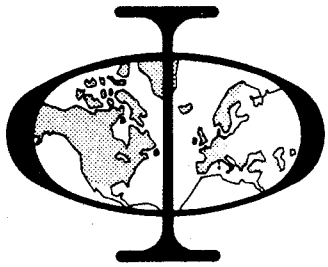

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NUMERICAL METHODS FOR REACTOR CALCULATIONS

R. ORTIZ FORNAGUERA

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EUROPEAN NUCLEAR ENERGY AGENCY, O.E.C.D.
38, Boulevard Suchet - PARIS 16e

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R. Ortiz Fornaguera

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INTRODUCTION

Although some general comments on the role of numerical analysis techniques in nuclear reactor calculations were made in Section IV of the EACRP report "Review of Reactor Physics Problems", the Committee felt that numerical methods deserved a more detailed consideration. The objective of this report is to give a brief and somewhat sketchy review of current trends and advances in the field of numerical analysis as applied to nuclear reactor physics problems. The report is largely based on information provided by many laboratories in reply to a questionnaire which was sent last July to all EACRP members. Another very important source of information and comments has been the valuable discussions with many scientists organized on the occasion of visits to the following centres: EIR, Würenlingen, Switzerland; Centro di Calcolo, CNEN, Bologna, Italy; EURATOM, CCR, Ispra, Italy; Centre de Saclay, CEA, Saclay, France; AERE, Winfrith, Dorchester, Dorset, U.K.

The questionnaire mentioned above referred to the following three points: A) information on the present work being done in the field of numerical methods for reactor calculations; B) anomalies observed, if any, in the behaviour of currently used nuclear programmes; C) directions in which substantial improvements could be reached as compared with the present approaches. The report is accordingly divided into three sections:

Section A: Present trends in numerical methods.
Section B: Do some codes show a "pathological" behaviour?
Section C: Possible improvements.

This report does not claim to be complete. Only some trends and some directions have been discussed and the author is well aware that many important items remain untouched.

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A. PRESENT TRENDS IN NUMERICAL METHODS

A.1. Finite difference methods

General

There exists a large variety of methods for obtaining numerical solutions to a given system of differential or integro-differential equations. In particular, the partial differential equations of the multigroup-diffusion model are replaced over the region in which the solution is sought by finite difference equations over a set of mesh points within the region. The reduction of the problem posed in a continuum set to a problem posed in a discrete set (the so called discretization of the problem) is carried out by replacing the differential operators involved with finite difference operators related to a given mesh imposed on the domain of the independent variables. In this manner a finite difference analog of the continuous space problem is derived which is actually used in numerical computations. It is possible to control the accuracy of the numerical results either by increasing the number of mesh-points and/or by improving the approximation of the finite difference operators.

The accuracy of the numerical solution, however, refers to the solution of the mathematical model of the actual physical system. In fact, it is important to bear in mind that it does not always follow that improving the accuracy with which a particular (approximate) reactor model is solved necessarily improves the accuracy in real terms of the final answer. Thus whilst it is possible to improve the accuracy of the numerical solution of the homogeneous reactor calculations by increasing the number of mesh points, etc., it does not follow that by doing this one is improving the solution to the original physical problem.

The discretization of a given problem poses some general questions of practical character[1]. Thus,

a) Although there are in principle many meshes which might be used, the behaviour of the solution, and the form of the domain and its boundaries, severely limitthe number of possible choices . This is an important point, since a wrong selection could imply, for example, the use of an unnecessarily large number of mesh points.Even more, it has been pointed out[2] that, in using standard discretiza - tion methods as applied to heterogeneous systems, it may give erro - neous results to use a mesh bearing no relation to the heterogeneous lattice geometry and that better results should be obtained with mesh points at channel centres. On the other hand, the physical notion of "characteristic length" should be mentioned as a guideline to mesh spacing. Characteristic length and radius of curvature of boundaries are the two natural scaling factors on the length dimension.

b) There are many different difference approximations to a given differential operator. The selection of a particular approxima tion is largely determined by the mesh structure and by the nature of the truncation error associated with the approximation. However , the selection is not unique in the sense that the difference opera - tor need not necessarily be the same throughout the mesh.

A proper handling of hexagonal geometries, for example,has led to a formulation of multigroup-diffusion equations in terms of a uniform triangular mesh. However, in some cases the restriction to uniform spacing resulted in a need for an excesive number of mesh points, whereas the use of a non-uniform triangular mesh enables to reduce this number considerably. Ritz variational methods have been applied to derive the corresponding finite difference operator[3].

c) It would be very convenient to find the means of automa tically choosing both the mesh and the difference operator approxima tion "best" suited to a given situation (of course, after defining what is meant by "best"). In particular, it has been possible to cons

truct codes in which mesh doubling takes place as iteration proceeds.

d) There are available various numerical methods for solving the system of equations of the discrete finite difference analog. The choice of the numerical method will depend not only on the nature of the problem to be solved, but also on the computing hardware to be used. In other words, the problem requirements plus the computer available often determine the broad strategy of the solution, and this in turn determines the numerical method that is most appropriate.

Inner-outer iterations

Two basic procedures have been used for solving the finite difference analog of the multigroup diffusion equations: inner-outer iterations and the Equipoise iterative procedure. The algebraic equations to be solved can be written in the matrix form

$$A\phi = \frac{1}{\lambda} F\phi , \qquad (1)$$

where ϕ is a vector whose GxN components ϕ_n^μ (μ =1,2,...,G; n=1,2,...,N) are the approximations for the G fluxes $\phi^\mu(x)$ at the N prescribed mesh points; A is a matrix representing leakage, absorption, out- and in-scattering; F is a matrix representing the fission source. The usual process of solving (1) consists of guessing an eigenvalue and a source distribution, computing the G fluxes at each mesh point, and recomputing the source and the eigenvalue. This computation, called an outer (or fission-neutron source) iteration, is repeated sucessively, stopping when it is felt that consistency has been reached according to pre-established criteria (convergence indicators). When direct inversion of A is not practical, as it can be the case when the value of N dealt with is too large, iterative techniques will be used in computing the flux from a given fission source. These iterations are referred to as inner iterations (or mesh sweeps).

