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Juni 1973 KFK 1821

Institut für Neutronenphysik und Reaktortechnik

Review of Current Problems for Multidimensional Reactor Statics Calculations

R. Fröhlich

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REVIEW OF CURRENT PROBLEMS FOR MULTIDIMENSIONAL REACTOR STATICS CALCULATIONS

R. Fröhlich

Gesellschaft für Kernforschung mbH., Karlsruhe

Abstract

It is attempted to place the current mathematical and computational methods development efforts into an appropriate perspective by giving a short review about the accuracy requirements and present capabilities of predicting physical parameters for fast and thermal reactors. The mathematical properties of the neutron transport and diffusion equations and of their exact solutions are considered and their relevance to the development of numerical methods is sketched. The theoretical foundation of numerical solution methods is discussed. Typical computational difficulties based on characteristic physics properties of various reactor types are presented and the benefits, difficulties, and the reliability of several computational methods are reviewed. In addition, new methods and possible future trends are discussed. Finally some of the outstanding mathematical and computational problems for fast and thermal power reactor calculations are mentioned.

Kritische Besprechung der gegenwärtigen Probleme bei mehrdimensionalen, stationären Reaktorberechnungen

Zusammenfassung

Es wird versucht, die gegenwärtigen Anstrengungen auf dem Gebiet der mathematischen und numerischen Methodenentwicklung sowie der Rechenprogrammentwicklung in eine angemessene Perspektive zu rücken. Dazu werden die gegenwärtigen Genauigkeitserfordernisse und die Möglichkeiten der Vorhersage physikalischer Kenngrößen für schnelle und thermische Reaktoren kurz erörtert. Die mathematischen Eigenschaften der Neutronen-Transport und -Diffusionsgleichungen sowie ihrer exakten Lösungen werden betrachtet, und ihre Bedeutung für die Entwicklung numerischer Methoden wird skizziert. Die theoretische Begründung der verschiedenen numerischen Methoden wird diskutiert. Typische rechentechnische Schwierigkeiten für verschiedene Reaktortypen, die auf charakteristischen physikalischen Eigenschaften beruhen, werden dargestellt, und die Vorteile, Schwierigkeiten und die Zuverlässigkeit etlicher numerischer Methoden werden erörtert. Außerdem werden neue Methoden und mögliche zukünftige Trends diskutiert. Schließlich werden einige wichtige ungelöste Probleme für die Berechnung schneller und thermischer Reaktoren erwähnt.

1. Introduction

One of the most important tasks for the design of large fast and thermal nuclear power reactors is the determination of the neutron flux distribution as a function of space and energy. It is well known that the neutron flux can be obtained as a solution of the linear Boltzmann transport equation, but very often the rigorous numerical solution of the transport equation is not practical, because of excessive computer time requirements. It has been assumed for quite some time that the multigroup diffusion approximation gives sufficient accuracy for various reactors, especially large fast and thermal power reactors, by using an appropriate homogenization of the heterogeneous fuel pin and fuel subassembly cell structures. Presently very sophisticated homogenization methods are in use for thermal reactors based on differential transport theory (e.g. discrete ordinates) or integral transport theory (e.g. collision probabilities). For fast reactors the homogenization methods presently in use are much less sophisticated. Indeed, for fast reactors this problem is of less importance than for thermal reactors, because fast neutrons do not see the small heterogeneities due to their much larger mean free path.

Zum Druck eingereicht am 2.5.1973.

The few remarks about homogenization show already characteristic differences of fast and thermal reactors. It is intended to focus the attention on characteristic differences of calculational difficulties for fast and thermal reactors. Before one such characteristic difference is discussed let us mention some problems of specific interest in fast and thermal reactor physics.

Problems of specific interest for fast reactors are for example: control rod worths and shadowing effects, heterogeneity effects of control rod followers, power prediction in and near blankets, Na-void effects.

Problems of specific interest for thermal reactors are for example: Improved homogenization methods for fuel subassemblies; prediction of power distributions in large power reactors; spectrum calculations for fuel pins near water holes, control rods, or plutonium loaded rods; resonance shielding in the presence of Pu and fission products; temperature coefficients; boron worth.

Let us consider /1/ the determination of global power distributions in liquid metal cooled fast reactors (LMFBRs) and pressurized light water reactors (PWRs). It is assumed that an appropriate homogenization has been performed and the macroscopic cross sections are regionwise known. For large 3000 MW(thermal) power reactors one observes that the diameters, measured in diffusion lengths, are approximately 36 for an LMFBR and 190 for an PWR. This indicates the well known fact that the fuel subassemblies in large PWRs are very loosely coupled. Computationally this fact has serious consequences for difference approximation methods:

1) One needs much more spatial meshpoints for PWRs than for LMFBRs to achieve a given accuracy. By utilizing one mesh per diffusion length one would need approximately seven million spatial meshpoints for a PWR but only approximately 5o thousand spatial meshpoints for an LMFBR.

