol{\Sigma}_{ggj} \; \; . \end{array}$$

Writing the one-group equations in matrix form we get

$$Ax = By$$
,

$$x_{i} = V_{i} \phi_{i}$$

$$y_{i} = V_{i} T_{i}$$

$$B_{ij} = P_{gji}$$

$$A_{ij} = \sum_{i}^{T} \delta_{ij} - \sum_{i}^{S} B_{ij}$$

Applying the physical restrictions

$$\Sigma^{T} > \Sigma^{S}$$
 and Sum  $B_{ji} \leqslant 1$ ,

it can be seen that the transpose of A is an M-matrix (Varga 1962) with a positive inverse and hence, in particular, that  $A^{-1}$  exists and that all elements of  $A^{-1}$  are positive.

We may therefore write C = A-1 B and the one-group equations are reduced to the form

$$x = Cy$$
.

The matrix C is the same size as the original matrix of collision probabilities and to compute this matrix requires the inversion of a k x k matrix, and the multiplication of two k x k matrices. In exchange for this computational labour we have obtained, for the purely downscattering problem, the partitioned equivalent of the Gauss-Seidel iteration scheme in the simple example. In the more general problem where upscattering exists, the formulation above is consistent with a block relaxation scheme which we shall now consider.

We can partition the vector x into the set of n subvectors  $x_i$  each of length k so that  $x_i$  contains the spatial fluxes of group i.

The set of equations can then be written

$$A_i x_i = B_i y_i$$

and for the non-fissionable case

$$y_i = VS_i + Sum_{j \neq i} D_{ij} x_j$$
,

where Dij is a diagonal submatrix with elements

$$(D_{ij})\ell\ell = \sum_{ii}\ell$$
.

Hence the matrix equations can be written:

$$A_i X_i = B_i (VS_i) + Sum_{j \neq \ell} B_i D_{ij} x_j$$

$$= b_i + Sum_{j \neq i} E_{ij} x_j ,$$

and ultimately as

$$\mathbf{F} \mathbf{x} = \mathbf{b}$$

where

$$F_{ii} = A_i$$

$$F_{iij} = -E_{ij} .$$

In the case of pure downscattering  $F_{ij}=0$  for j>i and the Gauss-Seidel solution is correctly obtained from the first iteration. In the more general problem some of the lower energy groups do have upscattering and the matrix F can then be written in the reducible (Varga 1962) form:

$$\begin{pmatrix} F_{11} & 0 \\ F_{21} & F_{22} \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} b_1 \\ b_2 \end{pmatrix}$$

where x2 in this partitioning contains all the groups to which upscattering is permitted. This equation is solved in the order

$$F_{11} x_1 = b_1$$

which requires no iteration since F11 is lower triangular and

$$F_{22} x_2 = b_2 - F_{21} x_1 .$$

The matrix  $F_{22}$  is irreducible and the second equation requires an iterative scheme for its solution. Since the Gauss-Seidel iteration matrix derived from  $F_{22}$  is no longer 2-cyclic, which is a prerequisite for Property A (Varga 1962), it will not be possible to determine efficiently an over-relaxation parameter  $\omega$  for use in an SOR scheme on  $F_{22}$ . From numerical experiments previously reported (Doherty 1968) it seems likely that the Gauss-Seidel and the Aitken double-sweep iterative schemes would be about equally efficient and that both would be capable of acceleration if sufficient storage could be made available.

#### 5. EIGENVALUE PROBLEMS

We shall now return to a discussion of the eigenvalue problem posed by the presence of fissionable material in the system. Neglecting for the present the possibility that a fixed source is also present in the system the equations can be written:

$$A_i \times_i = \underset{j \neq i}{\text{Sum}} B_{i} D_{ij} \times_j + \frac{1}{\lambda} \underset{j}{\text{Sum}} B_{i} G_{ij} \times_j ,$$

where Gii is diagonal with elements

$$(G_{ij})\ell\ell = \chi_i \nu \Sigma_{j\ell}^F$$
.

