THE MULTI-LEVEL ITERATIVE SCHEME

ON THE APPLICABILITY OF THE MULTI-LEVEL ITERATIVE SCHEME TO TWO GROUP NEUTRON DIFFUSION PROBLEMS

By

GARY KURT ALBERT, B.Eng.

A Project Report
Submitted to the School of Graduate Studies
in Partial Fulfilment of the Requirements
for the Degree
Master of Engineering

McMaster University

1982 February

MASTER OF ENGINEERING

McMASTER UNIVERSITY
Hamilton, Ontario

TITLE: On the Applicability of the Multi-Level Iterative Scheme to Two Group Neutron Diffusion Problems

AUTHOR: Gary Kurt Albert, B.Eng. (McMaster University)

Supervisor: Doctor D.A. Meneley

NUMBER OF PAGES: vi, 43

ABSTRACT

This report concerns the applicability of the Multi-Level iterative scheme to the neutron diffusion problem. In the process of this study the iterative scheme is analyzed in modal form. The results of this analysis are used to derive the Single Mode Extrapolation scheme and give mathematical support to the Multi-Level theory. A program was written to test this theory and the results of test cases are discussed.

ACKNOWLEDGEMENTS

I wish at this time to express my gratitude to Dr. D.A. Meneley for both the design of this project and the supervision received during its completion. I would also like to thank the Department of Engineering Physics at McMaster University and Ontario Hydro of Toronto, Ontario for the opportunity to participate in an Off Campus Project in partial fulfilment of my Master of Engineering Degree.

TABLE OF CONTENTS

TABLE OF FIGURES

1.0 INTRODUCTION

Since relaxation schemes were first used, different schemes to reduce the overall effort in reaching the final result have been developed. The most successful method for accelerating convergence rates in iterative eigenvalue problems has been the single mode extrapolation technique developed by M.R. Wagner[5]. This scheme takes advantage of the modal characteristics of the solution process to subtract off the first error mode in the approximate solution during the iterative cycle. Extensions to more than single mode subtraction have been attempted but have yet to be proven more successful than the single mode approach. The possibility that multi-mode error subtraction may improve convergence rates significantly, if properly applied, has led to this investigation of a new method which we shall call the Multi-Level Iterative Scheme. Achi Brandt[2] has developed and analysed this method for matrix problems of the form:

$$Ax = b \tag{1}$$

and reports significant decreases in computational effort. An example given solving the Dirichlet problem for the Poisson equation on a rectangle was solved with ten times less computational effort on a six level structure than on the single level. Gauss-Seidel iterations where used on all levels in this example. You will note that the

merit of this system has been considered in terms of computational effort rather than in terms of convergence rates. The reason for this distinction will become obvious once we discuss the method itself. It will, however, be advantageous to first analyze the iterative process in modal form.

2.0 MODAL ANALYSIS OF THE ITERATIVE PROCESS

To analyze the iterative process it is convenient to represent the partial solution of the problem as a sum of orthogonal vectors of increasing frequency. It can then easily be shown that the zeroth mode (lowest frequency component) will dominate the solution as higher frequency components decay away with successive iterations. The approximate solution can be represented as a sum of Fourier components, Bessel functions or orthogonal eigenvectors of the problem. The latter approach is most suitable for our purposes.

Although this analysis is generally applicable our attention will be directed toward the neutron diffusion equation. The equation to be solved can then be written as

$$\left[R - \frac{P}{k_o}\right]\Phi_o = 0 \qquad (2)$$

Here R is the removal matrix and P the production matrix. Φ_o is the zeroth order eigenvector for which we are searching and k_o is a constant related to the eigenvalue of the problem which divides the production matrix such that a critical system is

obtained. In the process of iterations we search for this eigenvalue using the relationship

$$k^{(n+1)} = k^{(n)} \frac{\langle x^{(n+1)}, x^{(n+1)} \rangle}{\langle x^{(n+1)}, x^{(n)} \rangle} \qquad (3)$$

Throughout this report a number of iterations will be indicated by a superscript in rounded brackets. Here the new value of k corresponding to the (n+1)th iteration is calculated using the (n)th value of k and the values of the vector x found at the (n)th and (n+1)th iterations. The angular brackets indicate an inner product which is defined as

$$\langle a,b \rangle = \sum_{i=1}^{N} | a_i b_i | \qquad (4)$$

the subscript indicating the ith value of the corresponding vector.

Letting the vector $x^{(n)}$ be the solution of equation (2) found after n iterations, it can now be represented by a sum of the orthogonal eigenvectors of the problem such that

$$x^{(n)} = \sum_{m=0}^{\infty} A_m \Phi_m \qquad (5)$$

where A_m is the coefficient multiplying the mth eigenvector.

There are an infinite number of eigenvectors associated with any real physical system but only N of these can be represented in any numerical problem, where N is the number of equations to be solved. The modes neglected determine the accuracy obtainable with our N point approximation. Equation (5) is then more appropriately written as

$$x^{(n)} = \sum_{m=0}^{N} A_m \Phi_m \tag{6}$$

Assuming that after n iterations a value $k_g^{(n)}$ for the problem criticality has been found, equation (2) can be written using the approximate result giving:

$$\left[R - \frac{P}{k_g^{(n)}} \right] x^{(n)} = 0 \tag{7}$$

The subscript g indicates that this value is a current guess value. Using simple matrix algebra a relaxation scheme yielding the next best set of x values can be defined as:

$$x^{(n+1)} = \frac{R^{-1}P}{k_g^{(n)}} x^{(n)} \tag{8}$$

Substituting for $x^{(n)}$ with the modal expansion in equation (6) gives the following relationships:

$$\begin{aligned} x^{(n+1)} &= \frac{R^{-1}P}{k_g^{(n)}} \sum_{m=0}^{N} A_m \Phi_m && \text{i} \\ &= \sum_{m=0}^{N} A_m \frac{R^{-1}P}{k_g^{(n)}} \Phi_m && \text{ii} \\ &= \sum_{m=0}^{N} A_m \frac{k_m}{k_g^{(n)}} \Phi_m && \text{iii} \end{aligned} \tag{9}$$

where k_m (m = 0, 1, ...N) are the criticality eigenvalues corresponding to each individual eigenvector Φ_m.

Using these results similar relationships for the next iteration can be derived:

$$x^{(n+2)} = \frac{R^{-1}P}{k_g^{(n+1)}} x^{(n+1)} \qquad \text{i}$$

$$= \sum_{m=0}^{N} A_m \frac{k_m}{k_g^{(n)}} \frac{R^{-1}P}{k_g^{(n+1)}} \Phi_m \qquad \text{ii} \qquad (10)$$

$$= \sum_{m=0}^{N} A_m \frac{k_m^2}{k_g^{(n+1)} k_g^{(n)}} \Phi_m \qquad \text{iii}$$

From these results one can deduce a general expression for the iterative process:

$$x^{(I)} = \sum_{m=0}^{N} A_m \frac{k_m^I}{\prod_{j=0}^{I-1} k_g^{(j)}} \Phi_m \qquad (11)$$

the usual choice of $k_g^{(o)}$ being unity.