2) Fast reactor calculations require more energy detail. If 26 energy groups are used for the LMFBR and 4 energy groups for the PWR, then the number of group-space meshpoints for the PWR is still by more than a factor 20 higher than the corresponding number for the LMFBR.

3) In addition, the convergence of the socalled power iterations for the solution of the difference equations is much worse for large (measured in diffusion lengths) reactors.

After having discussed some of the typical problems and differences for fast and thermal reactors several explicit comments to the title of this review paper are necessary.

The question whether or not multidimensional calculations are needed has been discussed by several authors in the past /2,3,4/. It has been confirmed that two and three dimensional reactor calculations can have a great economic incentive, especially in connection with burnup studies, for large power reactors. Presently there are multidimensional computer programs in use which employ (in the case of fast reactors) in excess of 20 energy groups and (in the case of thermal reactors) in excess of a hundred thousand spatial meshpoints.

Current problems in multidimensional reactor calculations have various aspects. Let us name some of these aspects:

- mathematical and numerical problems
- computational problems
- accuracy and reliability of methods and computer codes
- accuracy of data libraries
- accuracy of experimental results and comparison with theoretical predictions.

In this paper the last two aspects will not be considered because they are somewhat divorced from the scope of this topical meeting and they have been discussed during a recent topical meeting of the reactor physics division of the American Nuclear Society in Kiamesha Lake, NY, USA (September 1972). Also some of the computational problems, e.g. the benefits of modular code systems and the computer independence of reactor codes (see for example /5/), will not be discussed here. The first three aspects will be discussed in some length. The attention will be focussed on characteristic difficulties and differences for fast and thermal reactor calculations.

The material is presented in the following order: In Section 2 some comments on accuracy requirements and on present capabilities for predicting physical parameters of fast and thermal reactors will be presented. This is done in an attempt to place the current mathematical and computational methods development efforts into the right perspective. In Section 3 the basic understanding of the mathematical equations, boundary value problems, and properties of exact solutions is shortly discussed and references to more detailed papers are given. In Section 4 the theoretical foundation of various approximative methods is reviewed. Specific attention is given to difference approximation methods and synthesis methods in a discrete formulation. In Section 5 physics properties of various reactors and their relevance to computational difficulties are considered. In Section 6 the benefits and difficulties of various numerical methods are summarized. Finally in Section 7 some of the outstanding problems for reactor calculations are listed and several conclusions are drawn.

2. Comments on Accuracy Requirements and on Present Capabilities for Predicting Physical Parameters of Fast and Thermal Reactors.

Considerable progress has been achieved during the last years in predicting physics parameters for fast and thermal reactors /2,3,6,7/. This was accomplished by improving the basic nuclear data, by developing better calculational methods and programming techniques, and by using modern high speed computers. It is not attempted to seperate the benefits of all these developments, but one should be aware that the computing power of high speed computers increased by more than one order of magnitude during the last five years.

One crucial question to ask is the following:

"What are the motivations for improving the predictive accuracy for the physics parameters still further ?"

To be more specific, let us first list some of the physical parameters of interest:

- reactivity (k_{eff} for initial core and during burnup)

- power distribution (peak to average)
- breeding ratios
- control rod worths
- temperature and power reactivity coefficients
- void effects
- streaming effects
- temperature hotspots

During July 1971 an IAEA panel of experts assembled in Vienna to discuss "Reactor Burn-Up Physics". This Panel attempted to define the key accuracy objectives (targets) for both theoretical and experimental methods, as well as the present capabilities with respect to these objectives. The assessment was restricted to thermal reactors only, and it was considered of a preliminary nature. Table I shows the capabilities and target values for the theoretical methods. The accuracy is a function of reactor type and is stated for well developed reactor systems. Differences in magnitude of the reactor parameters for some systems made it necessary to indicate a range of uncertainty or to give two values. For example, the smaller change in reactivity with burnup for the heavy water and gas cooled as compared to the light water moderated reactors, results in greater percentage uncertainties in reactivity lifetime for the same magnitude differences.

Table I shows that k_{eff} can be predicted with an uncertainty of ± 1 percent; the target values are less than 0.5 percent. The reactivity lifetime would need some improvement for gas cooled reactors and heavy water reactors. Most of the improvement is needed for predicting the power distributions.

In Table II, extracted from /4,8/, the present predictive uncertainties and the target values for evaluating fast reactor physics parameters are estimated. Table II contains these values for the German prototype reactor SNR-300 and for the large (2000 MW(e)) LMFBR power reactor concept presently under study in Germany.

Table II indicates that the predictive accuracy of k_{eff} needs some improvements for LMFBRs, especially for the large power reactors. Most significant is the improvement needed for predicting the control rod worths and the Na-void effects.

It is interesting to note that the present capabilities of predicting some fast reactor physics parameters appear to be almost better than the corresponding capabilities for thermal reactors (see for example peak to average core power). On the other hand one should not overrate the reliability of the values given in both tables. Especially the target values must partly be considered as short range objectives and all the entries of both tables are not free of personal judgement. I would also be somewhat sceptical about the values quoted for the present predictive uncertainties; they are certainly only achievable by the best methods presently available.