These equations can be written

$$F x = \frac{1}{\lambda} H x ,$$

where

$$F_{ii} = A_i$$

$$F_{ij} = -E_{ij}$$
 as before

and

$$H_{ij} = B_i G_{ij}$$
.

Writing this equation as  $F^{-1}$  H x =  $\lambda$  x, this eigenvalue problem is the same one encountered in neutron diffusion and transport codes. The matrix T =  $F^{-1}$  H corresponds to the process of obtaining the new flux iterate from the old one. In the purely downscattering problem one pass through the equations produces precisely the result

$$x^{n+1} = T x^n / \lambda^n$$

where

$$\lambda^n = \| T x^n \| / \| x^n \|$$

 $\| x \|$  being some suitable norm of x. The usual norm applied is based on the fission production rate at each iteration since this quantity is needed to preserve neutron balance in the course of the calculation.

When upscattering problems are considered, the relation

$$\lambda^n x^{n+1} = T x^n$$

is no longer exact because the vector T  $x^n$  is not exactly evaluated by the inner iteration scheme with the matrix  $F_{22}$ . We nevertheless assume that the relation is exactly satisfied and proceed to a simple method of accelerating the outer iteration which converges the eigenvalue and eigenvector problem.

The matrix T can be shown to be non-negative and irreducible. Hence, from the Perron-Frobenius results for non-negative matrices (Varga 1962), T has a largest real eigenvalue with an associated real positive eigenvector — the persistent flux distribution that we seek to establish. The non-negative property is due to the fact that the elements of H and F<sup>-1</sup> are non-negative, the latter result being established with the aid of a Neumann expansion of F<sup>-1</sup> in block diagonal form. The irreducibility of T can be asserted on physical arguments because fission neutrons are emitted in the topmost energy groups and cause further fissions in all lower energy groups. It is not difficult to establish irreducibility with mathematical rigour but the physical argument should suffice.

#### 6. CONVERGENCE OF THE OUTER ITERATIONS

The outer iteration convergence problem is the same as that encountered in  $S_n$  transport programs and diffusion programs, though the inner iteration schemes of these are markedly different. Two methods of acceleration are of particular interest — the simple Aitken procedure of removing the subdominant eigenvector, and the more elaborate Chebyshev extrapolation prodecure.

Let the eigenvalues of T be  $\lambda_1$ ,  $\lambda_2$  . . . .

such that

$$\lambda_1 > |\lambda_2| \geqslant |\lambda_3| \dots$$

with corresponding eigenvectors xi satisfying

$$T x_i = \lambda_i x_i$$
.

Let y be a given starting vector and decompose y into the eigenvectors of T (which are assumed to span the space)

$$y = a_i x_i \text{ (dummy suffix summation)}$$

$$Ty = a_i \lambda_i x_i$$

$$T^m y = a_i \lambda_i^m x_i$$

$$= \lambda_1^m \left[ a_1 x_1 + \left( \frac{\lambda_2}{\lambda_1} \right)^m a_2 x_2 + \left( \frac{\lambda_3}{\lambda_1} \right)^m a_3 x_3 + \dots \right]$$

Since we have assumed  $\lambda_1 > |\lambda_i|$  for  $i \neq 1$ , this simple powering procedure will ultimately yield correct values of both  $\lambda_1$  and  $x_1$ .

The Aitken procedure has been outlined by Fox (1964). The assumption underlying the procedure is that the subdominant eigenvalue is real and that the presence of the associated eigenvector is the main hindrance to convergence.

$$T^{n}y = a_{1} \lambda_{1}^{n} x_{1} + a_{2} \lambda_{2}^{n} x_{2} + \dots$$

$$T^{n+1}y = a_{1} \lambda_{1}^{n+1} x_{1} + a_{2} \lambda_{2}^{n+1} x_{2} + \dots$$

The estimate of the eigenvalue obtained at this point, which we denote by  $\mu^n$  is simply

$$\mu^{n} = \frac{T^{n+1} y}{T^{n} y} = \lambda_{1} \left\{ \frac{a_{1} x_{1} + \left(\frac{\lambda_{2}}{\lambda_{1}}\right)^{n+1} a_{2} x_{2} + \dots}{a_{1} x_{1} + \left(\frac{\lambda_{2}}{\lambda_{1}}\right)^{n} a_{2} x_{2} + \dots} \right\}$$