The interrelationship between inner and outer iterations appears to be very complex and poses the problem of how to reach an optimum strategy between inner and outer iterations. An optimum strategy here means a combination of inner and outer iterations in such an order and number that the time required to solve the problem on a given computing system be a minimum. In this sense, inner and outer iterations have to be tailored to the computer being used. It has been pointed out[4], for example, that problems for which the inner iteration can be contained in fast memory are often solved most efficiently by imposing stringent error reduction requirements on the inner iteration. This enables more effective Chebyshev extrapolation of the outer iteration. When the inner iteration is not memory contained, an effective strategy is to perform relatively few inner iterations with restricted extrapolation on the outer iteration.

Two basic outer iteration procedures are being widely used for solving the discrete multigroup-diffusion equations: the Wielandt's method and Chebyshev extrapolation. As is well known Wielandt's method (also called fractional iteration or inverse power method) substitutes the matrix equation

$$(A - \frac{1}{\lambda_e} F)\phi = (\frac{1}{\lambda} - \frac{1}{\lambda_e}) F\phi \qquad (2)$$

for the matrix equation (1). If the estimated eigenvalue λ_e is greater than the true fundamental eigenvalue λ_o by order of magnitude a few percent, the dominance ratio is sharply reduced thus improving the rate of convergence. When direct inversion may be applied to (1) or (2), to invert $(A - \lambda_e^{-1} F)$ is perhaps more trouble than to invert A. However, the increased difficulty involved in the inversion of $(A - \lambda_e^{-1} F)$ rather than A appears less significant than the sharp reduction in the dominance ratio. No instability has been reported thus far in the application of this method[5].

Although some of the assumptions on which the Chebyshev extra-

polation is based have not been shown to be valid in all conceiva - ble practical cases (e.g., the assumption that the eigenvalues of $A^{-1}F$ are real and non-negative and that the eigenvectors form a complete set[6]), this method has been, and is being, widely used quite sucessfully. As a matter of fact, the theory of Chebyshev extrapolation has been extended[7] to consider complex eigenvalues and the relationship between the convergence rate and certain acceleration parameters has been determined. In particular it has been shown that Chebyshev extrapolation is the best acceleration scheme in the com - plex eigenvalue case provided the eigenvalues lie within a particu - lar region of the complex plane.

Two general methods are currently used as iterative techniques for inner iteration: successive overrelaxation (either point successive, SOR, or line successive, SLOR, or 2-line successive, S2-LOR, overrelaxation) and alternating direction implicit iteration (ADI). Both represent mathematical advances which have largely de - creased the number of iterations needed to solve neutron-diffusion problems. The improvement is specially evident when one has to deal with problems with a very large number of mesh points. Methods are now available for improving all points on a mesh line simultaneously without any increase in arithmetic effort in passing from point to line successive overrelaxation. Other partitionings of the matrix A which leave A in block tridiagonal form allow the simultaneous solution for all points on two and even three adjacent mesh lines, each iteration requiring only 20-40 percent more computer time than does each iteration in the case of SOR. By increasing the rate of convergence, the use of all these block iterative methods have greatly brought down the number of iterations required to reduce the norm of the error vector to a specified fraction of the norm of the initial error vector.

Many variants of alternative direction implicit iteration

have been developed and often provide very powerful techniques for solving finite difference analogs of partial differential equations of elliptic type. Although general convergence proofs have been given, the theoretical explanation for the success of ADI iteration techniques is incomplete. The theory is in fact so unsatisfactory that it is often not possible to predict whether a suggested ADI scheme is likely to converge or not. On the other hand, many discussions of the ADI and SOR techniques are at least implicitly restricted to two dimensional considerations.[68] Under these circumstances it is probably worth mentioning that extrapolation of the schemes to three-dimensional situations is not clear.

As said before, the general problem of finding an optimum strategy between inner and outer iterations which would minimize the computer running time is a very complex problem. As a consequence, great efforts have been made to analyse the outer iteration and its relationship to the inner iteration. It has been pointed out[4] that poor convergence of the inner iteration leads to complex eigenvalues in the matrix relating successive fission source distributions, which in turn adversely affects the convergence of the outer iteration. To escape this situation, in a code for one-dimensional calculations Wielandt method has been used to accelerate the convergence of the outer iteration, whereas inner iteration is based on analytical methods. However, at the same laboratory, in a second code for solving two-dimensional problems, SLOR was used as the inner iteration scheme.[69]

The opinion has also been expressed that programming theory aproaches should be recommended in discussing the relationship between inner and outer iterations. In other words, it should be possible after iteration to "evaluate" the results within a monitoring subroutine, thereby "learn" what is the best combination.

The Equipoise method

Either the original version of the Equipoise iterative procedure or some variants of it have been applied both to diffusion and transport theory. These techniques contrast with the conventional inner-outer iteration methods in that blocks of equations are forced to satisfy overall neutron balance conditions. Although this method looks rather simple to apply, no proof has been given that the iterative processes it represents will always converge.

Direct inversion techniques

Work in numerical analysis has been reported[8,9] on direct (non-iterative) solution of large systems of linear equations with block-tri-diagonal coefficient matrix by stable numerical procedures. At the same time, convergence acceleration by variational coarse mesh methods has been applied to burn-up codes because the region wise averaged fluxes converge rapidly[10]. Thus, a new one-dimensional equilibrium-cycle burnup code has been developed using the direct inversion technique for block-tri-diagonal matrices mentioned above[11]. The thermal groups are solved simultaneously, no inner iterations being necessary. The same method is used in a one-dimensional depletion code with and without reload features. An extension to seven groups (4 thermal groups) is also available[12]. Development has been reported also of a few group, two dimensional diffusion code for hexagonal geometry (constant mesh size), in which direct inversion technique is used to calculate the fluxes in the interior of very large sized diffusion blocks. This procedure leads to an improved convergence rate of the spatial iterations[13]. The development of a three dimensional diffusion code, using the direct inversion techniques for large sized diffusion blocks is presently under way at General Atomic.