Let us come back to the crucial question: "What are the motivations for improving the predictive accuracy for the physics parameters still further ?" Some of the motivations are:

- to improve the reactor economy (lower the cost of generating electricity)
- to ease reactor licensing procedures and to decrease the time requirements for the licensing process

- to decrease the safety margins (or to increase the predicted safety)
- to reduce the overdimensioning of plant components and fuel requirements
- to save time during startup experiments
- to increase the predictive accuracy of future large power reactors
- to increase the basic understanding of the phenomena involved (academic basic research)

Several of the motivations are closely related to cost, i.e. to the improvement of reactor economy, but for others, e.g. the safety related motivations or the increase of the basic understanding of the phenomena involved, it is very difficult to express the gain explicitly in cost figures.

Attempts have been made to establish some cost benefit analysis of certain improvements in the predictive accuracy of physical parameters /9,7,1o/, but one has to realize that this problem is a very complex one. Table III was extracted from a paper by JONSTONE and SCOTT /1o/ and contains cost benefits from certain improvements of the predictive accuracy for high temperature reactors (HTRs).

Let us consider the temperature coefficient for an HTR somewhat more in detail by following the comments given in /1o/. An improvement in the knowledge of the fuel temperature coefficients is usually considered to lead to a reduction in the required number of control rods. However, there is a less obvious but more important relationship between the operating temperature of the fuel and the temperature coefficient. In the HTR, the fuel kernels are separated from the coolant gas by layers of graphite, and hence the thermal time constant of the fuel is significantly longer than for a metal clad fuel. Consequently the response of the outlet gas thermocouple to an increase in fuel temperature is relatively low. This is an important feature in examining the behavior of the reactor under fault conditions. As the power temperature coefficient becomes less negative so the amplitude of the fuel temperature transient increases before the gas outlet temperature reaches the trip level. For one particular design, with a prompt fuel temperature coefficient of -2.5 mN/°C, a change of the coefficient to -2.0 mN/°C would lead to a further increase of 25°C in the fuel temperature before the trip operated (1 mN = 10^{-5} $\Delta k/k$). The present intention is to operate the HTR with a "clean" gas circuit. It is therefore imperative that the fuel temperature transients do not lead to temperatures in old fuel at which a significant number of fuel kernels rupture due to the high fission gas pressure. Consequently the fuel must operate with a large margin between the fuel temperature and the failure temperature. An improvement of the predictive accuracy of the temperature coefficient from ± 1.0 mN/°C to ± 0.5 mN/°C would allow a reduction of the temperature margin by approximately 25°C. This increase in operating fuel temperature is worth about $ 1.0/kW, or $ 10^6 for a 1000 MWe reactor. This is almost 2 orders of magnitude greater than the saving due to reduction in the required number of control rods.

Table III displays also the cost benefits due to an improvement in accuracy for predicting power distributions. The details should be omitted here.

The cost benefit numbers of Table III show, that a small improvement could have a high economic incentive, especially as the number of operating reactors increases. But the story about the temperature coefficient shows also that the relation of accuracy improvement to cost benefit is generally speaking not an easy one.

Up to now it has not been mentioned here that it might cost a lot of money to do the research and development for achieving the improvements in predictive accuracy for certain physical reactor parameters. Several attempts have been made to estimate such expenses (see for example /1o/). Naturally, these expenses increase very rapidly for extremely high accuracy requirements.

The "global" problem of finding the minimum of the total expenses for building and operating reactors is a very complex task. But it is the opinion of the author of this review paper, that one should first more vigorously attack the "local" problem of finding the cost relationships for accuracy improvements of single physical parameters and of doing the necessary research and development work to achieve these improvements.

While looking over the three tables I, II, and III one could be somewhat pessimistic how much more effort should be expended in this area of research. Therefore, this section should be concluded by mentioning one example - full core light water reactor (LWR) statics and burnup calculations in three dimensions - where obviously a lot of future work is required to develop calculational methods which are accurate and economic at the same time:

A comparison of the many types of three dimensional codes was proposed at the IAEA burn-up physics panel in July 1971. As explained with more détail in /11/, this led to an exercise where a 3D reactor core was defined as a mathematical benchmark problem. The reactor was a medium sized LWR with two types of fuel elements, with 9 control rods wholly and 4 partially inserted. All material constants were defined regionwise through two group reactor physics data. Calculations were performed in seven countries with seventeen 3 dimensional codes.

The codes, which were partly not especially tailored to this LWR problem showed a deviation in the range of 20 - 40 percent for the power distributions. It was found - as was proved by two dimensional test calculations - that the numbersof meshpoints used were insufficient. MICHEELSEN /11/ states that no "correct" answer to the simple 3D benchmark problem has been seen yet. It should be possible to generate a correct solution with PDQ-7 or a comparable code, but it might be a somewhat time consuming task. Indeed, the accurate determination of flux and power distributions for large light water power reactors is a very difficult task (see also section 3 of this paper), especially if one wants an accurate and economic solution at the same time. That an economic solution technique is required results from the fact that a complete depletion calculation requires many (20 to 100) steady state calculations.