This can be expanded to give

$$\mu^{n} \approx \lambda_{1} + \left(\frac{\lambda_{2}}{\lambda_{1}}\right)^{n} (\lambda_{2} - \lambda_{1}) = \frac{a_{2} x_{2}}{a_{1} x_{1}} + \dots$$

$$\mu^{n} - \lambda_{1} \approx \left(\frac{\lambda_{2}}{\lambda_{1}}\right)^{n} (\lambda_{2} - \lambda_{1}) = \frac{a_{2} x_{2}}{a_{1} x_{1}}$$

$$\mu^{n+1} - \lambda_1 \approx \left(\frac{\lambda_2}{\lambda_1}\right)^{n+1} (\lambda_2 - \lambda_1) = \frac{a_2 \times a_2}{a_1 \times a_1}$$

$$\frac{\mu^{n+1} - \lambda_1}{\mu^n - \lambda_1} = \frac{\lambda_2}{\lambda_1} = \frac{\mu^n - \lambda_1}{\mu^{n-1} - \lambda_1}$$

From these equations  $\lambda_1$  can be determined, and then  $\lambda_2$ . The eigenvector  $x_2$  can also be eliminated from the solution by noting that

$$T^{n+1}y - \lambda_2 T^n y \approx (\lambda_1 - \lambda_2) \lambda_1^n x_1$$
.

A difficulty with the use of this acceleration procedure is to know when to apply it. In deriving the procedure it has been assumed that  $\lambda_2$  is real and that by the time iteration n is reached the eigenvectors higher than  $x_2$  can be ignored in the expansion of  $T^n$  y. The only gross check that can be performed when applying the procedure is to check  $\lambda_2 < \lambda_1$ . If the latter is not satisfied the assumptions used in the derivation of the procedure are violated and the 'acceleration' is not applied. Such a procedure has been used in the WDSN program (Green 1967) and found to be an efficient acceleration device.

Chebyshev polynomial extrapolation has been employed in many large neutron diffusion programs for converging the outer iterations. A full description of the method, which will be summarised below, is given by Varga (1962).

It is assumed that at iteration n the estimate  $\lambda^*$  of the eigenvalue is a close estimate of the true eigenvalue  $\lambda_1$  of T. This is usually a valid assumption as it is the flux eigenvector rather than the eigenvalue which is varying most rapidly. Then the iterative procedure can be written, with  $\psi^n = T^n y$ ,

$$\left(\frac{\mathbf{T}}{\lambda^*}\right)\psi^{\,\mathbf{n}} \ = \ \psi^{\,\mathbf{n}+1}$$

and

$$\left(\frac{T}{\lambda^*}\right)^r \psi^n = \psi^{n+1} .$$

The matrix  $\frac{T}{\lambda^*}$  has spectral radius unity. If we consider polynomials  $p_r(x)$  for which  $p_r(1) = 1$ , then the matrix  $\left(\frac{T}{\lambda^*}\right)^r$  corresponds to the polynomial  $p_r(x) = x^r$ .

If the eigenvalues  $\lambda_i$  of T are all real and non-negative

$$0 \leqslant \lambda_n \leqslant \lambda_{n-1} \quad \ldots \quad \leqslant \lambda_2 \leqslant \lambda_1 = \lambda^*$$

and if the corresponding eigenvectors  $\mathbf{x}_j$  span the n-dimensional space, then  $\psi^{\mathrm{m}}$  can be expanded

$$\psi^{m} = C_{i} x_{i}$$

$$\psi^{m+n} = P_{n} \left(\frac{T}{\lambda^{*}}\right) \psi^{m}$$

$$= C_{1} x_{1} + Sum_{j > 1} C_{j} P_{n} \frac{\lambda_{j}}{\lambda^{*}} x_{j}$$

The sum on the right represents the error in the estimate of x1 so we minimize

max 
$$|p_n(x)|$$
 in the range  $0 \le x \le \frac{\lambda_2}{\lambda_1}$ 

subject to the restriction  $p_n(1) = 1$ .

