

MATHEMATICAL METHODS IN  
THEORETICAL REACTOR PHYSICS

A draft by

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## I. STATE-OF-THE-ART OF THEORETICAL REACTOR PHYSICS

During the last few years the development of theoretical reactor physics has neared the final goal of solving reactor problems from first principles of neutron transport. Not only a deeper understanding of concrete problems has been reached and many problems have been practically solved, but even the mathematical foundations of nuclear reactor theory are now much more well understood than they were, say, ten years ago. For example, a considerable amount of effort has gone into the development of the spectral theory of the transport Boltzmann operator, and the existence and completeness of a set of eigendistributions (in particular, eigenfunctions) has been demonstrated for a few, though important, elementary cases. Nevertheless, the character of the spectrum and the possibility and uniqueness of the expansion of an arbitrary state defining the initial neutron-precursors population into a series of eigendistributions (or eigenfunctions) has not been solved to date, for the general case, in a satisfactory way.

On the other hand, it must be recognized that due to the complexity of obtaining exact solutions of the Boltzmann equation, all reactor calculations are practically based on mathematical and physical approximations. The structure of the rigorous transport equations makes it very difficult to find explicit solutions. As a consequence, recourse must generally be had either to numerical calculations or to the introduction of simplified models based on simplifying

assumptions. But, first, computers are quite expensive and, second, simplified models could eventually turn out to be untrue. Therefore, from a practical point of view: a) it is extremely important to find and to employ the most efficient numerical techniques in nuclear reactor calculations as well as to develop simplified and still reasonably accurate methods - e.g., recipe-calculations; b), models have to be tested, either against experimental results obtained in well defined situations, or against rigorous theoretical results referring to simple, clean cases. Of course, the agreement between results is only a necessary, but not sufficient condition for the model to be trusted. Although much remains to be done, there are several directions in which work has successfully proceeded on both fields during the last few years<sup>(\*)</sup>.

For example, exact solutions to the Boltzmann equation have been obtained as checks upon numerical procedures; new machine methods of reactor computation have been developed, and programs have been prepared for integration of the Boltzmann equation in space and energy with anisotropic scattering.

In the domain of resonance capture, accurate, rapidly computed numerical formulae for escape probabilities and broadened line shapes are now available; attention has been given to the effect of the interference on the resonance self-shielding of fissile nuclides at rather high concentrations, and to the Doppler broadening of resonances, including the de

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(\*) As to the mathematical methods, they will be considered in Section II.

pendence of resonance line shape upon position; studies have been reported aimed at resonance escape in two region cells by methods of moments, at generalized equivalence relations, and at improved rational escape probabilities.

Space dependent neutron spectra in heterogeneous systems have been actively considered in many centers; it is well known, that this poses a major problem in the case of small reflected reactors and for reactors with large temperature gradients; in particular, the process of neutron thermalization in moderators with non uniform-temperature distribution is now better understood than it was only a few years ago. Matrix methods have been applied to the space-dependent kinetic problem in arbitrary one-dimensional geometry in the two-group diffusion approximation.

Another area of time-dependent effects in which progress has been made from the theoretical point of view is that of neutron pulsing in critical and subcritical assemblies, in particular time-dependent transport effects, as in the asymptotic and transient behaviour of pulsed neutrons.

Attention has also been paid to the important problems of stability in the large, and the results obtained have proved extremely fruitful.

An important part of efforts has gone into the development of general optimization procedures of complex systems. One of these procedures was derived using nonlinear programming, and although originally developed to investigate

reactor stability questions, it is now being used in reactor evaluation studies. Another problem is that of optimization under arbitrary constraints, including the evaluation of the sensitivity of selected performance measures of systems to changes in parameters.

Methods have recently been developed to study the interrelation between hydrodynamics, thermodynamics, and neutron kinetics; in particular, the Bethe-Tait theory has been used in coupled hydrodynamics-reactivity theory. Finally, we shall mention the increasing interest in the theoretical analysis of noise as a means to understand, for example, the rôle of fluctuations in affecting instability.

## II. MATHEMATICAL METHODS IN NUCLEAR REACTOR THEORY

### A. General remarks.

In general the present section confines itself to developments carried out during the last four years, and considers only: 1) a few selected topics in mathematical methods and techniques as applied to nuclear reactor theory ; 2) problems of a general character, i . e, problems not essentially related to a particular type of reactor . No attempt has been made to go into the details.