It should be mentioned that most of the remaining problems in multi-dimensional reactor statics are of particular interest to the applied mathematician, the numerical analyst, and/or the programming specialist. These problems are indeed challenging. The physical phenomena in reactor statics, which are of relevance to power reactor calculations, are almost all very well understood. There is possibly only one exception, i.e. the theoretical understanding of the basic nuclear data.

3. Basic Understanding of the Mathematical Equations, Boundary Value Problems, and Properties of Exact Solutions

The basic mathematical equation for multidimensional reactor calculations is the neutron transport equation. This equation in its steady state form could provide a reference solution for all problems of interest in reactor statics. Unfortunately, the rigorous numerical solution of the transport equation, taking into account the full heterogeneity of the reactor configuration, is presently impossible and will be impossible for quite some time. This is so, because the steady state flux depends on six independent variables and reactors have frequently a rather complicated twofold or even threefold heterogeneous structure. Very frequently the transport equation is approximated by the diffusion equation, usually in its multigroup form. The scalar neutron flux (integrated over all angular directions) is now dependent on 3 space variables and the discrete energy group index only. In this section some basic mathematical properties of the transport equation and of the multigroup diffusion equation will be discussed.

The steady state neutron transport equation can be written in the following form:

$$\vec{\Omega}\cdot\nabla\psi(\vec{r},\vec{\Omega},E) + \Sigma_t(\vec{r},E)\,\psi(\vec{r},\vec{\Omega},E) = \int d\Omega' \int_0^\infty dE' \left[\frac{1}{k} f(\vec{r},E'\to E) + \Sigma_s(\vec{r},E'\to E,\mu_o)\right] \psi(\vec{r},\vec{\Omega}',E') \tag{1}$$

where

$\psi(\vec{r},\vec{\Omega},E)$	is the directional neutron flux
$\Sigma_t(\vec{r},E)$	is the total macroscopic interaction cross section
$f(\vec{r},E'\to E)$	describes the fission processes
$\Sigma_s(\vec{r},E'\to E,\mu_o)$	describes the scattering processes, $\mu_o = \vec{\Omega}'\cdot\vec{\Omega}$
k	is the eigenvalue of the problem

The directional neutron flux must fullfill certain boundary conditions on the outer surface S of a reactor assembly or on the surface of a reactor cell. For example, the boundary condition can be expressed as follows:

$$\psi(\vec{r},\vec{\Omega},E) = o \text{ for } \vec{r}\in S\ ,\ \vec{n}\cdot\vec{\Omega} < o \tag{2}$$

where $\vec{n}$ is the normal to S pointed outward. Equation (1) together with boundary condition (2) constitutes a boundary value problem for the continuous steady state neutron transport equation. One is looking for positive eigenvalues k so that (1) and (2) have a non-negative solution $\psi(\vec{r},\vec{\Omega},E)$. For a long time very little was known about the existence and uniqueness of a non-negative solution of this problem. More than ten years ago G. BIRKHOFF /12, 13/ summarized some of the difficulties and also some proof ideas for

these positivity and criticality properties.

The proof of the existence and uniqueness of a non-negative solution of (1) and (2) with a corresponding positive eigenvalue k, which is larger in modulus than all the other eigenvalues of this boundary value problem, would be of great theoretical and also practical importance. From a theoretical viewpoint a rigorous mathematical understanding of the criticality phenomena would be achieved; from a practical computational viewpoint these properties would guarantee the convergence of certain wellknown iterative numerical solution methods for this boundary value problem.

Several russian mathematicians have made important contributions to the solution of this problem. Especially S.B. SHIKHOV /14,15,16/ and V.S. VLADIMIROV /17,18,19/ have proved these positivity and criticality properties under certain restrictive continuity assumptions. Also F. EBERSOLDT /2o/ introduces some restrictive continuity assumptions, especially for the scattering transfer cross-sections.

K.M. CASE and P.F. ZWEIFEL /21,22/ show the existence, uniqueness, and positivity of solutions for the inhomogeneous form of the transport equation. C. CERCIGNANI /23,24,25/ considers the inhomogeneous linear Boltzmann equation for rather general boundary conditions and scattering operators and proves the existence, uniqueness and positivity of the solution.

More recently M. BORYSIEWICZ and J. MIKA /26/ have considered the neutron transport equation in multigroup form. This equation can be written as follows:

$$\vec{\Omega}\cdot\nabla\psi^{g}(\vec{r},\vec{\Omega}) + \Sigma_{t}^{g}(\vec{r})\,\psi^{g}(\vec{r},\vec{\Omega})$$

$$= \frac{1}{k}\sum_{g'=1}^{G} f^{g'\to g}(\vec{r}) \int \psi^{g'}(\vec{r},\vec{\Omega}')\,d\Omega' \qquad (3)$$

$$+ \sum_{g'=1}^{G} \int \Sigma_{s}^{g'\to g}(\vec{r},\mu_{o})\,\psi^{g'}(\vec{r},\vec{\Omega}')\,d\Omega'.$$

$g = 1, 2, 3, \ldots, G$

G is the total number of neutron energy groups.