The solution of this problem is given explicitly in terms of Chebyshev polynomials

$$p_{n}(x) = \frac{\left(C_{n} \frac{2x}{\lambda_{2}} - 1\right)}{\left(C_{n} \frac{2\lambda_{1}}{\lambda_{2}} - 1\right)},$$

where the Chebyshev polynomials satisfy

$$C_0(x) = 1$$
 $C_1(x) = x$ 
 $C_{n+1}(x) = 2x C_n(x) - C_{n-1}(x)$ .

Defining  $\sigma = \frac{\lambda_2}{\lambda_1}$ , the dominance ratio of the matrix T, a new recurrence relation can be derived for the Chebyshev extrapolated iterates  $\xi$ 

$$\xi^{m+1} = 2 \alpha_{m+1} (\frac{2}{\sigma} \psi^{m+1} - \xi^{m}) - \beta_{m+1} \xi^{m-1},$$

where

$$\alpha_{m+1} = \cosh m p / \cosh (m+1) p$$

$$\beta_{m+1} = \cosh(m-1) p / \cosh(m+1) p$$

$$p = \cosh^{-1}\left(\frac{2}{\alpha}-1\right) .$$

To begin the new iteration scheme for  $\xi$  put

$$\xi^{0} = \psi^{0}$$

$$\xi^{1} = \xi^{0} + \frac{2}{2-\sigma} (\psi^{1} - \xi^{0}) .$$

The recurrence relation defined is a three-term one involving  $\xi^{m-1}$  and  $\xi^m$  in the calculation of  $\xi^{m+1}$ . The extra iterate which must be stored would be a severe penalty if we were to attempt to apply this recurrence scheme to the flux vector, which has length equal to the number of groups times number of regions. However the extrapolation is usually applied to the fission emission vector which only has length equal to the number of regions. The storage requirements for the Aitken scheme of acceleration are the same, and the Aitken procedure can yield an estimate of the eigenvalue  $\lambda_2$  and hence the dominance ratio of the Chebyshev extrapolation scheme. Thus the general outer iteration procedure could be to perform unaccelerated outer iterations up to a specified number, then

to perform an Aitken acceleration with the subsequent choice of Chebyshev extrapolation or continuing with Aitken accelerations at specified intervals.

The Chebyshev scheme relies on the assumption that the eigenvalues of the iteration matrix are real and non-negative and normally distributed in the interval  $[0, \lambda_2]$ . It is usually possible only to establish that the real parts of the eigenvalues are non-negative, though the success of the scheme in diffusion codes suggests that the eigenvalues of the diffusion iteration matrix must have small or zero complex parts.

#### 7. CONCLUSION

The method of solution has been coded for the IBM 360/50H computer in the program ICPP, which incorporates the collision probability methods described by Doherty (1969). The range of geometries which the program can handle will be extended to include clusters and some other two dimensional configurations and it is hoped also to include an anisotropic scattering option.

Extensive running experience is still being accumulated but it appears that the flux solution is quite satisfactory for thermal lattice calculations and very rapid for purely downscattering problems. A typical 10-region, 15-group thermal calculation takes about 30 seconds to converge to a tolerance of 10-4 in the eigenvalue. An increase in the number of groups produces a roughly linear increase in solution time but an increase in the number of space points produces a roughly cubic increase in solution time, principally in the initial matrix inversion and premultiplication, so that the method is unsuitable for few-group many-region problems. However the rate of convergence, which is to be distinguished from the time for convergence, does not depend strongly on the number of regions in the problem, as the SOR method appears to do (Askew et al. 1966).

On the problems so far attempted Chebyshev acceleration has been found unnecessary, few problems even reaching the arbitrarily selected number of outer iterations (10) at which Aitken acceleration is applied. It appears that the block relaxation scheme may be effecting a considerable separation of the eigenvalues of the iteration matrix which is a distinct advantage in problems which would otherwise converge slowly.

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