From a fundamental point of view, one of the main characteristics of nuclear reactor theory is that the linear operators involved are not in general self-adjoint. This means, first, that the situation is mathematically much more complex than in quantum mechanics, and, second, that associated with the neutron and precursors population there are two different fields. In particular, we cannot neither assume the possibility of expansion into eigenfunctions, nor extend without proof some basic results of the theory of self-adjoint linear operators to nuclear reactor theory. It has to be recognized that many interesting attempts to bring some order "into the chaos of "obvious" or partially proved results" have attained their end in spite of the great complexity of the problem. Not only finite models, or multigroup diffusion models have been

considered, but also some transport theory problems in plane geometry have been solved. It does appear, however, that much remains to be done. As to the existence of two dual fields associated with the neutron and precursors population, the analysis of the situation has gone pretty far and the physical meaning of the "adjoint" field (the generalized importance field) has been greatly clarified, even in those cases in which both the conventional field and its adjoint are solutions of non-homogeneous linear equations. In particular, both fields play an important rôle in connection with variational techniques and with the reduction of more general models to few group models.

However important all these investigations may be, their interest is primarily a fundamental one. The theory of neutron transport is a mathematically too complicated subject to lead to simple, general and exact formulae. Because of the great complexity of this problem, in practice most of the methods used to obtain solutions are approximate, since, on the other hand, only relatively few problems in practical reactor design require a very high degree of accuracy. In other words, approximation methods play practically as important a rôle as accurate solutions. There is here a question urgently asking for solution: to determine the minimum accuracy which is acceptable, and to estimate the errors associated with the various approximate methods.

In Part B of this section we shall deal with several mathematical methods that have been applied during the last

few years to solve reactor problems. Although these methods will probably be applied also in the near future, no attempt will be made here to assess the errors inherent in their application. The problems listed in Part C are, in my opinion, worth-while to be seriously considered in the future development of nuclear reactor theory. No claim is made for the list to be complete.

### B. Mathematical methods

1.- Eigendistributions (in particular, eigenfunctions) method. In problems involving transport equations, the eigenfunctions may be distributions (in Schwartz sense) or generalized functions (in Gel'fand sense). Since the early papers on this method, much work has gone into this subject. Initially applied to one velocity, isotropic scattering in plane geometry, the method has been extended to anisotropic scattering and multigroup approximation, as well as to initial value problems involving monoenergetic neutrons in slab geometry. In particular, it has been shown that the assumption (based on physical arguments and analogy with other theoretical physics problems) of the existence of a denumerably infinite set of eigenvalues is wrong in slab geometry. Another example of how much things have changed is offered by the theory of scattering operators: In solving time-dependent problems of neutron thermalization, it was thought that scattering operators will possess an infinite set of discrete eigenvalues with no limit point other than the point at infinity. Instead, it has been shown that this assumption fails for the proton gas model and, probably, in almost all models. However, in fi



nite systems and under rather general conditions, the Boltzmann operator has a countable infinity of real eigenvalues accumulating at infinity. Therefore, one is tempted to ask once again: which general connections there exist between space-boundness, on the one hand, and the structure of the spectrum and the completeness properties of the eigenelements, on the other?. To the best of my knowledge, there is here a real need for further investigation.

2.- Integral ( in particular, singular integral ) equations method. The reduction of the integro-differential Boltzmann equation to an integral equation is a well known classical procedure of treating transport theory problems. As such, this method has been recently applied to show some existence and uniqueness theorems for the neutron transport equation and its adjoint. A very interesting result of these investigations is that there are many cases in which existence and uniqueness theorems can be proved for one or the other problem, but not both. This lack of symmetry between the flux and the importance fields should seem rather surprising. Another aspect of the integral equations method is related with the use of singular integral equations. For example, the application of boundary conditions to problems treated following the eigenelements method leads to singular integral equations in all cases considered for the present. Thus, in one application of the method the solutions to boundary-value problems are expanded in terms of singular solutions to the integrodifferential form of the homo-

geneous transport equation, but the determination of the expansion coefficients is achieved by solving singular integral equations.

The theory of singular integral equations and analytic continuation can have great importance for a number of fundamental problems of neutron transport theory and, in my opinion, deserve particular attention.