Since k_g approaches k_o as I goes to infinity and k_o, being associated with the zeroth mode eigenvector, is the largest eigenvalue, it can easily be shown that

$$\frac{k_m^{\infty}}{k_g^{(\infty)}} = 0 \quad \text{for } m \neq 0 \qquad \text{i}$$

$$\text{and} \quad x^{(\infty)} = \frac{A_o k_o^{\infty}}{\prod_{j=0}^{\infty} k_g^{(j)}} \Phi_o = A_o \Phi_o \qquad \text{ii} \qquad (12)$$

The important consequences of these two results are:

1. The higher order modes constituting the error in $x^{(n)}$, having the smallest values of k_m, will decay quickly in the iterative cycle followed by slower decay of modes with values of k_m close to k_o.

2. The value $k_g^{(n)}$ will approach the true value k_o before $x^{(n)}$ converges to Φ_o.

These results and the modal expansion method form the basis of the two methods to be discussed next.

3.0 SINGLE MODE ERROR EXTRAPOLATION

M.R. Wagner has taken advantage of the modal view of the iterative process to accelerate convergence of a problem by subtracting the first error mode in $x^{(n)}$. To do this he relies on the assumption that the first error mode predominates in the total error of the approximate solution at sometime in the iterative process. This assumption follows naturally from consequence number one since the first error mode has the second largest eigenvalue and would, therefore, decay away last. From the iterative cycle one notices that once the first error mode predominates in the solution, any change in the vector $x^{(n)}$ is dictated by the k_1/k_o decay of this first mode. This region of uniform change is known as the asymptotic convergence region and represents very slow progress toward a converged result. It is within this region then that the extrapolation method becomes effective. To see how the extrapolation method develops consider equations (9) iii and (10) iii assuming domination in the asymptotic region.

$$x^{(n+1)} = \frac{A_o k_o}{k_g^{(n)}} \Phi_o + A_1 \frac{k_1}{k_g^{(n)}} \Phi_1 \qquad \text{i} \qquad (13)$$

$$x^{(n+2)} = \frac{A_o k_o^2}{k_g^{(n+1)} k_g^{(o)}} \Phi_o + \frac{A_1 k_1^2}{k_g^{(n+1)} k_g^{(n)}} \Phi_1 \qquad \text{ii}$$

Now subtracting (13) i from (13) ii,

$$x^{(n+2)} - x^{(n+1)} = A_o \left[\frac{k_o^2}{k_g^{(n+1)} k^{(n)}} - \frac{k_o}{k_g^{(n)}} \right] \Phi_o + A_1 \left[\frac{k_1^2}{k_g^{(n+1)} k_g^{(n)}} - \frac{k_1}{k_g^{(n)}} \right] \Phi_1 \tag{14}$$

Assuming by consequence number two that $k_g^{(n+1)} \approx k_g^{(n)} \approx k_o$ and eliminating $A_1 \Phi_1$ with equation (13) ii gives

$$A_o \Phi_o = x^{(n+2)} + E \left[x^{(n+2)} - x^{(n+1)} \right] \tag{15}$$

This equation represents the extrapolating formula with extrapolation coefficient

$$E = \frac{k_1}{k_o - k_1} = \frac{\sigma}{1 - \sigma} \text{ , where } \sigma = \frac{k_1}{k_o} \tag{16}$$

The value of k_1 can be found by introducing a third iteration:

$$x^{(n+3)} = A_o \Phi_o + \frac{A_1 k_1^3}{k_o^3} \Phi_1 \tag{17}$$

Eliminating $A_o\Phi_o$ and $A_1\Phi_1$ using relationships (13) i and (13) ii gives.

$$\left[k_1 - k_o\right] x^{(n+3)} = \left[k_1 - k_o\right] x^{(n+1)} - k_o\left[x^{(n+2)} - x^{(n+1)}\right] \qquad (18)$$

$$+ \frac{k_1^2}{k_o}\left[x^{(n+2)} - x^{(n+1)}\right]$$

Rearranging the terms results in a quadratic equation in k_1 of the form

$$ak_1^2 + bk_1 + c = 0 \qquad \text{i}$$

$$a = \frac{1}{k_o}\left[x^{(n+2)} - x^{(n+1)}\right] \qquad \text{ii}$$

$$b = -k_o\left[x^{(n+3)} - x^{(n+1)}\right] \qquad \text{iii}$$

$$c = k_o\left[x^{(n+3)} - x^{(n+2)}\right] \qquad \text{iv} \qquad (19)$$

In this form, however, we would require the storage of three successive iterations of x values to evaluate k_1.

A further simplification is to assume that $k_o \approx 1.0$, which is true of most realistic reactor systems, for which the relationship reduces to

$$k_1 \approx \frac{x^{(n+3)} - x^{(n+2)}}{x^{(n+2)} - x^{(n+1)}} \qquad (20)$$

Providing the first error mode is truly the only significant error mode, k_1 can be calculated at any given point of the problem. A usual method is to calculate an average value over a set of points. With careful programming the storage requirements can then be reduced to essentially two vector lengths.

The extension of this system of extrapolation to more than one mode requires additional storage of successive iterations, the minimum for two mode extrapolation being three consecutive iterations. This immediately points out a major disadvantage in extending this method to higher modes. The Multi-Level scheme to be discussed now is intrinsically a multi-mode method requiring, at its worst, storage in the neighbourhood of three solution vector lengths. The number of modes that can theoretically be subtracted by this method amount to N/2-1 modes.

4.0 THE MULTI-LEVEL SCHEME

One of the most fundamental methods of saving computational work in the iterative cycle has been to start off with an extremely good initial guess for Φ_o, thereby saving iterative steps outside of the asymptotic convergence region. One way in which this could be achieved was to iterate the problem on a mesh structure of much fewer points than the structure at which the solution is desired, and interpolate the result to the finer mesh as an initial guess. The Multi-Level scheme also utilizes a fine mesh structure and several coarse mesh structures but for a different purpose.

The Multi-Level algorithm proposed by Achi Brandt uses a hierarchy of coarser mesh levels to compute corrections to the solution found on the fine level. Each level provides a correction to the problem on the previous finer level. This system provides us with a number of advantages over normal iterative cycles. The first and most important of these is that calculation of the error vector on the coarser grid structure requires fewer computational steps since normally half as many points are employed. A second advantage is the possibility of increased diagonal dominance of the problem at the coarser level, further enhancing convergence rates. Other advantages include improved accuracy of the final solution and the ability to accurately predict beforehand the amount of computational work required to solve a problem to desired accuracy. These aspects of the system are thoroughly discussed in Brandt's paper and will not be developed here, the iterative scheme itself being our main concern.