Response matrix methods

Response matrix method is another interesting approach to the problem[14,15,16,17]. It has been applied to criticality calculations of two-dimensional systems in a few group model. In this method the reactor is assumed to consist of a number of infinitely high, rectangular homogeneous blocks, the composition of which may change from block to block. The response matrix method treats the motion of neutrons in a block rigorously except for the assumed form of the intensity distribution of the current incident on the block. The response matrices of component blocks in the reactor are calculated first analytically with group-diffusion approximation. Then the multiplication factor and the associated eigencurrents, together with mean flux in all the blocks, are determined from these matrices by an iterative method. The time required for a typical problem (two groups, two-dimensional) is reported to be less than 1 min, whereas it takes about 20 min for PDQ to do the same calculation with the same accuracy. However, the application of the method to multigroup problems has not yet been successful.

Heterogeneous methods(*)

There are many systems, such as substitution lattices, mixed lattices and lattices with several control rods or channels that contain important areas in which it can be difficult to define cells with geometrically simple boundaries. For this kind of problems, heterogeneous source-sink methods are well suited to obtain accurate flux distributions. As is well known, in this method the flux is expanded into a Fourier series in the azimutal angle around each channel. The monopole term describes absorption and production characte-

* The following comments were written prior to the EACRP-CEA meeting on the application of heterogeneous methods to burnup calculations held at Saclay, 16-18 January 1967.

ristics of the channel; the dipole sine and cosine terms represent effects due to radial leakage and streaming as a result of radial buckling.

In one version of these methods[18], neutron flux distribution evaluated at several points around every fuel element is correlated to the harmonic components of a neutron flux from a sink multipole, and then the iteration between the source and the sink strength is carried out until a sufficient convergence is attained. In another version[19], a solution of the heterogeneous neutron flux equations is superimposed upon the macroscopic solution of the homogeneous neutron diffusion equations obtained using a coarse finite-difference mesh. The macroscopic distribution is used to provide boundary conditions on the subregions of the reactor which will then be treated by a heterogeneous method.

Quite recently an extension of the source-sink method to finite fuel elements has been developed and reformulated in terms of the conventional finite difference equations plus some extra terms[2]. In such an approximation to the fully heterogeneous method, the equations are converted to finite difference form with one mesh point per channel and direct coupling between all mesh points. The correction terms to the terms of the conventional finite difference homogeneous type depend on the distant mesh points representing the heterogeneity effects.

A.2. Variational methods

General

Variational methods are of growing interest in all fields of reactor calculations. The development of variational principles for general linear operator equations is therefore, very important. Variational principles for general inhomogeneous linear operator

equations and for eigenvalue equations in case of general linear operators have been derived recently[20,21,22].

From a less general point of view, it is best to point out that several approximate methods have been developed based on variational principles. Variational techniques not only offer a means for reducing the Boltzmann equation to approximations which are computationally more convenient, but provide criteria for selecting "best" approximations to partial differential operators or finding "best" trial vectors for nonlinear iteration techniques. Thus, Ritz variational methods have been used[3] to derive difference equations for the case in which the set of mesh points does not form a rectangular pattern. On the other hand, variational principles have been applied[23] to provide a basis for nonlinear acceleration of linear iterative methods. Linear combinations of the elements of a sequence of successive approximations obtained by a linear iterative procedure are used as trial functions for the functional equivalent to the given linear problem.

Considering again the multigroup-diffusion equations, these equations have been solved by applying Ritz and Kantorovich methods to appropriate functionals associated with these equations[24, 25,26]. Both methods have been compared, with regard to accuracy and computing time, with the finite difference methods used in present nuclear codes[27]. Variational techniques have been applied also to the solution of reactor kinetics problems[28]. Thus, the multigroup solution of time-dependent diffusion equations by variational methods has received much attention during the last few years. The resulting set of ordinary differential equations for the time-dependent coefficients in the trial function can be solved by well known numerical techniques, such as the implicit (or backward difference) method or the implicitly explicit method. The implicit integration technique, in particular, has been widely used (see, e.g.,70) because such a

technique is more stable than an explicit integration technique (in fact it is unconditionally stable); therefore, a large time mesh can be used regardless of spatial mesh size, and the computation time is reduced correspondingly[29]. However, it has been pointed out that the extension of such an implicit technique to more than two groups of neutrons becomes a very time consuming procedure. Quite recently[30], an unconditionally stable one-dimensional multigroup-diffusion code has been designed which requires 4 min of computer time on an IBM-7094 for solving problems involving 4 energy group, 6 delayed neutron groups, 100 space points and 300 to 500 time steps.

The various perturbation methods are closely related to the concept of variation of a functional. The non-self-adjoint nature of nuclear reactor problems involves several technical mathematical difficulties. The situation is much more complicated than say, in quantum mechanics. Nevertheless, the recent developments of non-self-adjoint perturbation methods for reactor physics has substantially increased the amount of information that can be obtained from a given criticality calculation. This is valuable because the number of these complex and expensive calculations is thereby reduced in the long run. The full complexity of reactor calculations, however, is better revealed by the burnup problem than by the criticality problem, since the usual flux calculation must be repeated at each time step. Consequently, work is now in progress on the application of perturbation theory to the burnup problem[31].

The last application requires extending the concept of an adjoint from the fluxes to the isotopic concentrations. The difficulty that the burnup problem is no longer linear, because the isotopic concentrations that multiply the fluxes are now variables as the fluxes themselves, may be overcome by basing the treatment on the linear equations that determine the small departure from a known solution of the burnup equations. The difficulty that the multipli-

cation factor is no longer appropriate to use as the quantity whose perturbations are sought may be overcome by using for this purpose some specially significant property of the burnup history, such as the burnup exposure or lifetime beyond which the fuel is too depleted to maintain a critical reaction. A theory has been developed in detail[32] for a simple two-group point burnup model that allows variable composition for nine isotopes, including four heavy isotopes and five fission products. This theory is the basis of a new code which solves a burnup problem specified in the input, and then computes the adjoints for the neighbourhood of this solution and uses the solution and the adjoints to calculate derivatives of the burnup lifetime with respect to the input parameters.