M. BORYSIEWICZ and J. MIKA prove the existence and uniqueness of a non-negative solution of equation (3) together with the boundary condition

$$\psi^{g}(\vec{r},\vec{\Omega}) = o \text{ for } \vec{r}\in S \text{ and } \vec{n}\cdot\vec{\Omega} < o. \qquad (4)$$

The corresponding eigenvalue k is larger in modulus than all the other eigenvalues of this boundary value problem.

The proof was established under very weak assumptions, i.e. the system should have spectrum regenerating properties.

Frequently the multigroup diffusion equations are used for the determination of fluxes and power distributions in reactor assemblies. These equations can be written as follows:

$$-\nabla\cdot(D^g(\vec{r})\nabla)\ \phi^g(\vec{r}) + \Sigma_R^g(\vec{r})\ \phi^g(\vec{r})$$
$$= \frac{1}{k} \sum_{g'=1}^{G} F^{g'\to g}(\vec{r})\ \phi^{g'}(\vec{r}) + \sum_{\substack{g'=1 \\ g'\neq g}}^{G} \Sigma_s^{g'\to g}(\vec{r})\ \phi^{g'}(\vec{r}). \qquad (5)$$

The boundary conditions are:

$$\frac{\partial\phi^g(\vec{r})}{\partial n} + \alpha^g(\vec{r})\ \phi^g(\vec{r}) = o \text{ for } r\epsilon S. \qquad (6)$$

G.J. HABETLER and M.A. MARTINO /27,28/ proved the existence and uniqueness of a non-negative solution of equation (5) together with the boundary conditions (6). The corresponding eigenvalue k is positive and larger in modulus than all the other eigenvalues of the problem.

The proof was established under some restrictive assumptions, i.e. $F^{G\to 1}(\vec{r}) \not\equiv o$ and the transitivity of the problem. In addition, the diffusion regions must be the same for all energy groups.

The properties of the exact solution of the neutron transport equation (1) or (3) and of the boundary condition (2) are not very well known. The exact solution will have singularities for the derivatives. For discontinuous material properties DAVISON /29/ and V.S. VLADIMIROV /3o/ have discussed the singularities of the exact solution for a one dimensional problem in spherical geometry with discontinuous material properties; T. KULIKOWSKA (personal communication) has rederived these singular properties more directly. I. BABUSKA and R.B. KELLOGG /31/ will discuss the properties of the exact solutions for both the transport equation and for the diffusion equation in two dimensional rectangular geometry. For the diffusion equation singularities do for example occur at cornerpoints between different materials.

It can be very important for a high accuracy numerical solution to take the characteristic singular behavior into account for the specific numerical solution technique. I. BABUSKA and R.B. KELLOGG /31/ will address this problem also. Various numerical difficulties can be explained by the singular behavior of the exact solutions. J. MIKA /32/, T. KULIKOWSKA /33/, and J.J.ARKUSZEWSKI /33a/ have discussed the relevance of such singularities to the numerical solution of the transport equation.

4. Theoretical Foundation of Numerical Solution Methods

The multigroup transport equations or the multigroup diffusion equations could be solved numerically by discretizing methods. For the transport equation the discrete ordinates methods are the most frequently used methods. Very powerful and flexible computer programs have been created based on the methods of discrete ordinates, see for example /34/. For the multigroup diffusion equations difference equation techniques have been used for one, two, and three dimensions and very powerful computer programs were developed, see for example /35/. Many other methods, e.g. synthesis methods, finite element methods, collission probability methods, etc. have been created during the last decade and gain importance for numerical reactor calculations.

4.1 Finite Difference Equation Methods

For the discrete ordinates equations of the transport equation K.D. LATHROP has discussed the properties of these discretized equations in several publications and review articles, see for example /34,36/. With respect to positivity properties, there is a basic difficulty, because the positive difference equations have a higher discretization error than, for example, the diamond difference equations. The very interesting problem, whether or not the discrete solution converges for certain mesh refinements to the solution of the continuous problem will not be discussed here in any detail. But it should be mentioned that H.B. KELLER, see for example /37/, N.K. MADSEN /38/, and also C. CERCIGNANI /25/ have contributed to a solution of this problem.

One other result for the discrete form of the transport equation should be mentioned here. G. LINDENMAYER /39/ proved the following properties for the discrete form of the multigroup transport equation in spherical geometry: The discrete transport equation possesses a unique positive solution (eigenfunction) and the corresponding eigenvalue k ($k_{effective}$) is positive and larger in modulus than all the other eigenvalues of this equation. The proof uses a matrix theorem which was derived in /40/. It is not known whether similar properties, at least for the eigenvalues, hold for the general discrete form of the transport equation especially in two or three dimensions.