In matrix notation we start with an initial problem of the form:

$$A\phi = b \tag{21}$$

After n iterations an approximation of ϕ, $x^{(n)}$ is found such that

$$Ax^{(n)} = f+b \tag{22}$$

where f is a residual vector ensuring equality of left and right hand sides. Subtracting equation (21) and (22) gives the result

$$A(x-\phi) = f \tag{23}$$

An error vector can now be defined as $v = x - \phi$ which upon substitution into (23) results in the relationship

$$Av = f \tag{24}$$

To solve for the vector v on the fine grid would show none of the advantages previously mentioned. The problem is, therefore, rediscretized on a coarser level (half as many grid points) resulting in a new relationship

$$A_2 v_2 = f_2 \tag{25}$$

the subscript 2 indicating the second grid level. Since the residuals are calculated at the fine level they will have to be interpolated to the coarse level. The interpolating formula should be of the same order as the differential equation being solved to maintain sufficient accuracy. The relationship between first and second level points for cell centred nodes are indicated in Figure 1.*

One of the most important criteria for a level transition is that the significant modes of the residual vector be representable on the coarse grid level. For example, if a fourth order mode of the residual has a wavelength of less than four mesh spacings on the fine grid level it could not be represented on the two equivalent mesh spacings of the coarse level without significant loss in accuracy. By consequence number one of Section 2 these higher order modes would decay quickly in the iterative cycle and the asymptotic convergence region could be considered a suitable transition point.

---

* for cell-edge meshpoints no interpolation would be required

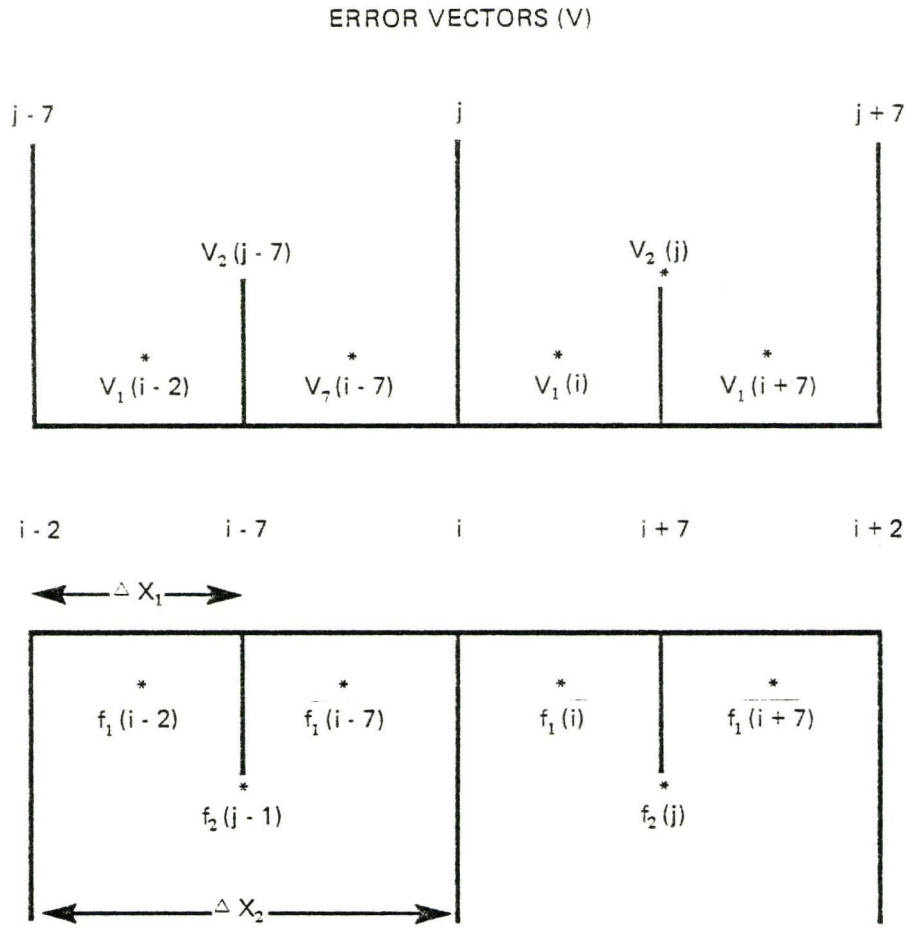


FIGURE 1
Relative Position of Mesh Points
Between Two Levels

Once v_2 has converged at the coarse level it is interpolated back to the fine level at which point we solve for $\phi = x^{(n)} - v_1 = x^{(n-1)}$. If the transition between levels has been executed accurately the new values of $x^{(n+1)}$ will be significantly closer to the ideal solution ϕ than those obtainable after an equivalent amount of computational work at the fine level.

This cycle can be extended to more than two levels by simply treating the new coarse level as a fine level for the next coarser level. This procedure further enhances computational work savings by in effect converging the problem on as coarse a level as accuracy between levels can be maintained.

The solution scheme outlined here does not take into account the peculiarities of the neutron diffusion problem such as the eigenvalue search process. To see how this fits into the Multi-Level scheme a modal view of the problem will again be used.

5.0 MODAL ANALYSIS OF THE MULTI-LEVEL NEUTRON DIFFUSION PROBLEM

Rewriting equation (2) in the form

$$M\Phi_o = 0 \ , \text{ where } M = \left[R - \frac{P}{k_o} \right] \tag{26}$$

indicates that this problem is a special case of equation (21) with vector b = 0. On this basis one can assume the Multi-Level scheme is applicable to our problem. The effects of the eigenvalue search and criticality at each level of the problem still have to be determined.

After n iterations equation (7) can be more precisely written as

$$\left[R - \frac{P}{k_g^{(n)}} \right] x^{(n)} = f \tag{27}$$

Substituting for $x^{(n)}$ in modal form gives

$$\left[R - \frac{P}{k_g^{(n)}} \right] \sum_{m=0}^{N} A_m \Phi_m = f \tag{28}$$

Separating the zeroth mode from the rest of the summation results in the relationship

$$\left[R - \frac{P}{k_g^{(n)}} \right] A_o \Phi_o + \left[R - \frac{P}{k_g^{(n)}} \right] \sum_{m=1}^{N} A_m \Phi_m = f \qquad (29)$$

Subtracting the exact relationship for the zeroth order equation and substituting

$$v = x^{(n)} - A_o \Phi_o = \sum_{m=1}^{N} A_m \Phi_m \qquad (30)$$

as the error vector gives

$$\left[R - \frac{P}{k_g^{(n)}} \right] v = f - A_o \left[\frac{1}{k_o} - \frac{1}{k_g^{(n)}} \right] P \Phi_o \qquad (31)$$

Since k_o is not known exactly and zero order components are undesirable in the residual a criteria for grid level transitions can be defined as

$$\left| k_g^{(n)} - k_g^{(n-1)} \right| < \xi \qquad (32)$$

implying for suitable ξ that $k_q^{(n)} \approx k_o$. This criteria cannot be met for small enough ξ before the solution process enters the asymptotic convergence region. By consequence number two the magnitude of the error in $x^{(n)}$ at this stage would still be large enough to make a level transition worthwhile. The equation to be solved can now be written as

$$\left[R - \frac{P}{k_o}\right] v = f \tag{33}$$

The next step in the process is to reformulate the problem at the next coarser level

$$\left[R_2 - \frac{P_2}{k_v}\right] v_2 = f_2 \tag{34}$$

The residual f_2 is interpolated to the new level as previously described. The subscript v on the eigenvector k indicates that the same criticality cannot be maintained between both levels. This is in general true between any two discretizations of the same problem.