Synthesis methods

Although not always based explicitly on variational principles, synthesis methods have been evolving into more and more accurate techniques. Apart from the conventional variational synthesis methods, even the multichannel synthesis method, originally based on heuristic methods, has recently been derived from a basic functional by using variational techniques[33]. As is well known, in the multichannel flux synthesis method, regions are represented by nodes and nodal-difference equations are derived with the aid of the lower dimensional results. The nodal equations are a system of simultaneous linear equations which may be solved by conventional methods. In the new variational formulation the trial functions used are, in general, not continuous, and nodal-difference equations are derived from a variational principle.

In the particular case of continuous trial functions and a single channel, the procedure is equivalent to the conventional variational synthesis. In the case of one trial function per channel, the nodal-difference equations are identical in structure to the conventional multichannel synthesis.

An interesting feature of this approach to the flux synthesis is the increased efficiency in the use of the two-dimensional base functions forming the three-dimensional discontinuous trial functions for the variational synthesis computation. Since the machine time consumed in obtaining the two-dimensional base functions is a large fraction of the total time required by the overall computation, the above mentioned increase in efficiency leads to a reduction in computing time.

A new method for solving the space-time problem in terms of a synthesis formulation of the multigroup-diffusion equations has been also reported [34,35]. The method considers techniques as used in a one-dimensional multigroup code for the S_n solution to the transport equation as well as diffusion theory. The technique has been intended to incorporate nonlinear temperature feedback [36].

A.3. The S_n method

A few words on the S_n method. Although existing two-dimensional S_n-type transport codes have not always proved entirely satisfactory (see Sec.B), much effort is going into the development of new versions which might allow to overcome the difficulties one encounters in using them. Nevertheless, the value of the various proposed improvements on the general method cannot be ascertained until they have been incorporated in new transport codes and tested in a wide variety of problems [37].

However, it might be said, that from a practical point of view, the S_n method is far and away the most popular and widely used method for solving the transport equation-especially in one dimension. It is a most powerful tool and enables anisotropic events, the effect of boundary conditions to be readily studied and lends itself without difficulty to adjoint and perturbation method solutions. As a consequence , it is thought that the DSN and SNG techni-

ques will continue to play a vitally important rôle in future com - putational methods for handling transport problems [38].

A.4. Collision probabilities methods

The methods of collision probabilities seem at present to be among the prevalent forms of integral transport theory. These methods are becoming more and more important as a useful and practical tool in reactor calculations. Thus, methods of calculating the neutron flux within a lattice cell as a function of space and energy have been developed based on a representation of neutron transport in terms of first collision probabilities without recourse to the Boltzmann integro differential equation [39].

An essential part of a calculation according to all these schemes is the evaluation of the collision probabilities to a fair degree of accuracy and with a reasonable amount of computing time. In fact, the practical applicability of the collision probability techniques depends heavily on the availability of methods adequate for calculating these probabilities. An exact method for calculating collision probabilities in square and hexagonal lattices has been developed and applied to the calculation of the thermal spectrum following the matrix factorization technique [40]. On the other hand, several approximative schemes have been proposed in order to facilitate the evaluation of collision probabilities in the particularly important case of annular geometry [41]. It has been found, however, that some of the approximations (e.g., behaviour of the angular flux distribution at boundaries between regions) are not really necessary [42,43,44].

Quite recently, a new, purely numerical technique has been developed to deal with complicated fuel element geometries [45]. The collision probability routine PIJ may be used to compute collision probabilities in two dimensions in all practical geometries. In par

ticular, PIJ includes specific representation of individual rods in cluster geometry with internal subdivision of the rods if required. This routine is available within the WIMS framework. The WIMS code [46] (Winfrith Improved Multi-group Scheme) is a general code for reactor lattice cell calculations applicable to a wide range of reactor types including both thermal and fast reactors. Solution of the transport equation is provided either by use of the Carlson DSN method or by collision probability methods. The differential solution is performed by the discrete coordinate code WDSN [38]. The integral solution is achieved by the generation of collision probabilities for which the PIJ routine may be used. Having obtained the collision probabilities, the next problem of course is to solve the resulting equations. These are solved numerically in the PIP [47] routine which uses a successive overrelaxation method.

A.5. Semi-analytic methods

There is a tendency in many laboratories to substitute semi-analytic techniques for direct, "brute force" numerical methods in reactor calculations. Although there is no sharp separation between numerical and non-numerical methods, it should be stressed that several different problems could be solved at a lower cost just by simply pushing forward the analytical work as far as possible. Of course, the right answer to the question could a given problem actually be solved by analytic or semi-analytic methods at a lower cost than by resorting to "brute force" numerical techniques is strongly space- and time-depending. Here and now, the answer might be in the affirmative, here and tomorrow, in the negative, etc. The view has been expressed, for example, that even if the analytic method is conceptually feasible, the question of whether it is cheaper to solve the problem this way as opposed to use of computers really depends on the availability of specially skilled staff on the one hand and computer time on the other. There are cases in which computer time is cheaper. Another point going more deeply into the funda

mentals is that of whether in fact a problem of real practical significance is conceptually capable of being solved by analytic or semi analytic methods, and whether there is any evidence which indicates that these techniques are of benefit for real systems or for any significant generality.

Whatever the answers to these questions might be -and perhaps, as has been said before, the answers are not unique, there are two good examples of the semi-analytic approach, which were developed quite recently: the multiple collision method and the Lie series method.

The multiple collision method [48,49] is an analytical approach based on a viewpoint different from that of the Boltzmann equation, that is, the life-cycle (or random-walk) approach in contrast to the neutron-balance viewpoint. Physically significant solutions which, for example, describe reflection and transmission through a subcritical slab are obtained analytically by making use of expansions in spherical Bessel functions. Numerical results are obtained from these expansions by truncating the series (the so called j_n approximation). As a result of the introduction of discontinuity factors, problems for finite systems can be dealt with in a manner similar to those for an infinite system. The method has been further developed and applied to neutron transport problems for a bare spherical reactor (up to 18 energy groups). In particular, it has been shown that the j_3 approximation gives results comparable in accuracy to the S_4 approximation of transport theory.