Much more is known about the discrete form of the multigroup diffusion equations. Let us apply difference equation methods to the multigroup diffusion equation (5) and the boundary conditions (6). In this way the numerical solution of the continuous problem can be reduced to the solution of an eigenvalue problem for a system of linear algebraic equations, the discrete form of the multigroup diffusion equations. In matrix form these equations can be written as follows:

$$A\underline{\phi} = \frac{1}{k} B\underline{\phi} \ . \qquad (7)$$

The order I of the square matrices A and B is equal to the number of energy-space meshpoints, and $\underline{\phi}$ is a column vector representing the (approximate) neutron flux at the I energy-space meshpoints. k is the eigenvalue(an approximation of k-effective) of the problem.

The matrix A includes the diffusion, removal, and scattering processes, and the matrix B represents the fission processes within the discrete formulation chosen.

In 1957, BIRKHOFF and VARGA /41/ proved for the discrete form of the few-group diffusion equations the existence of a unique (normalized) positive flux vector $\underline{\phi}_1$ and of a corresponding single positive eigenvalue k_1 (k-effective) larger than the absolute value of any other eigenvalue of the problem. BIRKHOFF and VARGA achieved by these results a major break-through for mathematical reactor physics. From a theoretical viewpoint a rigorous mathematical understanding of the criticality phenomena for the discrete diffusion theory model was achieved; from a practical computational viewpoint this article stimulated the development of mathematically wellfounded numerical solution techniques, making the solution of one and two dimensional complicated heterogeneous reactor problems on high-speed digital computers possible and a matter of routine.

BIRKHOFF and VARGA proved these properties under some restrictive assumptions (few group problems, multiplicative form of the fission transfer matrix, i.e. $F^{g' \to g} = \chi^{g} \nu \Sigma_f^{g'}$, transitivity[1] of the problem, etc.). In 1968, these important existence and positivity properties have been proved /4o/ under very weak assumptions for the discrete form of the multigroup diffusion equations. In fact, these assumptions cover for the most widely used difference approximations all problems of practical interest. Some of the features are:

1) Arbitrary up- and downscattering is permitted.
2) A general fission transfer matrix ($F^{g' \to g}$) is possible, which is important for the inclusion of (n,2n) reactions, a fission spectrum dependent on the incident neutron energy group g', etc.
3) Interior non-diffusion regions with logarithmic boundary conditions at their surfaces are allowed.
4) The diffusion regions for different energy groups must not be the same.
5) For some energy groups the diffusion regions need not be connected.
6) The problem can be nontransitive.

The condition of transitivity has been replaced by weak conditions of connectedness. The existence and positivity theorem has been formulated and proved as an independent matrix theorem. This has the advantage that unnecessary physics assumptions are eliminated. In addition it has been shown that the weak conditions of connectedness are not only sufficient conditions for the existence, unity, and positivity statements, but they are also necessary conditions. In this sense, a problem which does not fulfill the necessary and sufficient assumptions given in /4o/ is not formulated properly. A more careful review of the contributions of other workers in this field can be found in /4o/. A more recent paper about this subject is /42/.

For a discussion of the discretization error of various difference equations see for example Lecture 3 in /43/.

Iterative solution methods for the eigenvalue problem (4o) have been discussed in detail in /44,45/. Z. WOZNICKI /46/ recommended the socalled "two sweep techniques" for the iterative solution of the difference equations for each energy group (inner iterations). This method was studied more carefully in /47/ and looks very promising. The method is similar to the "forward elimination and backward substitution technique" which has been used for the direct solution of one dimensional problems. One great advantage of the method appears to be its excellent performance for nonuniform meshspacings or for extremely heterogeneous material properties.

4.2 Flux Synthesis Methods for the Multigroup Diffusion Equation

Variational flux synthesis methods /48/ and multichannel flux synthesis methods /49/ were in competition since 1962/3. Later, the use of discontinuous trial functions for variational flux synthesis methods and the use of the

1) A reactor problem is transitive if a neutron of any energy introduced anywhere in the reactor has, potentially, nonzero progeny at all energies and locations of the reactor.

blending procedure for multichannel flux synthesis methods unified the two competing efforts /5o/.

In the present paper flux synthesis methods will be discussed in a very general formulation which includes all the above mentioned methods as special cases. But by using the trick to consider flux synthesis methods in a discrete formulation only, many of the difficulties are avoided which were a matter of controversies in the past /51,52/.

Two rectangular I **x** R($R \leq I$) matrices T and W of rank R are considered. The column vectors of T (W) may represent the R basic trial (weight) functions which are assumed to be known. Then the flux vector $\underline{\phi}$ can be expanded as follows

$$\underline{\phi} = T\,\underline{d} \tag{8}$$

$\underline{d}$ is an unknown column vector of order R (driving coefficients). If one multiplies Equation (7) from left by W^* (the transposed matrix W) and inserts $\underline{\phi}$ from (8) in the resulting equation, one obtains the general form of the discrete flux synthesis equations:

$$(W^*AT)\underline{d} = \frac{1}{\lambda}\,(W^*BT)\underline{d} \tag{9}$$

This is an eigenvalue problem for the unknown column vector $\underline{d}$ of order R. The eigenvalue λ has been distinguished from k because in general the eigenvalues λ of (9) might be different from the eigenvalues k of (7). For most synthesis methods R is much smaller than the number of group-space meshpoints I. Therefore, it should be much easier to solve the eigenvalue problem (9) of order R than to solve the original discrete problem of order I.