3.- Variational methods. Because of the great complexity of the problem posed by neutron transport theory, several approximate methods have been developed based on variational principles. The structures of these variational principles are largely different, and depend on the particular nature of the problem to which they refer to. The trouble with some of the variational methods consists in that the variational expressions involved are not of the maximum or minimum type. Rayleigh functionals can be used directly to obtain upper or lower bounds for the quantity of interest by the appropriate choice of trial functions. Regrettably, the situation is essentially different in some applications to neutron transport problems: the only condition is that a given functional be stationary with respect to arbitrary variations in a given functional space (or in its dual space). Although general procedures have been outlined for using variational methods in connection with nonself-adjoint problems, not too much can be said about the "worth" of the "best" function of a given set of trial functions. Nevertheless, if the interest is in an integral involving the unknown function, quite often

a variational principle is constructed and the variational method applied in an heuristic way.

It is not at all clear at the present time to what accuracy these methods can lead, and it would be very interesting to investigate not only the mathematical background of the whole procedure, but its practical reliability.

4.- Symmetrization methods. The search for the value of a physical quantity means, strictly speaking, to look for two numerical values: a lower and an upper bound for the "real" value. With this fact in mind, symmetrization methods have been introduced in neutron transport theory to provide inequalities referring to quantities which are set functions -for example, critical masses. Two such inequalities allow us not only to set lower and upper bounds for the quantity of interest, but to estimate the maximum possible error. During the last years some attention has been paid to these methods in connection with nuclear reactor theory, in particular to Steiner and Schwarz symmetrization. The central problems is that of finding the effects of symmetrization on a given set function. For example, which are the effects of Steiner symmetrization on the critical multiplication or on the multiple collision probability?

The generalization of these methods from bare, homogeneous convex solids with isotropic scattering to reflected systems with anisotropic scattering will undoubtedly increase the range of applicability of these fundamentally simple, although rather subtle methods.

5.- Invariant imbedding. Originally applied to the diffuse reflexion of light by a foggy medium, the method of invariant imbedding has been systematically exploited to give a new formulation to many classical transport equations, in particular to neutron transport theory. As is well known, so me transport problems can be transformed via invariant imbedding from eigenvalue problems to initial value problems. In this way, problems of critical mass were solved, and the distribution functions for the reflected and transmitted fluxes, and the energy and the time dependence for plane geometry have been computed. Using the standard arguments of imbedding theory, functional equations for the correlation function in energy space and also in time space have been obtained, and the existence and uniqueness of the solution of the trans - port equation has been proved.

However, and although the invariant imbedding equa - tions were derived from the Boltzmann equation for certain simple cases of the time-independent slab geometry, failed a general rigorous justification of the method. Recently a de rivation from the Boltzmann formulation has been given for the time dependent transport in a rod, time-independent trans - port in a slab, and time-independent transport in a solid sphere, a hollow spherical shell, and a spherical shell en - closing a perfect absorber. The rigorous derivation has dis closed the existence in the final expression of extra terms which were overlooked in the original derivation obtained by elementary physical arguments. As a new mathematical techni que; invariant imbedding is an interesting and useful tool when carefully applied.

6.- Group theoretical methods. Some ten years ago, Wigner proposed a group theoretical method for the exact evaluation of appropriate moments in problems of multiple scattering when the elementary scattering law is invariant under a group of transformations. There is no need to emphasize the success of group theoretical methods in quantum mechanics and, more recently, in the theory of elementary particles. As in these cases, in neutron transport the group theoretical methods afford a unifying point of view based on the symmetry of the problem. For example, each reactor possesses its own symmetry group, and the eigenfunctions of the diffusion operator provide the basis for a representation of the group. This representation enables one to determine in the conventional way the degeneracy and symmetry properties of the reactor eigenfunctions.

Another application of the method we can mention is that of the study of the time dependent slowing down of neutrons by elastic collisions with free moderator nuclei initially at rest. Using the representations of the group of symmetries associated with the slowing down model chosen, it is possible to express in a closed form the Laplace transform with respect to lethargy of the  $m$ th space and  $n$ th time moments of the  $l$ th Legendre component of the distribution function.

Not only to gain a deeper insight into the nature of some problems in nuclear reactor theory, but also to provide an alternative mathematical tool to be possibly used when other exact methods fail, further investigations to determine the capabilities of the application of the group theoretical methods should be very useful.