As to the Lie series method [50,51,52], the basic idea might be summarized as follows. Take for instance the multigroup-diffusion or P_n approximation in cylindrical geometry. The computer would use a power series expression for the Bessel functions in cylindrical geometry. Since the solution is a linear combination of Bessel

functions, the computer will numerically combine several power series into a single series with combined coefficients. In view of this it seems justified to skip the intermediate step and to calculate the final expression directly in terms of a single Lie series, whose coefficients are generated by the basic differential equations of the problem. The coefficients are derived from algebraic recursion relations. Thus, very brief computing times are needed to determine solutions even if many terms in the series expansion have to be kept. In most applications, the accuracy of the solution can be controlled by an input parameter. Difficulties of convergence are avoided by analytic continuation.

A.6. The Case method

Although the Case method should be considered an analytical one, brief mention will be made of some applications of the method of Case. In the one-group transport problem for slab geometry, the general solution of the Boltzmann equation is expressed as a superposition of eigenfunctions. A system of singular integral equations is derived for the coefficients and the solution can be obtained, for example, by two methods, one based on the Hilbert problem approach, and the other on the reduction to a Fredholm integral equation of the second kind. The application of this method to the transport problem in a multi-region reactor of a slab geometry has been reported [53]. Another application is that to the solution of the energy-dependent Boltzmann equation. It is known that under certain assumptions the energy-dependent Boltzmann equation can be reduced to a "one velocity" equation by means of a Fourier transformation with respect to lethargy. When finite media problems are to be solved, the resulting "one-velocity" equation in the space variable could be solved by the procedure suggested by Case, were it not because the number of secondaries in the one-velocity equation is now a complex function of the transform variable instead of a real number. The method of Case has then to be extended to complex numbers

of secondaries. The process of work has been reported on this problem[54]. For an infinite medium, however, the solution may readily be obtained by a Fourier transform with respect to the space coordinate. The exact result is a double Fourier inversion integral, which can be calculated numerically.

A.7. Monte Carlo methods

Monte Carlo methods are among the most powerful techniques available for solving the transport equation. In fact, there are given areas where the space and energy detailed to be studied is enormous and where Monte Carlo techniques provide the only feasible tool. But the application of these techniques is by no means straightforward.

It is known that the main drawback of Monte Carlo methods is the great amount of computer time it takes, the large number of arithmetical operations involved and the statistical errors one gets from the results. There are also the convergence problems in the Monte Carlo approach resulting from either insufficient or inadequate sampling procedures. The question of errors other than statistical errors (round-off errors) is important too, and due attention has to be paid to the question of stability. To the usual possibility of the growth of round-off errors adds the possibility that statistical errors may contribute to errors which grow with time.

An important part of any Monte Carlo calculation is estimating the variance of the quantities which are being averaged over the population of histories. The feasibility of the calculation hinges on a sample size sufficiently large to produce an adequate number of successful events to permit a statistically valid result. Were this to be done in a straightforward manner (using the exact physical analog), this sample size would be so large to preclude its use in any reasonable length of time, even on the most sophisti

cated digital computers.

Consider, for example, the transmission of particles through a shield. If one could exclude from the sample all those particles which have little or no chance of producing a successful event, he would reduce this sample from some enormous number to one for which the calculation is quite feasible (biasing). The particles remaining in the sample, however, must be assigned statistical weights so as to preserve the expected values of the results. The most obvious effect of biasing, therefore, is in this case to increase the sample size of the escaping particles (per unit of computation time). What is less obvious is that it matters significantly exactly how this increase is obtained. Merely getting more particles to escape does not ensure satisfactory results, and using techniques which do this can yield very misleading information. What will, in general, be satisfactory is a procedure which will emphasize those random-walks which produce the greatest contribution to the escape probability in the true problem [55].

It should also be borne in mind that the average event taking place in the biased calculation bears little resemblance to the average event taking place in the actual (unbiased) situation. If, therefore, one were to compute the variance, as well as the result, in a biased calculation as means of establishing confidence limits on the result, such confidence limits would be highly questionable and, in extreme cases, would be meaningless. A technique has been reported [56] for evaluating the quality of the confidence limits obtained in a standard manner from a set of estimates of a given result. This technique has been used with success and can be considered a step in the right direction. It does not, however, prescribe a method for obtaining good results but rather is a method for warning when the results obtained are poor.

Variance reduction techniques, therefore, are among the

most powerful means of bringing down the machine time required to solve a given problem by a Monte Carlo calculation. Although the improvement in convergence resulting from optimization of a given biasing technique can be quite impressive, it requires, in general, a time consuming study in itself. However, it has been shown [57] that it is possible to develop empirical or semi-empirical relationships for obtaining nearly optimum biasing in deep penetration problems in a nearly geometry independent manner. Incorporation of such a relationship into a large Monte Carlo shielding code should eliminate any anomalous or misleading results which are sometimes obtained.

Many other devices for improving the efficiency of the sampling technique are being developed in many laboratories as well as a number of codes to be used to exploit the advantages of the Monte Carlo method. For example, a number of variance reducing sampling techniques have been incorporated into the TIMOC code [58] for the calculation of characteristic reactor parameters in three-dimensional assemblies. The splitting of the integral form of the Boltzmann equation into neutron generations reflects the actual calculation mechanism of the Monte Carlo techniques used in the present case. As to the variance reducing methods, the "standard" weight estimator, the method of fractionally generated neutrons, the method of expected leakage probability, as well as the semi-systematic sampling and the double sampling have all been used in the new versions of the TIMOC code [59].