To understand how the residual vector is transformed in a level change consider a linear interpolation of equation (28) with $k_g^{(n)} = k_o$ to the coarser level. The equation can now be written as

$$f_2 = \left[R'' - \frac{P''}{k_o} \right] \sum_{m=1}^{N/2} A_m \Phi''_m \qquad (35)$$

A few exemplatory problems quickly show that R" and P" in the above equation are indeed equivalent to R_2 and P_2 of equation (34) and the vectors have undergone the same interpolation as applied to the vector f. Considering the source-like nature of f it would necessarily have to be volume weighted in a level transition (see Appendix A). Substituting equation (35) for f_2 in (34) gives the result

$$\left[R_2 - \frac{P_2}{k_v} \right] v = \sum_{m=1}^{N/2} A_m \left[R_2 - \frac{P_2}{k_o} \right] \Phi''_o \qquad (36)$$

The limit in the summation accounts for the fact that only half as many modes may be represented on the coarse grid structure. No contradiction or loss of accuracy results because of this since higher order modes are assumed to have decayed to insignificance.

Consider a first iteration of this equation:

$$v_2^{(1)} = \frac{R_2^{-1} P_2}{k_v^{(o)} k_o} v_2^{(o)} + \sum_{m=1}^{N/2} A_m R_2^{-1} \left[R_2 - \frac{P_2}{k_o} \right] \Phi''_m \qquad (37)$$

A second iteration will yield

$$v_2^{(2)} = \frac{R_2^{-1} P_2}{k_v^{(1)}} \left\{ \frac{R_2^{-1} P_2}{k_v^{(o)} k_o} v^{(o)} + \sum_{m=1}^{N/2} A_m R_2^{-1} \left[R_2 - \frac{P_2}{k_o} \right] \Phi''_m \right\}$$

$$+ \sum_{m=1}^{N/2} A_m R_2^{-1} \left[R_2 - \frac{P_2}{k_o} \right] \Phi''_m \qquad (38)$$

Observing the iterative process illustrated by these two equations and implementing the usual error vector initialization.

$v_2^{(o)} = 0$, a general relationship for the iterative process can be written as

$$v_2^{(I)} = \frac{R_2^{-1} P_2}{k_v^{(I-1)}} \sum_{m=1}^{N/2} B_m R_2^{-1} \left[R_2 - \frac{P_2}{k_o} \right] \Phi''_m$$

$$+ \sum_{m=1}^{N/2} A_m R_2^{-1} \left[R_2 - \frac{P_2}{k_o} \right] \Phi''_m \qquad (39)$$

Simplifying this result gives

$$v_2^{(I)} = \sum_{m=1}^{N/2} B_m \left[\frac{k_m}{k_v^{(I-1)}} - \frac{k_m^2}{k_v^{(I-1)} k_o} \right] \Phi''_m$$

$$+ \sum_{m=1}^{N/2} A_m \left[I - \frac{k_m}{k_o} \right] \Phi''_m \qquad (40)$$

where B_m is a coefficient containing the accumulated effects of the criticality search at the coarser level.

The ideal result of these iterations at level two is

$$v_2^{(\infty)} = \sum_{m=1}^{N/2} A_m \Phi''_m \qquad (41)$$

This can only be true if $k_v = k_o$ and $B_m = A_m$ at $I = \infty$.
One can easily see that for problems with fixed values of k_m between levels and no criticality search that this indeed would be true. How our problem is affected by these variable parameters can only be determined through numerical tests.

6.0 THE PROGRAM

A 1-D diffusion code written by the author and verified by Cheby[3] and Sorghum[1] results was used as a basis for the application of a Multi-Level subroutine.

To test the scheme three iterative options were introduced into the code.

Option 1. Gauss Seidel iterations were used at all levels of the problem.

Option 2. Successive Overrelaxation (SOR) was implemented at all levels.

Option 3. An extrapolated weighting factor was applied to the error vectors calculated at any level in conjunction with either of the above options.

For Option 2 the optimum overrelaxation factor "w" for the fine level iterations was introduced as an input parameter. This factor would in general be larger than the optimum value at coarser levels but the decrease in convergence rates due to this discrepancy would be partially offset by the increased diagonal dominance of the problem at these levels. The reduced number of work steps required to converge the problem at these levels would also reduce the significance of this effect on the overall behaviour of the scheme.

Option 3 arose from previous investigations of the behaviour of the Multi-Level scheme which indicated that the error vectors calculated would attain the expected shape but were generally smaller in amplitude. This is supported by the modal analysis which indicates that the coefficients Bm of the coarse level cannot be expected to equal the fine level coefficients Am. The one norm of the error on the fine level was estimated by summing the absolute differences between two successive iterations and multiplying by Wagner's Extrapolation coefficient:

$$| v_f |^1 = E \left\{ \sum_{i=1}^{N} \left[\phi_i^{(n)} - \phi_i^{(n-1)} \right] \right\} \qquad (42)$$

The one norm of the error vector at the coarse level

$$| v_c |^1 = \sum_{i=1}^{N} v_i \qquad (43)$$

could then be used to weight the resultant error vector such that

$$v_c' = \frac{| v_f |^1}{2 | v_c |^1} v_c \qquad (44)$$

the factor "2" arising since there are half as many points at the coarse level.

The Multi-Level algorithm implemented follows closely the scheme known as Cycle C in Brandt's paper. The finite difference coefficients for each level were calculated using the subroutine supplied by the original program and were recalculated at each level change. This added iterative work equivalent to two iterations of the flux vector at the new level but reduced storage requirements by one half a flux vector length and simplified program bookkeeping.

7.0 RESULTS AND DISCUSSION

The 1-D infinite slab test problem used, and its properties are illustrated in Figure 2. Each region of the problem was divided into cells such that the number of cells could be evenly divided by two at least twice to provide easy accessibility to three levels of grid structure. All levels of the problem were considered to have converged when

$$\frac{\sum_{i=1}^{N}\left[\phi_i^{(n)} - \phi_i^{(n-1)}\right]^2}{\sum_{i=1}^{N}\left[\phi_i^{(n)}\right]^2} < \text{EPS} \qquad (45)$$

for a value of EPS = 1.0×10^{-5}.

