NEW COMPUTATIONAL METHODS FOR THE SOLUTION OF MULTIDIMENSIONAL
NEUTRON DIFFUSION PROBLEMS RELATED TO NUCLEAR REACTOR SAFETY ANALYSIS

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J. Dorning
University of Illinois at Urbana-Champaign
Urbana, Illinois 61801

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Abstract

The convergence, accuracy and computing times for the partial current balance (PCB) method have been studied for simple one-, and two-dimensional test problems based on an HTGR model. The PCB (linear) method was found to be three to thirteen times as fast as the finite difference method for a given accuracy for the one-dimensional problems, depending upon the degree of complexity of the problem. It was two to seven times as fast as the finite element (linear) method. The advantages of the PCB method over the other methods increased as the degree of problem complexity was increased, and as the required accuracy was increased.

The advantages of the PCB method over the finite difference method were even more dramatic when comparisons were made for the two-dimensional problems. The PCB (bilinear) method was four to fifty times as fast as the finite difference method for a given accuracy. Again the advantages of the PCB method over the finite difference method increased as the required accuracy was increased. A further improvement of a factor of about eight was obtained when the PCB (bilinear) calculation was replaced by a PCB (biquadratic) calculation.

The investigation of techniques for accommodating time-dependent changes of nuclear properties (feedback) are continuing. Special methods for the solution of stiff differential equations have been applied to the point kinetics equations. They have been found to permit extremely large time steps, however inefficiencies in the startup procedure and the early part of the calculations using these methods must be resolved. A technique which combines these stiffly stable methods with the PCB method in such a way that it will not be necessary to invert large matrices has been devised.

A method by which the "Green's function" matrix elements can be generated for heterogeneous volume elements has been devised.

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REPORT

Studies comparing the convergence, accuracy and computing times of the partial current balance (PCB) method with those of the finite difference method have been continued. Our initial estimates which indicated that the advantages of the partial current balance method over the finite difference method would be even more dramatic for two-dimensional problems than they are for one-dimensional problems have been verified by the problems run thus far. We have observed that, in general, as the degree of complexity (e.g., the number of groups, the number of regions, the number of dimensions) is increased the advantages of the PCB method over the finite difference method increase, even when only linear (bilinear) expansion functions are used in the PCB method.

In all of the one-, and two-dimensional calculations done thus far the advantages of the PCB method over the finite difference method and the finite element method (only one-dimensional finite element calculations have been done) have increased as the accuracy requirements have been increased. This, of course, is a desirable feature from the standpoint of applications to reactor safety research in which a high level of accuracy will often be required.

A two-dimensional PCB program, and a comparable finite difference program (same input, output, editing, outer iteration scheme, etc.) have been written and debugged. The matrix elements in the two-dimensional PCB code are being constructed from their series representations. These codes were used for the initial comparison studies which led to the general conclusions stated above.

One-, and two-dimensional k-calculations for very simple systems based on HTGR models have been done. In the one-dimensional calculations the ratio R_1 of the finite difference method computing time to the PCB (linear) computing time for the same accuracy increased as the system complexity was increased from one-dimension, one-region, one-group to one-dimension, two-region, one-group to one-dimension, two-region, two-group. This ratio for the one-dimension,

two-region, two-group system was approximately 12.7 (for an accuracy requirement of 10^{-6}).

The ratio R_1 also increased as the accuracy requirement on the eigenvalue and the solution was increased. It was found that this ratio is proportional to the reciprocal of the accuracy to a constant power ($R_1 \propto 1/\epsilon^c$, where $c \approx 0.4$). Similar results were also obtained for R_2 , the ratio of the finite element (linear) computing time to the PCB (linear) computing time.

In the two-dimensional calculations R_1 , the ratio of the finite difference computing time to the PCB (bilinear) computing time was also proportional to the reciprocal of the accuracy to a constant power, but here the exponent was approximately four times larger than in the one-dimensional case (that is, $R_1 \propto 1/\epsilon^{4c}$, where $c \approx 0.4$). We regard this as extremely encouraging, but the simplicity of the systems calculated and the limited number of the calculations done prevent us from assuming that this factor of four will appear in the exponent in all problems as the number of dimensions is increased from one to two. (In this case this factor happens to be the square of ratio of the number of dimensions. Whether this is general or not will be determined in the future.)

The two-dimensional finite difference calculations were done only for accuracies only up to $\epsilon = 1.6 \times 10^{-5}$. Beyond that, computing times were extrapolated for the finite difference method, since false convergence would occur for finer mesh calculations without acceleration techniques and poor accuracy would result. The PCB method is not plagued by this false convergence problem; hence PCB bilinear calculations were done for accuracies up to 10^{-6} . The ratio R_1 was 4.0 for $\epsilon = 1.6 \times 10^{-5}$, the last finite difference calculation. For higher accuracies the PCB (bilinear) results were compared with the extrapolated ideal finite difference results to obtain: $R_1 = 4.5$ for $\epsilon = 10^{-5}$, $R_1 = 11.9$ for $\epsilon = 4 \times 10^{-6}$, and $R_1 = 56.3$ for $\epsilon = 10^{-6}$. An additional improvement by about a factor of eight is obtained when a PCB (biquadratic) calculation is

done instead of a PCB (bilinear) calculation for this accuracy. More extensive calculations for more complicated systems based on HTGR models will be done in the future.

Studies on the accommodation of time-dependent changes of nuclear properties in the PCB method by developing the capability to do PCB static feedback calculations (i.e., criticality calculations at a given power) are being continued. The coding necessary for these studies has not yet been completed.

Work on combining the PCB method with a special solution technique for solving stiff differential equations has been started. One such special solution technique, Gear's method, has been applied to the point kinetics equations and compared with a standard theta-difference method. Using Gear's method, it was possible toward the end of the calculation to employ time steps which were more than fifteen times as large as those permitted for the theta-difference method. However, the actual computing times required when Gear's method was used were greater than those for the theta-difference calculations. This appears to be due to the large number of very small time steps taken during the startup procedure and early part of the calculation when Gear's method was used. The possibility of employing a different startup procedure and a different method during the early part of the calculation, such as a standard theta-difference method, and then switching to Gear's method will be explored.

The combination of Gear's method with ordinary finite difference methods in space appears to be unwise. Since Gear's method is a multi-step method the total storage space required for a realistic reactor kinetics problem would be prohibitive. On the other hand, when a coarse mesh method such as the PCB method is used for the space calculations the total amount of storage required is comparable to that required when a finite difference method in space is combined with a single-step method in time. However, there is

still another difficulty which arises in the direct application of a predictor-corrector method such as Gear's method. Large matrices of the order of the total number of spacial expansion coefficients in the entire assembly must be inverted in each corrector iteration for each time step. This, of course, makes the direct application of the method impractical. We have developed a scheme by which these matrices can be inverted iteratively rather than directly. The method is the logical extension of the directional spatial sweeps which we are currently using in the static PCB calculations for one-, and two-dimensional systems. Hence, no direct matrix inversions are required. Rather, only simple multiplication of very low order matrices, as in statics PCB calculations, are involved. This method will be used to combine the PCB method with a multi-step predictor-corrector method such as Gear's method after the problem of the small initial time steps has been satisfactorily resolved.

The problem of accommodating heterogeneous volume elements in the PCB method is being considered. A method by which the "Green's function" matrix elements can be calculated has been devised. It is quite simple and straightforward. However, it has now been recognized that a more severe problem is the proper representation of the source term in the PCB equations when the method is applied using heterogeneous volume elements. A similar problem also arises when attempts are made to apply the finite element method using heterogeneous volume elements. Work on this problem is continuing.