7.-Stochastic methods. Random functionals. Although the study of the physical behaviour of nuclear reactors by statistical techniques is not at all new, particular attention has been paid to these techniques in the course of the last years. In particular, statistical methods have been applied to the study of the kinetic parameters of subcritical assemblies based on neutron counting techniques (alpha-Rossi and alpha-Feynmann methods). Certain techniques of correlation analysis have been applied to the analysis of the measurements of reactivity of a subcritical reactor, the correlation functions being in general obtained from the linear differential equations describing the physical system. It has to be pointed out that the stochastic aspects of neutron behaviour in a reactor are of most concern when the reactor is being started up with a very small neutron source. There exist three fundamental neutron processes characterized by stochastic equations: neutron multiplication, neutron diffusion and neutron transport. The probability distribution generating function has been adopted to synthesize the corresponding stochastic equations. On the other hand, the prediction of statistical parameters associated with fluctuation in neutron population density in a reactor can be based on mathematical models. The measurement and analysis of the stochastic time series of the fluctuations allow then to determine by statistical techniques the reactor parameters and, therefore, to check the adequacy of the mathematical model. Another problem that has been treated by stochastic methods is that of time-dependent slowing down of neutrons. Neutron moderation is reduced to a stochastic process by regarding the time required

by the neutron to slow down to a given energy as the sum of a number of elementary random events. It has been proved that finding the neutron time-energy distribution is equivalent to finding the distribution of a random functional. Random functionals are playing an increasingly important rôle in theoretical physics and are likely to become a powerful tool to solve statistical problems related with nuclear reactors. We shall finally mention that it has been shown that, in principle, stochastic methods and those based on the Boltzmann formulation of the neutron transport are equivalent if we consider neutron migration phenomena as a stochastic process.

8. - Monte Carlo methods. Monte Carlo methods have been employed in solving neutron transport problems for many years. But only the availability of large, high-speed digital computers has permitted to push forward these methods to the present level. Now, it is widely recognized that even with modern high-speed computers, to keep running times within economically reasonable limits requires rather sophisticated mathematical tricks. These tricks affect the statistical errors in a not adequately known way, and there is here an important subject of investigation.

Apart from the approximations and idealizations made to reduce the inherent complexities of the problem to be solved, there exists a whole variety of Monte Carlo techniques that can be used, and one has to choose between them (or combine them). We are thinking, for example, of weighting (in particular, importance) sampling, systematic sampling, conditio-

nal Monte Carlo, rejection techniques, use of survival probabilities, etc. The usefulness of Monte Carlo methods for solving practical problems of neutron transport might be greatly extended if further powerful techniques of this kind were discovered.

One of the most important advantages of the Monte Carlo methods is that they can be used for a large variety of problems: critical size calculations, determination of resonance escape probabilities in a lattice, distribution of neutrons both in energy and space in a given system, shielding calculation, in particular gamma flux distributions, energy deposition from neutrons and gamma rays in a lattice cell, etc. On the other hand, one of the main disadvantages are that accuracy is limited and not always well estimated, and that quite often present codes are of too much complexity when applied to the complex geometries found in practice. Improvements in such directions are highly needed. In particular, some assessment of the reliability of existing Monte Carlo methods is desirable.

9.- Expansion methods. Although methods such as multiple scattering methods must be considered as expansion methods (expansion into a Neumann series) together with all eigenfunctions expansions methods, we shall here deal with only expansions of the neutron flux  $F(\vec{x}, u, \vec{\Omega})$  considered as a function of the (unit vector) variable  $\vec{\Omega}$ . Any complete orthonormal set of functions defined on the unit sphere can be used in principle as a basis for such an expansion method. Since all these sets are mathematically equivalent,



the only criterion for the choice of one these sets are the degree of convergence and the simplicity of treatment. To my knowledge, in the general case, i.e., when all three components of  $\vec{\Omega}$  are involved (that is, two independent angular variables), only the spherical harmonics set has been practically used. The resulting (general) spherical harmonics approximation has provided a powerful tool for solving many problems of neutron transport. However, although only in very special instances are higher order spherical harmonics expansions used in reactor calculations, the application of the method is far from trivial in the case of complicated geometries even for low order approximations.