The options run include Option 1, Option 2 and a combination of Option 1 and 3. Graphs plotting the relative execution time for each option versus the level change criteria values (from equation 32) are illustrated in Figures 3 through 5. The execution time required to converge the test problem at the fine level using Gauss Seidel iterations was used as the standard for comparison of the effectiveness of each option. Therefore the ordinates of the graphs represent the values

$$\text{Ratio} = \frac{\text{Execution Time of Option}}{\text{Execution Time of Standard}} \qquad (46)$$

The absicca values range from $\xi = .1 \times 10^{-1}$ to $\xi = .1 \times 10^{-10}$ with only fine level iterations occuring for the minimum value in all options.

A first indication of the merit of an option is whether or not two level convergence rates improved upon fine level results. This was not found to be so for options 1 and 2. The extension to three levels of iteration then showed further deterioration in convergence times. The results for two and three level iterations were found to merge at some value of ξ at which three level excursions ceased to occur. The only option that showed any promise was the combined Option 1 and 3 result.

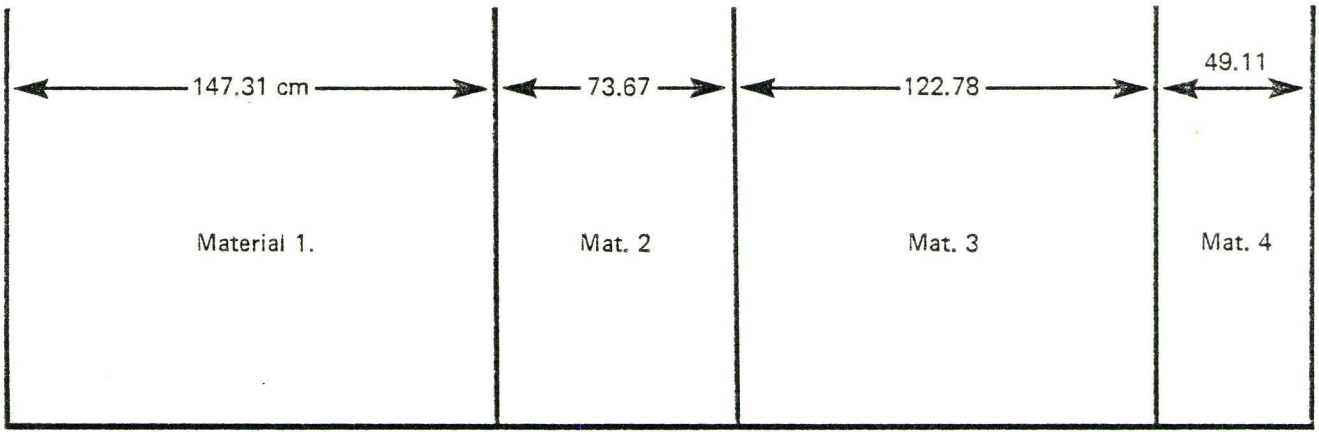
The two level results for this third option improved upon single level results for $\xi \geq .1 \times 10^{-4}$. It is, therefore, expected that a three level test would show a further improvement. Since there was no significant improvement in convergence times, tests were run to ensure that consistency between levels, as required in the discussion of the Multi-Level scheme, had been maintained. These tests indicated that three levels of iteration were valid for our test problem and that the problem lay in the application of the extrapolation coefficient.

Since Wagner's Extrapolation coefficient is not applicable until asymptotic convergence occurs the major component of the error in our Multi-Level problem would be the first error mode. This mode essentially becomes the fundamental mode at the second iterative level and corrections from the third level enhance only minimally the overall convergence rate. The failure of this system, therefore, lies in the inability of Wagner's Extrapolation coefficient to accurately obtain an estimate for the "one norm" of the error vector before asymptotic convergence takes place.

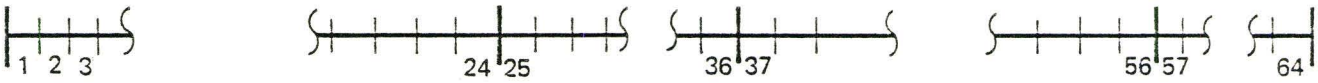
The application of an Option 2 and 3 combination did not show any improvement over Option 1 results. This could again be attributed to an inaccurate estimation of the Extrapolation Coefficient during SOR iterations. Figure 6 compares the two level results of each of the three options discussed showing optimum SOR iterations to excel. Wagner's Extrapolation method was also applied and matched or exceeded SOR results for the test cases run.

8.0 CONCLUSIONS

The mathematics of the Multi-Level scheme developed has proven the feasibility of the scheme as applied by Brandt. It has, however, also pointed out the problems associated with the application of this scheme to the iterative eigenvalue search problem. These problems were partially overcome with the use of an extrapolated weighting function for the error vectors. The applicable range of this weighting function unfortunately reduced the basically multi-mode method to a single mode method, losing any advantage over the single mode extrapolation method. In all cases the Multi-Level scheme has shown no advantage over SOR or the already proven results of Wagner's extrapolation technique. Considering the increased programming and storage requirements of the method it cannot be recommended for application to the Neutron Diffusion problem at this time.