For a successful synthesis method a solution $\underline{d}_1$ and λ_1 of Equation (9) should be such that λ_1 is a good approximation of the fundamental eigenvalue k_1 and the vector $T\underline{d}_1$ should be close to the fundamental eigenvector $\underline{\phi}_1$ of Equation (7). This problem will be more carefully discussed. For most synthesis methods T and W are nonnegative matrices.

This formulation of flux synthesis methods is indeed rather general and does include the various synthesis techniques /53,48,5o,54/ as special cases. Only some examples can be mentioned here:

The <u>blending method</u> discussed by S. KAPLAN /48/ is considered for a one group three dimensional problem

$$\phi(x_i, y_j, z_k) = \sum_{n=1}^{3} Z_n(z_k)\, H_n(x_i, y_j) \tag{1o}$$

The matrix T can be written for this problem as follows:

$$T = \begin{bmatrix} x\,x\,x & & & 0 \\ x\,x\,x & & & \\ \vdots\,\vdots\,\vdots & & & \\ x\,x\,x & & & \\ & x\,x\,x & & \\ & x\,x\,x & & \\ & \vdots\,\vdots\,\vdots & & \\ & x\,x\,x & & \\ & & \ddots & \\ & & & x\,x\,x \\ & & & x\,x\,x \\ & & & \vdots\,\vdots\,\vdots \\ 0 & & & x\,x\,x \end{bmatrix} \begin{matrix} z_1 \\ \\ \\ \\ z_2 \\ \\ \\ \\ \vdots \\ z_K \end{matrix} \qquad (11)$$

$$H_1H_2H_3 \quad H_1H_2H_3 \quad \cdots \quad H_1H_2H_3$$

The order R is equal to 3 x K in this case (3 is the number of basic functions $H_n(x_i, y_j)$ and K is the number of axial planes considered). More general blending methods, including methods with and without group collapsing, are also special cases of our general flux synthesis formulation.

The coarse mesh methods: It will be assumed that the group-space meshpoints {1,2,...,I} are partitioned into R disjunctive subsets S_r, socalled coarse meshes,

$$\{1,2,3,\ldots,I\} = S_1 + S_2 + \ldots + S_R \qquad (12)$$

A given (approximative) flux vector $\underline{\phi}_a$ is partitioned correspondingly

$$\underline{\phi}_a = \underline{\phi}_1 + \underline{\phi}_2 + \ldots + \underline{\phi}_R \qquad (13)$$

where the components of $\underline{\phi}_r$ are defined as follows

$$\phi_r^{(i)} = \phi_a^{(i)} \text{ for } i\varepsilon S_r, \quad \phi_r^{(i)} = 0 \text{ otherwise.} \qquad (14)$$

If the vectors $\underline{\phi}_r$ are used as the R columns of T, then the method is called a coarse mesh method.

The coarse mesh rebalancing weighting: This is a special choice of the weighting matrix W. A partitioning of the type (12) is considered and the R column vectors $\underline{\delta}_r$ of W are defined as follows:

$$\delta_r^{(i)} = 1 \text{ for } i\varepsilon S_r, \quad \delta_r^{(i)} = 0 \text{ otherwise.} \qquad (15)$$

The Galerkin methods are characterized by W = T.

If a coarse mesh method is combined with a coarse mesh rebalancing weighting scheme for the same coarse mesh, the short description coarse mesh rebalancing method will be used.

If a coarse mesh method is used as a Galerkin method the short description coarse mesh Galerkin method will be used.

The state of the art for the theoretical foundation of the flux synthesis methods will now be reviewed for the various methods and physics situations.

It will be assumed that the matrices T and W are nonnegative. For a successful synthesis method it appears to be necessary that Equation (9) has a positivity property (P), i.e. Equation (9) has a unique (normalized) positive eigenvector $\underline{d}_1$ and a corresponding single positive eigenvalue λ_1, which is larger then the absolute value of any other eigenvalue of Equation (9).

The positivity property guarantees also that the synthesized flux $\underline{\phi} = T\underline{d}_1$ is nonnegative. It is also wellknown that the positivity property (P) assures the convergence of the source iteration procedure for Equation (9) to the eigenvector $\underline{d}_1$ and the eigenvalue λ_1.

The following two theorems have been proved /53/

Theorem 1 If $\underline{\phi}_a > 0$ and the coarse mesh rebalancing method is used, then the synthesis equations (9) have the positivity property (P).

Theorem 2 If $\underline{\phi}_a > 0$ and $A\underline{\phi}_a = \underline{S} \geq 0$, $\underline{S} \neq 0$, and the coarse mesh Galerkin method is used, then the synthesis equations (9) have the positivity property (P).

The following two theorems show /55/ that the additional assumption $A\underline{\phi}_a = \underline{S} \geq 0$, $S \neq 0$, can be omitted under certain circumstances.

