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

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ABSTRACT

The generation of the matrix elements which appear in the partial current balance method (PCB) equations is being studied. For one-dimensional problems two methods of constructing these matrix elements, i.e. directly--from exact expressions, and approximately--via a variational principle, have been used. Both are very efficient. For two-dimensional problems directly generating the matrix elements from their series representations has been found to be satisfactory since the series have good convergence properties. Work is continuing on the generation of accurate approximate matrix elements via the variational principle for two-dimensional problems.

Convergence, accuracy, and computing times for the PCB method have been studied for simple one-dimensional test problems and compared with those for the finite difference and finite element methods. The PCB method was superior in all of the cases studied. For given accuracy it was five to ten times as fast as the finite difference method and two to six times as fast as the finite element method.

The two-dimensional PCB equations are being coded, and similar studies for them is beginning. Initial estimates indicate that the advantages of the PCB method over the other methods will be significantly greater in two-dimensional problems than it is in one-dimensional problems.

The investigation of techniques for accommodating time-dependent changes of nuclear properties (feedback), and for combining the PCB method with special methods for the solution of stiff differential equations has begun.

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REPORT

The first problems studied to determine the value of the partial current balance (PCB) method as a computational technique for reactor statics and dynamics calculations were those related to the generation of the required Green's function matrix elements, and those concerning convergence and computing times for simple source iteration schemes used to solve the PCB flux and partial current equations for k-calculations. Considerable progress has been made on both problems.

The required matrix elements are double integrals of the local "group removal and diffusion" Green's functions weighted by simple polynomials in the source point and the field point variables. For simple one-dimensional geometries, the exact Green's functions and matrix elements can be easily generated from analytic expressions. However, an approximate method, based on a variational principle, has also been developed to directly generate the matrix elements. The approximate matrix elements generated by this method are very accurate for the "volume-volume", "volume-surface", and "surface-volume" matrices. Those for the "surface-surface" matrix are less accurate (as would be expected when a variational principle is used), but can be made very accurate simply by using a slightly higher order expansion when generating the matrix elements than is used to solve the PCB equations for the system fluxes and partial currents. (See C00-2461-2 for details.) Very little computer time is required to generate the matrix elements either exactly from the analytical expressions or approximately via the variational principle for one-dimensional problems. For two-dimensional problems in which the system is decomposed into volume elements with reasonably simple geometries the matrix elements can be calculated quickly from their series representations. This

would be extremely inefficient if it were necessary to construct the Green's functions themselves. However, that is not necessary. Since the matrix elements are double integrals of the Green's functions their series representations have better convergence properties. (The series representations for the "volume-volume" matrix elements converge as n^{-5} , "volume-surface" and "surface-volume" matrix elements as n^{-4} , and "surface-surface" as n^{-3} .)

Hence, the computer time necessary to construct the matrix elements in simple two-dimensional problems is small compared to the time required to solve the PCB equations. Nevertheless, there is still motivation to further develop the method for the approximate generation of the matrix elements for two-dimensional problems. It would permit the matrix elements to be constructed even more rapidly when simple two-dimensional volume elements are used. More importantly, it will also make possible the use of irregular volume elements in two-dimensions for which simple series representations for the matrix elements cannot be obtained. The variational principle presently being used to generate the matrix elements for two-dimensional problems results in accurate "volume-volume", "volume-surface", and "surface-volume" matrix elements, but the "surface-surface" matrix elements are in error by a few percent when calculated for two adjacent surfaces. This results in an unacceptable error in the solution to the PCB equations. However, it may be possible to correct this difficulty by simply scaling the approximate matrix elements to ensure neutron balance. It may also be possible to use a slightly more complicated approximation scheme for the generation of the "surface-surface" matrix elements. These ideas will be examined in detail in the future. For the present, the series representations will be used for the two-dimensional matrix elements since they can be accurately summed in

reasonable amounts of time. This will permit the early evaluation of the overall PCB method as a computational scheme in multidimensional problems.

The convergence, accuracy and computing times for the iterative solution of the PCB equations definitely compare favorably with those for the finite difference and finite element methods. So far, very simple one-dimensional, one-group bare and reflected systems, and one-dimensional, two-group, reflected systems based on HTGR models have been studied. The one-dimensional PCB equations have been coded, and one-dimensional finite difference and finite element programs which have the same input, output, editing, etc. have been written. The simple test problems described above have been run using linear, quadratic, and cubic expansions in the PCB and finite element calculations. For a given accuracy, the PCB method was approximately five to ten times as fast as the finite difference method, depending upon the particular problem. The advantage was greatest for reflected systems. For a given accuracy, the PCB method was approximately two to six times as fast as the finite element method. Here the advantage was greatest when linear expansions were used in both methods. The advantage of the PCB method over the finite element method was smallest (only about a factor of two in computing time) when higher order expansions, i.e., quadratic and cubic, were used in both methods.

The two-dimensional PCB equations are being coded and debugged, and a comparable finite difference program (same input, output, editing, outer iteration scheme, etc.) is being written. The matrix elements calculated in the two-dimensional PCB code are being constructed from their series representations. Initial estimates indicate that the advantages of the partial current balance method over the finite difference method are more dramatic for

two-dimensional problems than they are for one-dimensional problems, and that the increase in this advantage as we go to two-dimensions may be very substantial.

The investigation of the ability of the PCB method to accommodate time-dependent changes of nuclear properties is initially being carried out by developing the capability to do PCB static feedback calculations (i.e., criticality calculations at a given power) using a simple temperature feedback model for the system thermo-hydraulics. This will determine whether, and how often, it is necessary to recalculate the Green's function matrix elements as the cross sections change due to feedback. After this, capability to do load-following transient calculations via the PCB method will be developed. Such calculations will test the ability of the PCB method to accommodate both time-dependent changes of nuclear properties (via feedback) and reactor geometry (via control rod motion). After it is demonstrated that the PCB method can accommodate such changes, a full reactor kinetics calculational capability based on the method will be developed. For this reason the possibility, and desirability, of combining the PCB method with a special solution technique, Gear's method, for solving stiff differential equations is concurrently being studied.

The value of combining Gear's method, a predictor-corrector method, with the PCB method for kinetics calculations is being investigated by initially applying Gear's method to the point kinetics equations and comparing the computing times required by this method with those required by a standard theta-difference method. If Gear's method proves to be favorable both techniques will then be applied to the PCB equations using a few spatial volume elements. The fact that Gear's method (and most other fruitful

methods for treating stiff differential equations) is a multi-step method causes some initial concern in connection with the computer storage space necessary to implement the method (such methods) for practical multi-dimensional reactor kinetics calculations. However, if this method can be combined with an accurate coarse mesh method for multigroup spatial calculations, such as the PCB method, the total storage space required will not exceed that necessary for ordinary finite difference methods (in space) when combined with single-step methods (in time), due to the large saving of the PCB method over the finite difference method in the storage space necessary for the spatial calculations. The advantages of using Green's functions in time, analogous to the use of Green's functions in space in the PCB method, over special methods for stiff differential equations will be examined in the future.