LEVEL 1 MESH STRUCTURE



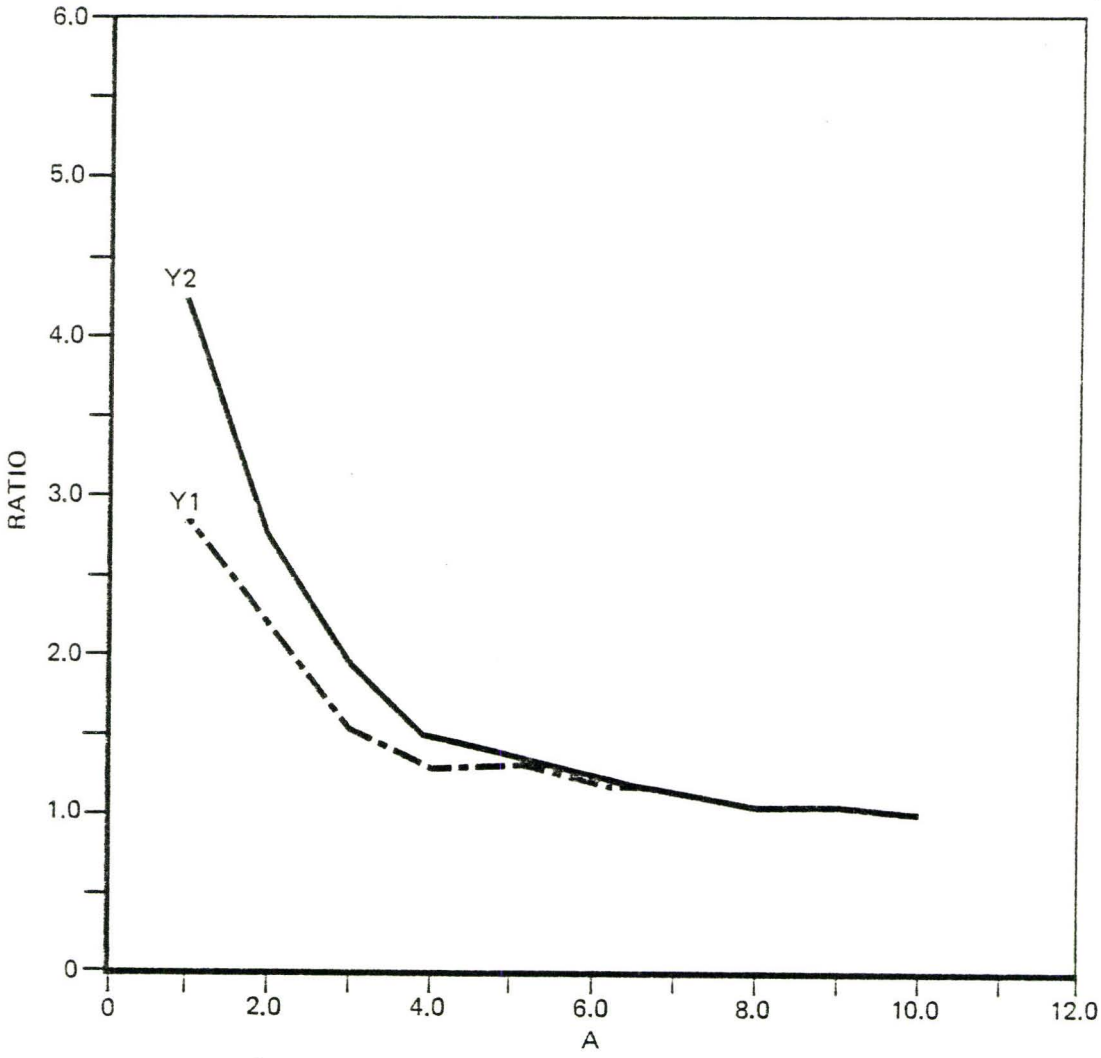
TWO GROUP MATERIAL PROPERTIES

Mat	$\Sigma_T(7) \times 10^{-2}$	$\Sigma_T(2) \times 10^{-2}$	$\Sigma_s^{(2\ 1)} \times 10^{-2}$	$\Sigma_f(2) \times 10^{-2}$
1	.856434	.418640	.768350	.485170
2	.856434	.411440	.768350	.485170
3	.856434	.404230	.768350	.485170
4	7.07970	.854870	1.01970	0.0

DIFFUSION CONSTANTS

D (1) 1.2657
D (2) .9329

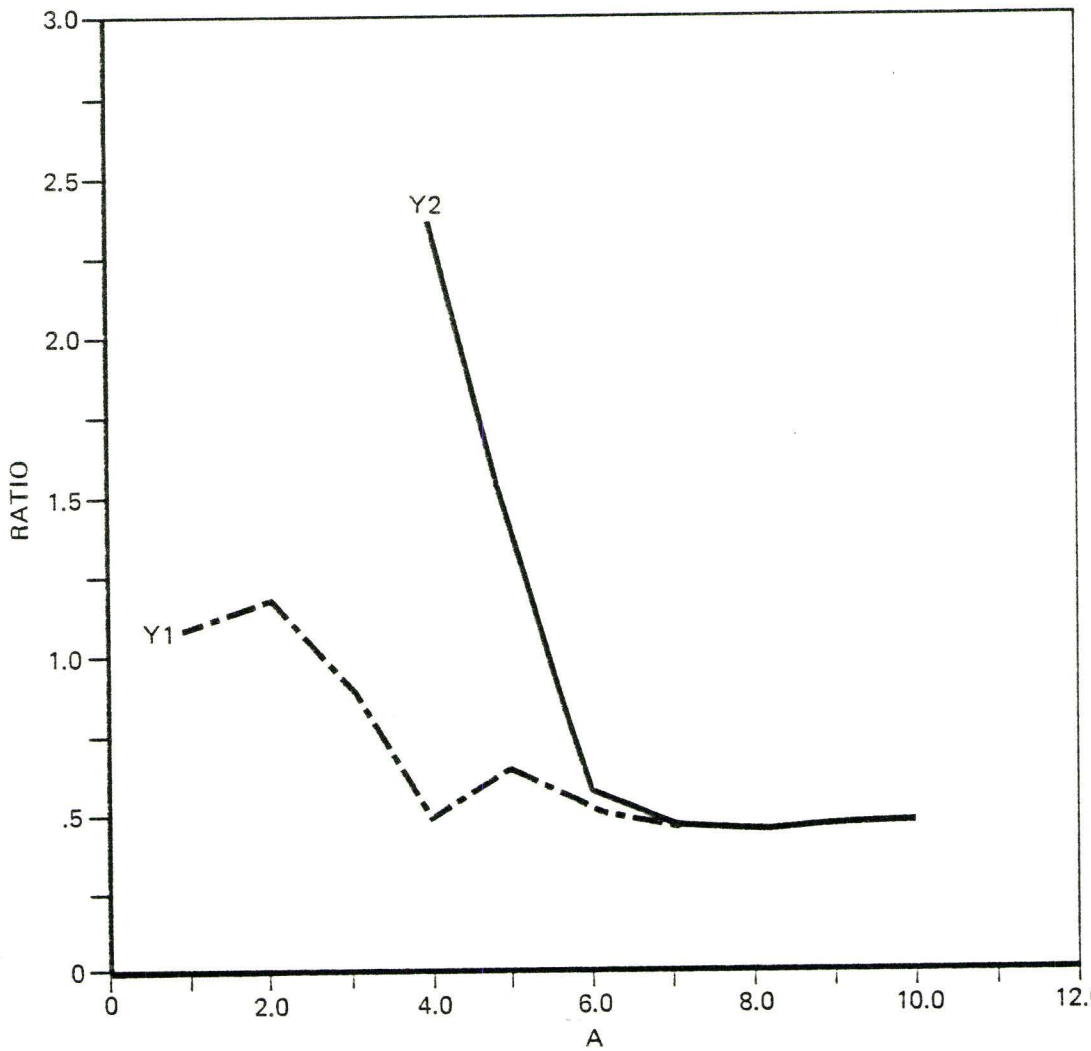
FIGURE 2
Test Problem Configuration and Properties