On the other hand, the feasibility of Monte Carlo criticality calculations has also been established by the application of a recently developed code [60] to critical experiments, criticality hazards problems and to the HWOCR lattice analysis. Convergence of k to better than one per cent was obtained in ten minutes on a IBM 7094 computer in the latter case. The speed of the code has been attributed to careful attention to the specific problems considered,

in contrast to the extreme generality usually incorporated into such codes. Comparison runs on identical problems were made between this code and other Monte Carlo codes of a more general nature which make an indiscriminating and abundant use of region and energy de - pendent importance sampling. Comparable statistics were obtained with the "tailored" code in about one-fifth of the computation time, indicating that biasing in criticality and reactor analysis problems should be used sparingly and with extreme care.

This is a good example of a well known conflicting situation. On the one hand, the usefulness of Monte Carlo methods for practical problems may be greatly extended by improving the effi - ciency of the sampling techniques. In fact, some problems can be handled with present computers only by suitable weighting. But, on the other hand, indiscriminate use of variance reduction can result in a poor statistical analysis and in excessive computational ti - mes. It is by no means exceptional that a given variance reduction technique works well for one problem, whereas it may actually increase the variance in another problem. In other words, the variance reduction device, the problem to be solved and the computer on which the calculations are performed are all closely interrelated. Now, it is not easy to decide which of several variance reduction techniques is the most efficient, in the sense that it leads to the smallest computing time when applied to the solution of a given problem on a given computer. For the time being, it is in these areas where Monte Carlo techniques offer challenging new problems.

Summarizing, it may be said that much effort is going in - to, and has been concentrated on improving the computer time impli - cations of Monte Carlo techniques, variance estimates, etc. It has been pointed out that such techniques as those of source superposi - tion and adjoint methods can reduce the variance of Monte Carlo me - thods in an unbiased manner and produce valuable results for speci -

fic problems.

A.8. Error analysis

Finally, there is another important and difficult problem : that of estimating the errors of all types present in a given numerical procedure. Let us take, for example, the discretization of a given continuous model. How to estimate the discretization error for an approximate solution of a partial differential equation?.In fact, only in a few cases reliable estimates for the error are obtainable. As a consequence, numerical experiments, comparisons between numerical and analytical results for single problems are necessary, and such procedures will remain among the better practical means for testing the accuracy of the approximations involved. Development of iteration independent error analysis will be extremely useful. For each somehow calculated approximate solution a procedure should be available to estimate the error. Such a procedure would be extremely valuable for flux synthesis techniques and for iterative methods with an incomplete understanding of the convergence behaviour.

B. DO SOME PROGRAMMES SHOW A "PATHOLOGICAL" BEHAVIOUR ?.

There appears to be some kind of a general agreement in that usual programmes do not show any really "pathological" behaviour if properly used. "pathological" behaviour here means an unexpected, abnormal, or wrong behaviour -e.g., lack of convergence in asupposedly convergent iterative procedure. Nevertheless , that codes are all intrinsically "well-behaved" sounds somewhat strange. In fact, they sometimes incorporate procedures that are still waiting for a more rigorous foundation. Thus, basic numerical processes are being used without exactly knowing whether they would work correctly or not in a given particular case. Although this situation poses many unanswered mathematical questions of numerical analysis, it is not the first time in history when mathematics in

Their applications to physics proceeds without paying too much attention to their rigorous foundation.

It has to be recognized, however, that the situation is particularly obscure with respect to the fundamental problem on wether any given numerical technique produces a solution which converges to the "true" solution. There are two questions involved here. The first refers to the discretization process: given a finite difference representation of an analytic equation, does the solution of the finite difference scheme approach the solution of the analytic equation as the maximum distance between neighbouring mesh points tends to zero?. If so, as the maximum mesh spacing tends to zero, does the approximate solution tend to the analytic solution uniformly throughout the region?. The second question refers to the finite difference equations proper: do the convergence and iteration procedures used produce a solution of the finite difference system?.

The basic difficulty, from the practical point of view,in answering the first question is the lack of analytic solutions in all but the most elementary problems. As a consequence, one is forced to compare numerical solutions with other numerical solutions . For example, it has been reported that a method using time integration of the few-group, one-dimensional S_n equations is presently under development at Atomics International primarly as a check on the results obtained by synthesis. To facilitate in a general way the comparison process the Mathematics and Computation Division of the ANS commissioned a sub-committee to formulate a library of "bench - mark" problems and solutions. These problems would be designed so that a user of the library could solve a standard problem by whatever method he chose and compare his results with results obtained by a variety of methods. The problem would be of varying degrees of complexity so that, in elementary problems results might be compared with analytic solutions, and in more complex problems with other

numerical results. A report of this committee was given last November at the Pittsburgh ANS meeting [61]. Some of the items for discussion were the classification of reactor calculations, the format for the problem presentation, intended use of the benchmark problems,and suggestions for a collection of benchmark experiments.

As mentioned above, a prevalent views on the abnormal behaviour of a code is that in most cases it has to be traced to a careless use of the programme, and that a more thorough effort to make the code's limits and assumptions clear could be a remedy. In other words, it is quite probable that for any code it will normally be possible to find a problem on which the code will break down or fail in some sense. In many cases it will be possible to define the area in which success is guaranteed but certainly not in all cases. On the other hand, pathological behaviour would sometimes be due to the failure to anticipate, at the time the programme is designed and coded, the full range of the variables which may occur during the numerical solution process. A third reason for code problems is that, occasionally, "almost trivial" mathematical errors exist in the code formulation. These errors give no difficulties to the test problems, but propagate into large errors in other classes of problems for which the correct theory should be valid.

As a first example take a two-dimensional diffusion code (like PDQ2) based on difference methods and a certain iterative technique. It has been reported that if the mesh spacing is pathologically non-uniform, or the diffusion constant has large discontinuities, the method has a very very slow convergence behaviour, and a semi-convergence with completely wrong results can appear to an unexperienced user. A similar behaviour shows a two-dimensional multigroup diffusion code that essentially uses the Equipoise method for criticality problems. In this particular code, however, the iterates λ_t are defined by

$$\lambda_t = \frac{(\phi_t, A\phi_t)}{(\phi_t, F\phi_t)}, \qquad (3)$$

where (,) denotes scalar product, instead of being defined by the more conventional formula

$$\lambda_t = \frac{(e, A\phi_t)}{(e, F\phi_t)}, \qquad (4)$$

where $\underline{e}$ is the vector with all components equal to unity. In cases of divergence , the programme gradually switches over to the always converging power method. However, since the convergence is often rather slow, in some cases the programme assumes divergence and stops, although it should not.