In recent years new techniques have been developed to deal with simple geometries, i.e., with geometries for which  $\vec{\Omega}$  can be expressed in terms of a single co-ordinate,  $\mu$ , ( $0 \leq |\mu| \leq 1$ ). In this connection two approaches have been followed: that of full range approximations, and that of partial ranges approximations. In the first case, the same analytic approximation for the flux as a function of  $\mu$  is taken over the whole interval of variation of  $\mu$ ; in the second case, the whole interval is divided into a certain number of partial intervals, and with each partial interval there is associated a different analytic approximation. A typical full range approximation is the  $P_N$  approximation; a typical double-range approximation is the  $DP_N$  approximation. In a certain sense, even the  $S_N$  method can be considered as a partial range approximation (of course, with two dimensional ranges (cells) on the unit sphere in the general case).

It has been known for many years that, if convergent, the rate of convergence of successive  $P_N$  approximation to the true distribution is very slow in plane geometry. In Milne's problem, the truncated expansion in Legendre polynomials even leads to the appearance of negative neutron fluxes. There is some evidence, therefore, that the  $P_N$  method is not always a good approximation and certainly it is not a satisfactory approximation at distances within the order of a mean free path from a free surface, in a boundary region, and, generally, for highly anisotropic fluxes. As a consequence, attention has been paid to alternative complete orthonormal polynomial sets in order to improve the convergence of the whole procedure. Thus, the Tchebyshev polynomial method was already proposed in 1958, and its capabilities have later been investigated by several authors. Now, since Legendre and Tchebyshev polynomials are, together with Gegenbauer polynomials, particular cases of the hypergeometric polynomials of Jacobi, the expansion of the flux into a (truncated) series of Jacobi polynomials  $F_N(\alpha, \gamma, \mu)$  has been considered as a basis for a general discussion of the subject. In particular, some effort has gone into the analysis of the influence of the choice of  $\alpha$  and  $\gamma$  on the linear extrapolation distance and the critical size of a bare slab reactor. It has been found, for example, that Gegenbauer polynomials  $C_N^\nu(\alpha = 2\nu, \gamma = \nu + \frac{1}{2})$ , with a properly chosen value of  $\nu$ , give better results in low order,  $N$ , than the Legendre polynomial expansion in computing the above mentioned quantities. Some work has also been

reported on the behaviour of Jacobi polynomial approximations for  $N \rightarrow \infty$ , in particular concerning the failure of neutron conservation associated with the general truncated Jacobi approximations. As it ought to be expected, the introduction of two more degrees of freedom (the parameters  $\alpha$  and  $\gamma$ ) besides the conventional  $N$  makes the play more subtle, but opens new questions. Perhaps one of the most important is that of the generalization of the Jacobi polynomial method to more complex geometries than the plane or slab geometry. Is it possible? If not, this would mean a drastic limitation to the method.

There is another point of even more general and fundamental character in that it refers to all procedures based on truncated expansions. The point is this. In neutron transport theory, interface and boundary conditions are physically and mathematically well defined concepts, but it turns out that it is impossible to satisfy these conditions completely when dealing with an approximation of the truncated type. As a consequence, there are many a priori possible ways in which boundary and interface conditions can be selected to uniquely define the solution to the given problem in its approximate version. In other words, these conditions cannot be deduced in a unique and logical fashion from the corresponding transport conditions, and, therefore, there is no single "best" method to derive them. For example, for the  $P_N$  approximation two sets of approximate free-surface boundary conditions have been used for many years, (Mark's and Marshak's conditions), the choice between the two being ge-

nerally decided by the nature of the problem or the order of the approximations. Although Marshak's conditions have been derived a few years ago (1961) from a variational principle, there remains some degree of arbitrariness: in fact, also using the variational calculus, free-surface boundary conditions have been obtained other than Marshak's. The situation is, thus, rather involved, and there is a real need for further investigation. The very root of this difficulty consists probably in that when the  $P_N$  approximation is not valid in one of two contiguous media (e.g., vacuum - material medium) or is generally valid in both, but not on the interface and its neighbourhood (that is, when the  $P_N$  approximation is only asymptotically valid), there are no compulsory reasons to select a given type of conditions on the interface. The situation is not so bad when the two contiguous media are physically similar and possess good scattering properties, because then continuity considerations usually lead, unambiguously, to well defined boundary conditions on the interface. Of late some attention has been paid to the general problem on finding appropriate interface boundary conditions (in particular for Wigner-Seitz cell calculations), but there remains much work to be done.