$\xi = 0.1 \times 10^{-A}$

Y1 = 2 LEVELS
Y2 = 3 LEVELS

FIGURE 3
Option No. 1



$\xi = 0.1 \times 10^{-A}$

Y1 = 2 LEVELS
Y2 = 3 LEVELS

FIGURE 4
Option No. 2

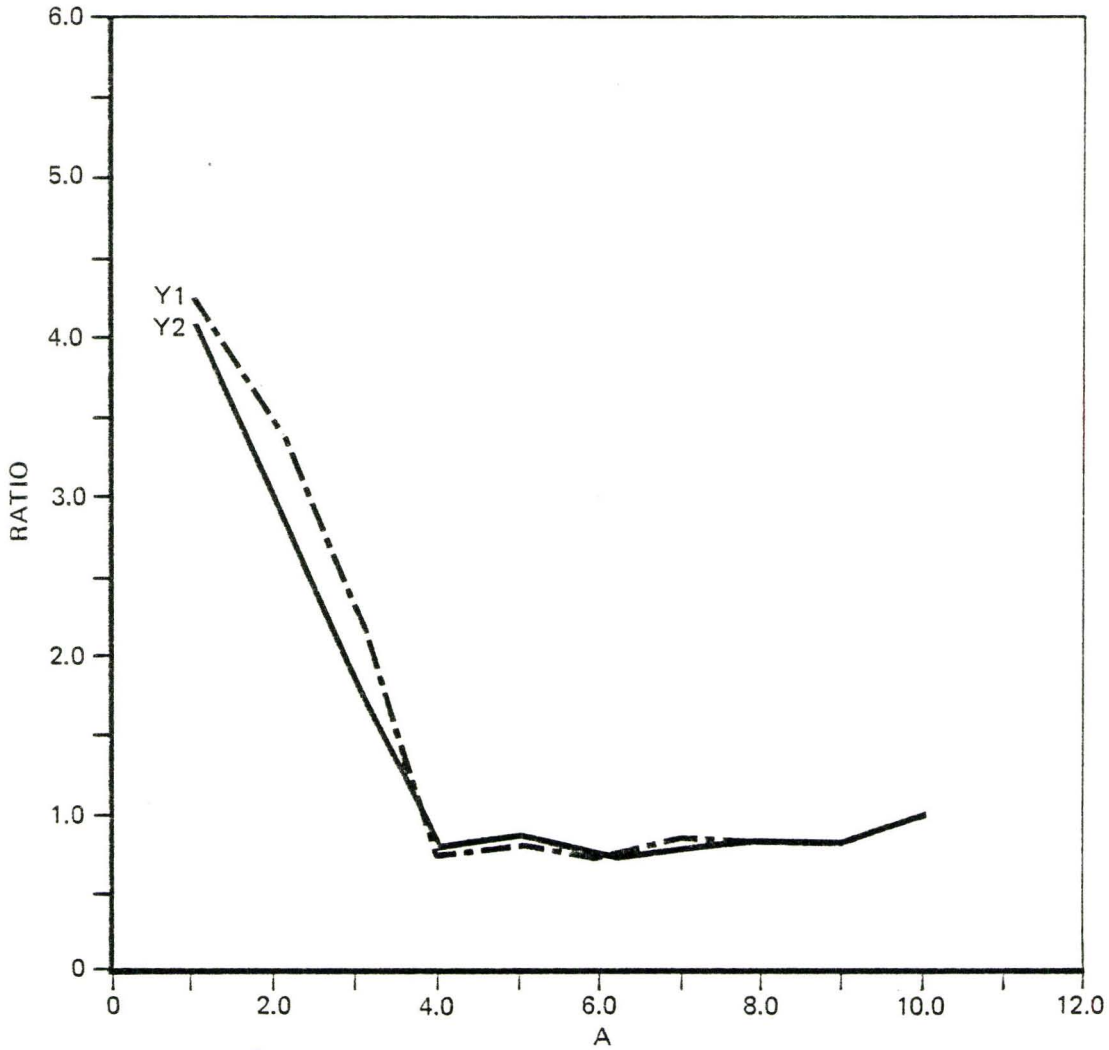
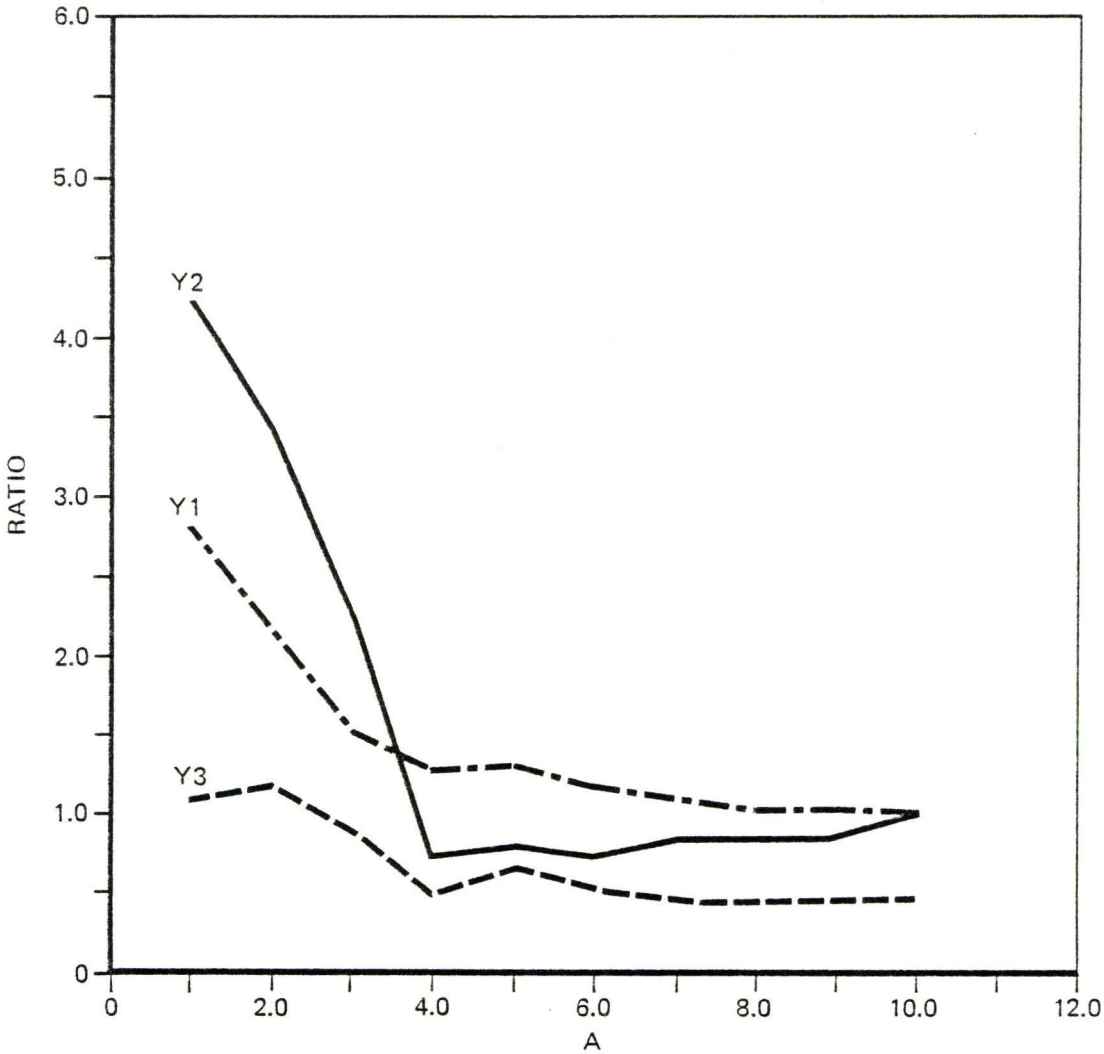