Another potential source of troubles possible with iterative processes is the selection of the initial guess. In some cases, it has been proved that the iteration method used is a convergent process and, independently of the initial guess, converges to the right solution. Unfortunately, there are other cases in which convergence depends on the initial guess being an element of a certain set, and it may demand a very complicated analysis to determine precisely the class of the elements admissible as initial guesses. On the other hand, even when the process is convergent from a theoretical point of view, its use may be severely limited in practice by bad starting guesses and, in general, by the problem of round-off. It is well known, for example, that the question of the growth of rounding errors is very important when using Wielandt method, and that this method can conceivably lead to instabilities . Some instability characteristics have been also reported in the case of the ADI method when using a 4-point acceleration factor, although convergence is obtained with a 16-point acceleration factor.

Other examples somewhat akin to the just mentioned are the effects of poor trial functions in synthesis methods.

The existing two-dimensional, S_n -type transport codes offer a very interesting example of an inter-relation between the physical and the mathematical aspects of a problem which could explain some observed anomalies [37]. An unsatisfactory feature of the-

se codes is that at times the discrete ordinates angular representation gives rise to "ray effects" in certain highly absorbing media, that is, the iterates and final flux solution show abnormal peculiarities in shape. This solution is, however, the solution to the difference equations and the trouble is simply that the difference equations do not adequately represent the physical problem, that is, typically, too few discrete ordinates are chosen. From a slightly different point of view, it can be said that discrete ordinates method is to be regarded as a neutron grouping technique and not as a method which selects and treats isolated neutron directions. This means that the flaw here lies in the mathematical model [37].

Multi- or few-group neutron diffusion calculations sometimes show a "pathological" behaviour as well. One reason for this can be the appearance of negative flux values. During the iterative process it is entirely possible that negative fluxes will occur, especially during the early iterations. If those are not detected and corrected, they will be used in the calculation of the neutron source and will thus propagate the error. The problem will be aggravated by the extrapolating schemes used to accelerate convergence. It is therefore necessary to include in diffusion and transport calculations means of detecting and eliminating negative fluxes. It has been pointed out, however, that one needs that any correction or elimination of negative fluxes does not destroy conservation properties such as neutron balance.

Some anomalies have been encountered in using a programme based on a calculation of multigroup flux shapes from first-flight collision probabilities (integral transport theory) [62]. This programme extends the methods of integral transport theory to the epithermal neutron energy region, utilizing the numerical methods of the MUFT programmes to treat energy dependence. This same programme extends the homogenized cell migration area by Fourier-transform methods to the thermal neutron energy region. In the process of

checking out this programme, oscillations were noted in the spatial dependence of the epithermal cell flux at the boundary of a non-moderating, source-free material. Although the condition for stability was not known, the situation can be remedied by introducing the small moderation which actually exists for heavy regions and, on the other hand, it does not arise for codes like THERMOS which do not rely on a differential treatment of the slowing down operator. Therefore, this last mentioned approximation seems to lie at the root of the difficulty.

One other difficulty has been discovered. Although the equations of integral transport theory for thermal neutron spectra (THERMOS) appear to be unconditionally stable for isotropic scattering, introducing the transport correction for hydrogen as a negative diagonal element of the scattering operator leads to spectra which are numerically divergent, and which are not everywhere positive. This behaviour has been attributed to the negative elements of the scattering operator, since the difficulty vanishes if the transport approximation is not employed.

It is thought that these last two difficulties are probably related, and that undoubtedly could both be understood if a general treatment of the convergence criteria for the integral transport equation were available which encompassed the usual forms of the energy transfer operator.

In fact, from a general point of view it can be said that some techniques currently being used do not fulfill the presently known theoretical requirements for assuring a convergent process.

Finally, a few quite concrete anomalies will be pointed out. Two centres have reported that some S_n-type codes develop oscillatory behaviour, and lead to contradictory and even unacceptable results when applied to the thermal region. It has also been pointed

out that the two-dimensional S_n code SNARG2D has a tendency to predict negative fluxes at interfaces. At the same laboratory, the CRAM code in Rθ geometry with a coarse θ mesh was found to be unstable. With up-scattering, convergence in RZ geometry was extremely slow and during the first 25 hours of IBM-7090 time indicated alternating divergence. On the other hand, the EXTERMINATOR code showed no signs of converging for the EBWR plutonium core loading, whereas the PDQ shows no such difficulty.

In conclusion, it might be said that, even if programmes were intrinsically "sound", nevertheless their use can lead, and in fact do sometimes lead to strange situations and surprising results for which no explanation is known at present. To find a more rigorous foundation for the basic numerical processes is a challenging problem which deserves a large amount of effort. It should be extremaly valuable to attain a basic understanding to remedy the present situation in which many questions can be answered only by numerical experimentation.

C. DIRECTIONS OF POSSIBLE IMPROVEMENTS

Although there is no obvious direction which will lead to a break-through, it is generally believed that continued effort should be spent in the development of faster, more reliable analytical and numerical methods for solving reactor mathematics problems. The trouble is that many problems encountered are such that an accurate analysis is necessary case by case. Nevertheless, the situation is not so obscure as to preclude the presentation of some general trends.

It may be worth pointing out that some difficulties are not to be attributed to the mathematical methods proper, but to the nature itself of the problem to be solved. For example, the Cauchy problem for elliptic equations, or the Fredholm equations of the first

kind when treated by ordinary numerical methods usually lead to the problem of solving ill-conditioned linear systems. In such cases, instead of trying to adjust the numerical method to the proposed problem it may be more convenient to reformulate the latter by substituting for it another properly posed problem, the solution of which approximate that of the initial problem (regularisation methods).