In connection with the spherical harmonics method, some interesting results have recently been obtained applying even-order approximations. Although the  $P_{2N}$  approximation can not be said to be in general better than the  $P_{2N-1}$  approximation, the domain near the interface in which the  $P_{2N}$  approximation differs from the exact solution is much more reduced than the corresponding domain for the  $P_{2N-1}$  approximations. On the other hand, it seems to be not more difficult to apply

even-order approximations than the commonly used odd order theory. It has even been suggested to combine both even - and odd-order approximations to improve the results obtained with application of the conventional  $P_N$  theory ( $N$  odd).

Since the early work on  $DP_N$  approximation, some effort has gone into the investigation of the capabilities of several double range approximations, although the extension of the double range expansion method to more complicated geometries than plane geometry raises certain problems asking for solution. During the last four years, the logical structure of the discrete  $S_N$  method has been largely clarified, although no comprehensive numerical study for the completed  $S_N$  theory has been made as yet. In particular, with respect to convergence some  $S_N$  methods are not yet rigorously established and not much is known on the behaviour of the numerical solutions in the limit of very fine mesh resolution. From the practical point of view, one has to point out that  $S_N$  calculations are still quite time consuming, in particular for thermal reactors.

We shall finally mention two expansion methods that have been recently proposed which differ in certain aspects from the conventional ones. The first is an application of Lie series to reactor problems, in particular those the conventional treatment of which would involve the use of ill defined Bessel functions values. The second consists in an spatial expansion of the flux in series of known functions of the spatial variable. The coefficients are unknown functions of the angular variable. Two general formalisms

have been proposed (a variational method and a moment-conservation method) to obtain the necessary equations for the expansion coefficients.

10.- Heterogeneous methods. As early as during the First Geneva Conference, heterogeneous methods for nuclear reactor calculations were already proposed and discussed. Homogenization procedures must be used with great care when dealing with highly heterogeneous systems, and can lead to unacceptable errors if wrongly applied. As is well known, there are now in principle two ways in which heterogeneities can be treated: the kernel methods, and the mesh methods. At first, kernel methods considered fuel elements as sources and sinks, which contribution to the neutron field at any particular point is expressed by means of a suitable propagation kernel. However, to take into account the finite value of the radius of the (cylindrical) fuel element, in a recent version of the method two more parameters are introduced to characterize the fuel element as a dipole: the axial and radial polarization coefficients. Mesh methods describe each fuel element by a surface matrix connecting the surface fluxes and their normal derivatives on the surface. The resulting differential equations of multigroup theory within the moderator are solved following a finite differences scheme. Kernel heterogeneous methods provide a good example of an analytic approach to the solution of those reactor problems for which the conventional homogenization procedures are not particularly suited -for example, a reactor system with two zones of very different properties.

Although subjected to some limitations, heterogeneous methods are likely to evolve into a useful mathematical tool.

11.- Synthesis approximation methods. To avoid some drawbacks of the direct solution of three dimensional multigroup diffusion equations, several methods have been proposed to synthesize approximate three-dimensional flux distributions out of two-dimensional calculations. The mathematical basis of such methods is not so clear as would be desirable, although the application of variational techniques to the derivation of the fundamental formulae provides for some kind of justification. It has been pointed out that to find the "best" approximate solution among the elements of a set of trial functions depends on what is meant by "best" and on how to achieve it. Both questions are unsettled. Here again, the conceptual difficulties are intrinsically tied with the nature of the basic variational functional used: it is not of the maximum (or minimum) type.

In principle, synthesis methods should be considered as heuristic ones, the value of which can only a posteriori be assessed. However, from a practical point of view they could provide reasonably accurate results at reduced cost.

12.- Numerical analysis techniques. Because of the large number of variables involved, the mathematical complexities of the transport equation are considerable and one has usually to resort to numerical methods. The  $S_N$

method - essentially a numerical integration of the transport equation - and random sampling by a direct analog Monte Carlo procedure are typical numerical methods.

The trouble with numerical methods is twofold: a) they require computers as a powerful tool and large, high-speed modern computers are quite expensive; b) the convergence of the numerical solutions to the "true" solution, even the convergence of some iterative procedures has been not shown in most cases. For example, it has been reported that no proofs have been found to guarantee the convergence of EQUIPOISE, although - it is added - successful experience shows the method to be rapid and reliable. This example depicts pretty well, in my opinion, one of the general features of the present situation: with high-speed computers on scene, numerical methods are now the most versatile tools in the field of nuclear reactor calculations, but little is really known about their actual value.