FIGURE 5
Option No. 1 + 3



$\xi = 0.1 \times 10^{-A}$

Y1 = OPT. 1
Y2 = OPT. 1 + 3
Y3 = OPT. 2

FIGURE 6
2 Level Results

APPENDIX A

Residual Behaviour During Level Transitions

With respect to the interpolation of the residual from a fine to coarse level, we wish to show that

1. The residual behaves as a source term in the matrix equation and must be volume weighted in a level transition; and
2. The eigenvectors constituting the error in the approximate solution at the fine level are interpolated in the same manner as the residual.

To do this a simple problem using the point neutron diffusion equation has been devised:

$$-D\nabla^2\phi + \sigma_R\phi = S \qquad (a1)$$

This equation can be approximately solved by using some numerical method. Rewriting the above equation in 1-D slab central difference form gives

$$-D_i\left[\frac{\phi_{i-1}-2\phi_i+\phi_{i+1}}{\Delta x_i^2}\right] + V_i\sigma_{R_i}\phi_i = S_i \qquad (a2)$$

where

ϕ_i = neutron flux at meash point i

D^i = diffusion coefficent

σ_{R_i} = macroscopic removal cross section

V_i = volume of each mesh spacing

Δx_i = the width of a mesh spacing

$S_i = V_i \times s_i$ = total volume source

For simplicity, continuity of current boundary conditions leading to a linear result for ϕ have been chosen such that

$$\text{L.H.S.} - \phi_o = 2\phi_1 - \phi_2 \qquad \text{i}$$

$$\text{R.H.S.} - \phi_{N+1} = \phi_N \left(\delta - \frac{\Delta x_N}{2} \right) \Big/ \left(\delta + \frac{\Delta x_N}{2} \right) \qquad \text{ii} \qquad \text{(a3)}$$

where δ = the extrapolation distance from the outer surface.

For a six point one dimensional problem with the following values

$$D = .5$$

$$\Delta x = 1.0$$

$$V = 1.0 \qquad \text{for } i = 1, N \qquad \text{(a4)}$$

$$\Sigma_R = 1.0$$

$$\delta = .5$$

The resultant matrix equation at the fine level becomes

$$\begin{bmatrix} 1.0 & 0.0 & & & & \\ -0.5 & 2.0 & -0.5 & & & \\ & -0.5 & 2.0 & -0.5 & & \\ & & -0.5 & 2.0 & -0.5 & \\ & & & -0.5 & 2.0 & -0.5 \\ & & & & -0.5 & 2.0 \end{bmatrix} \begin{bmatrix} \phi_1 \\ \phi_2 \\ \phi_3 \\ \phi_4 \\ \phi_5 \\ \phi_6 \end{bmatrix} = \begin{bmatrix} V & & & & & 0 \\ & V & & & & \\ & & V & & & \\ & & & V & & \\ & & & & V & \\ 0 & & & & & V \end{bmatrix} \begin{bmatrix} s_1 \\ s_2 \\ s_3 \\ s_4 \\ s_5 \\ s_6 \end{bmatrix} = S \qquad \text{(a5)}$$

Since the solution $\phi = [6.0, 5.0, 4.0, 3.0, 2.0, 1.0]^T$ gives the result S = 0 for V = 1.0 the equation can be written in matrix notation as

$$D\phi - V\phi = 0 \tag{a6}$$

Rearranging this equation gives the result

$$D\phi - \frac{V}{2}\phi = \frac{V}{2}\phi = F = \left[3.0,2.5,2.0,1.5,1.0,-0.5 \right] \tag{a7}$$

which is in a form equivalent to the residual equation. Recalling that the residual should contain no zero mode components we can treat the vector ϕ as the error vector being sought in this derivation. The source like function of the residual is already obvious having been separated out of the original source term.

Rediscretizing the problem on a three point mesh results in the equation

$$D_2\phi_2' - \frac{V_2}{2}\phi_2' = F_2' \tag{a8}$$

where

$$D_2 = \begin{bmatrix} 2.0 & 0.0 & 0.0 \\ -0.125 & 2.25 & -0.125 \\ 0.0 & -0.125 & 2.2916 \end{bmatrix} \quad \text{i}$$

$$V_2 = \begin{bmatrix} 2.0 & 0.0 & 0.0 \\ 0.0 & 2.0 & 0.0 \\ 0.0 & 0.0 & 2.0 \end{bmatrix} \quad \text{ii} \qquad \text{(a9)}$$

Since we know the values of the error vector ϕ' at the fine level beforehand in this case, we can interpolate them to level two and solve for F'_2.

$$\left[D_2 - \frac{V_2}{2}\right] \begin{bmatrix} 5.5 \\ 3.5 \\ 1.5 \end{bmatrix} = F'_2 = \begin{bmatrix} 5.5 \\ 3.5 \\ 1.5 \end{bmatrix} \qquad \text{(a10)}$$

Interpolating F from level one to two using the same interpolation immediately shows that F_2 is just the volume weighted equivalent.

$$I^{1\rightarrow 2}(F) = \begin{bmatrix} 2.75 \\ 1.75 \\ 0.75 \end{bmatrix} = \frac{V_1}{V_2} F'_2 \qquad \text{(a11)}$$

where $I^{1\to 2}$ is the interpolating function from level 1 to 2. This simple problem illustrates points 1 and 2 clearly. These results have been shown to be true for problems of varying complexity and can be considered valid.

REFERENCES

1. Bailey C.M. et al., "The Sorghum Code: Program Description and User's Guide", TDAI-133, AECL - Engineering Company.

2. Brandt, Achi, "Multi-Level Adaptive Solutions to Boundary-Value Problems", Mathematics of Computation, Volume 31, No. 138, April 1977 Pages 333-390.

3. Private communication from Dr. Aziz Rehman: "Nuclear Studies and Safety Memorandum, July 30, 1975, File 91-41500-Cheby", Ontario Hydro, Toronto, Ontario.

4. Varga, R.S., "Matrix Iterative Analysis", Prentice-Hall, Englewood Cliffs, N.J., 1962.

5. Wagner, M.R., "The Application of the Block Inversion Technique to Multi-Dimensional Reactor Calculations", "Proceedings of Conference on the Effective Use of Computers in the Nuclear Industry", Knoxville, Tennessee, April 21-23, 1969, Pages 211-246.