One main problem is to obtain satisfactory agreement between the solution of the finite difference equations and those of the differential equations, without putting undue requirements to the computer. Methods have been established to choose the mesh size in such a manner as to minimize the requirements to computer space and time for any permissible deviation.

The opinion has also been expressed that it might be appropriate to look, not for new methods, but for old methods which were not practical on desk calculators and therefore are not used. In other words, it should be possible to gain considerable advantage by redoing old investigations with a broader scope of numerical methods in mind. In any case, as improvements are made in basic nuclear data and in theoretical models, and as computers of increased speed and versatility become available, numerical methods may become a weak link in our ability to perform reactor calculations.

One of the most important areas of need is in reactor kinetics. There is no entirely satisfactory calculational tool available at the present time for space dependent kinetic calculations. But even more basic than that, it is not even clear what numerical methods are best to use in space independent kinetic work. The existing codes use anywhere from the simplest first order Euler procedure to higher order methods such as fourth order Runge-Kutta. The Lie series method has also been applied to this problem [63]. It is not clear under what conditions the use of the more sophistica -

ted methods is necessary or justified.

Another somehow related outstanding problem is that of numerical integration of non-linear ordinary differential equations. These normally arise when one is considering the kinetic or dynamic behaviour of systems and one needs to integrate the equations with respect to time. Traditionally this sort of work has been on an analog computer because this is very suitable for performing time integrations and provides engineers with the sort of man/machine interaction which they find desirable. This last point can now be provided on digital computers [64], and the question therefore arises as to whether the integration of these equations might not be performed more efficiently on a digital computer. The problems here are essentially those of stability and convergence -especially when the equations contain small time constants. What is required are improved algorithms relating to the integration of these equations so that they may be performed in reasonable amounts of computer time.

It is also important to bear in mind that the optimization of the performance of a reactor, taking into account the complex nature of the processes involved, poses many difficult mathematical problems. A particular example of this is found in the field of fuel management, where the problem is to devise an optimum or near optimum, strategy for moving fuel and absorbers in a reactor for the whole life of a reactor. The algorithms of dynamic programming have been looked at, but it was found that these are not sufficiently powerful to deal with this sort of problem. At present it is possible to operate on a fairly heuristic basis by attempting to eliminate at each stage practically all the possibilities on fairly crude physical arguments. It is felt that what is needed is a new mathematical basis for optimising a path through such a complex problem.

Another important problem is that most of the large, multi- or few-group diffusion and transport codes were written keeping in mind the limitations of yesterday's computers, which are now being replaced by a new generation of machines. The numerical schemes and the calculational strategy were closely related to the relative speeds of the arithmetic using in-core data and of the speed at which data could be transferred from tape to core. The objetive was to keep the arithmetic unit busy even with somewhat wasteful calculations while the next set of data were transferred into the core memory. The situation is quite different on the computers now becoming available, for the following reasons:

1) Larger fast memories are available,

2) The data transfer rate to the fast memory is improving,

and most important,

3) Multi-programming capability is available.

The last improvement mentioned above means that the computer has the ability to work on several programmes at the same time. While one of the programmes is waiting for additional data being transferred into the fast memory, the arithmetic unit is kept busy with other programmes. It may therefore become possible to perform the calculations in a more straightforward and efficient manner. It will take a substantial amount of study and effort to make full use of the new computers.

On the other hand, generality and automation have been considered to be one of the most important requirements in the development of new methods for the solution of the reactor theory equation, in particular of the transport equation. Generality means here the ability to solve very complicated problems under very different possible conditions. For example, a transport code would

be general if it were able to solve the three dimensional, time dependent transport equation in a variety of geometries, with a variety of angular representations, and with a variety of scattering approximations. By automation it is meant that the solution technique should not require participation of the user for a satisfactory solution. That is, if a particular mesh scheme angular representation, trial function, etc. is to be used, depending on the characteristics peculiar to the problem at hand, the selection should be made automatically by the code and not by the user.

Another aspect of automation offers a broad field of activity into which much effort is going nowadays. Thus, there have been a number of attempts to automate computer usage in regard to performance of a sequence of inter-related calculations such as are commonly required in reactor physics studies. It has been pointed out that the KARE[65] system of KAPL and ANL MACHI[66] system which are early attempts in this direction suffer from some serious drawbacks. In particular, it is difficult to extend these systems, and many aspects of reactor theory are not incorporated in these rather specialized code packages.

The KAPL NOVA system is an attempt to eliminate these problems. An analogous system is being developed at Argonne and has been designated as the Argonne Reactor Computation System (ARC System[67]). It is intended for use on a next generation computer and represents a complete break with traditional computer methods in essentially all respects. This system consists of a collection of highly modular computation modulus which operate under the direction of a Central Operating System on an automated and unified manner.

As does NOVA, the ARC System uses a DATAPOOL which contains all external inputs, the computational modules, and the re-

sults generated by all of the computational modules. The storage and retrieval of data from the DATAPOOL is accomplished by the operating system. The route to be taken through ARC may be determined by selecting a previously Catalogued Standard Path, or by generating a non-Standard Path at run time. In the latter case, the full capability of the FORTRAN compiler is brought to bear on setting up the current ARC run. There is no limit to the complexity of the route to be taken through ARC other than imposed by the ingenuity of the user. The ARC System is open ended and can be extended indefinitely.

Finally, one particular direction of improvement is the use of computers with many parallel working arithmetical units. No doubt, today the data transfer speed (from tapes, discs or drums) is the limiting factor in case of large reactor problems, and parallel computing certainly is not helpful here. However, the use of large size bulk storage together with such multi-arithmetic unit processors seems to be worth considering. The sequential ordering of the arithmetical operations, at present used in most numerical schemes, is not required for such a computer with multi-arithmetic unit processors. Therefore, the development of completely different numerical schemes might be necessary. On the other hand, it has been pointed out that supporting the idea of the potential utility of parallel arithmetic machines is the matrix algebra formulation of the overwhelming fraction of all reactor problems. The reactor field might support the development of limited flexibility computers designed specifically for matrix inversion.

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