Nevertheless, a considerable amount of effort is going into development of new methods, and/or new versions of older ones, the reason being that although purely numerical procedures may be cumbersome, inaccurate and expensive, they are often the only means for getting an answer. Thus, new iterative methods have been derived for the solution of finite-difference analogs of the neutron diffusion and neutron transport equations for both steady state and burnout calculations. Anisotropic scattering is to be treated by construction of the complete discrete transfer matrix. An example of another still more complex problem is that of the rigorous analysis of the dynamic behaviour of a nuclear power



plant: to the space-dependent neutron kinetics equations for the reactor core there are added the time-dependent conservation equations of mass, energy and momentum for the coolant flow. These equations are interrelated and have to be solved all together. In this connection, numerical techniques are being developed to obtain the solution of a finite-difference approximation to the coupled nonlinear hydrodynamics, thermodynamics, and neutron kinetics equations for the particular case of a compact fast reactor.

There is a real need for further investigation to determine convergence conditions for both iterative and finite-differences techniques in order to decrease computing time and allow an estimate of the errors. On the other hand, it should be kept in mind that there are in principle many possible ways to solve a given problem following numerical techniques. For instance, one has to decide which difference scheme to use, what mesh intervals are mathematically and economically appropriate, how to solve the resulting finite-difference equations, etc. Therefore, comparisons between numerical and analytical results for simple problems would be very helpful in providing criteria as to the "best" decision to be taken in a given situation and for a given problem.

C. Specific problems

Some problems related to general mathematical methods have been considered in Part B. In the present part more specific problems are listed.

1. Better solutions  $F(\vec{x}, \vec{u}, t)$  of the complete Boltzmann equation are highly needed.
2. Exact solutions of the Boltzmann equation for as many special cases as possible to check theoretical simplified models, analytical approximations, and numerical methods.
3. Some assessment of the reliability of existing methods in new situations is desirable.
4. Theoretical error estimates are lacking at present for many simplified models and approximations. As a consequence, further mathematical development is needed in this direction.
5. The mathematical relationship between the variational and successive approximation methods should be clarified.
6. Production of a large library of Monte Carlo techniques, especially correlated sampling.
7. Automation of microscopic cross section data handling to produce multigroup cross sections.
8. Development of efficient group constant system calculations, in particular appropriate choice of weighting functions.

9. Models for calculating lattice properties for cells with complex fuel element configurations.
10. Search for calculations devices which can produce a large acceleration effect in group diffusion finite-difference programmes, and, generally, in the iterative solution of transport equations.
11. Accurate and rapid methods for the computation of the characteristics of heterogeneous assemblies of the complex character which real reactors possess.
12. To attain a basic understanding of what happens in a nuclear reactor in such a way that carefully build models and more efficient, perhaps even partially analytic methods can reduce the burden associate with a light-minded use of big computers.
13. Careful analysis of the physically and mathematically adequate interface and boundary conditions when dealing with approximations of the rigorous Boltzmann equation.
14. Study of the statistical distribution of level spacing in nuclides.
15. Calculation of resonance integrals for fissile nuclides in the statistical-energy range.
16. Theory of Doppler coefficients in fast reactors.
17. More refined methods for burn-up calculations.

18. Thermalization models to be used in connection with burn-up calculations so as to take into account the low energy Pu-resonances properly.
19. Develop an economical yet accurate method to calculate the secular behaviour of a reactor operating at power.
20. Examine the possibilities of the application of adjoint theory to reactor stability problems.
21. Improve the mathematical schemes for space-dependent kinetics and dynamics.
22. Develop methods for treating the nonlinear equations of reactor kinetics.
23. Setting up approximate though reliable mathematical methods for solving physical problems in reactor dynamics.
24. Improve practical methods of solving hydrodynamic problems.
25. Develop a heuristic program to "learn" a good way of maneuvering a very simple reactor under conditions where information feedback is noisy and imprecise, and under the assumption that the operator cannot look ahead into expected reactor responses except in the sense of predicting from past experience.
26. Study of noise analysis and statistical fluctuations in reactors including spatial effects.

27. Detailed theoretical treatment of noise fields.
28. Optimization of strategies in programs of reactor development.
29. Optimization procedures in general as applied to nuclear reactors.