Theorem 3 If $\underline{\phi}_a > 0$ and $\underline{\phi}_r = c_r\underline{\delta}_r$, (c_r real number), and the coarse mesh Galerkin method is used, then the synthesis equations (9) have the positivity property (P).

Theorem 4 If $\underline{\phi}_a > 0$ and Equation (7) is a problem without upscattering and the group-space meshpoints of each coarse mesh S_r, r = 1,2,...,R, belong to the same energy group (no group collapsing), and the coarse mesh Galerkin method is used, then the synthesis equations (9) have the positivity property (P).

Another interesting theorem is:

Theorem 5 If the general Galerkin blending method is applied to a one-group problem (7), then the synthesis equations (9) have a largest positive eigenvalue.

These theorems can be proved by showing that the necessary and sufficient conditions, which were derived in /4o/, are fulfilled for the matrices (W^*AT) and (W^*BT).

The review of the various theorems is now supplemented by the discussion of several anomalies of flux synthesis methods.

Anomalies for flux synthesis methods have been discussed by several authors in the past /56,53,57,55,58/. In /56/ an example has been analized which shows that adjoint weighting is not always preferable to Galerkin weighting. In /55/ an example has been presented which proves that the Galerkin blending method may give partly negative synthesized fluxes even for a one-group problem. Recently /59/ an example has been published which demonstrates that the general blending method without group collapsing, applied to a problem with downscattering only, does not always have a largest positive eigenvalue.

The first example justifies that the assumption $A\underline{\phi}_a = \underline{S} \geqq 0$, $\underline{S} \neq 0$, cannot generally be omitted in Theorem 2.

EXAMPLE 1

$$A = \begin{bmatrix} 10 & -1 \\ -9 & 2 \end{bmatrix}, \quad B = \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix}, \quad k_1 = \frac{9}{11}, \quad \underline{\phi}_1 = \begin{bmatrix} 2 \\ 9 \end{bmatrix}$$

$$T = \begin{bmatrix} 1 \\ 2 \end{bmatrix}, \quad (T^*AT)d = \frac{1}{\lambda}(T^*BT)d, \quad \lambda_1 = -1, \quad d_1 = 1.$$

The next example demonstrates that the matrix T^*AT can be singular for linear independent trial functions and a matrix A fulfilling all of the assumptions formulated in /4o/.

EXAMPLE 2

$$(1, 2) \begin{bmatrix} 12 & -1 \\ -9 & 2 \end{bmatrix} \begin{pmatrix} 1 \\ 2 \end{pmatrix} = 0.$$

The next example shows that the assumption "without upscattering" cannot be dropped in Theorem 4:

EXAMPLE 3

$$A = \begin{bmatrix} 40 & -1 & -8 & 0 \\ -1 & 10 & 0 & -48 \\ -38 & 0 & 10 & -1 \\ 0 & -8 & -1 & 50 \end{bmatrix}, \quad B = \begin{bmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}$$

$$T = \begin{bmatrix} 1 & 0 \\ 1 & 0 \\ 0 & 10 \\ 0 & 1 \end{bmatrix}, \quad (T^*AT)\underline{d} = \frac{1}{\lambda}(T^*BT)\underline{d}, \quad \lambda_1 = -\frac{1065}{56}, \quad \underline{d}_1 = \begin{bmatrix} 515 \\ 194 \end{bmatrix}.$$

The next example shows that the Galerkin blending method may give partly negative synthezised fluxes even for a one group problem:

EXAMPLE 4

$$A = \begin{bmatrix} 11 & -1 & 0 \\ -1 & 12 & -1 \\ 0 & -1 & 11 \end{bmatrix}, \quad B = \begin{bmatrix} 10 & 0 & 0 \\ 0 & 10 & 0 \\ 0 & 0 & 10 \end{bmatrix}, \; k_1 = 1, \; \underline{\phi}_1 = \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix},$$

$$T = \begin{bmatrix} 1 & 1 \\ 20 & 9 \\ 4 & 1 \end{bmatrix}, \quad (T^{*}AT)\underline{d} = \frac{1}{\lambda}(T^{*}BT)\underline{d}$$

$$\lambda_1 = \frac{1}{1.09012}, \; \underline{d}_1 = \begin{bmatrix} 10000 \\ 21294 \end{bmatrix}, \quad T\underline{d}_1 = \begin{bmatrix} -11294 \\ +8354 \\ +18706 \end{bmatrix}$$

$$\lambda_2 = \frac{1}{1.16558}, \; \underline{d}_2 = \begin{bmatrix} 10000 \\ -27910 \end{bmatrix}, \quad T\underline{d}_2 = \begin{bmatrix} -17910 \\ -51190 \\ +12090 \end{bmatrix}$$

The following example is very instructive because it shows a number of possible anomalies rather clearly.

EXAMPLE 5

$$A = \begin{bmatrix} 80 & 0 & 0 \\ -72 & 80 & 0 \\ 0 & -64 & 8 \end{bmatrix}, \quad B = \begin{bmatrix} 0 & 0 & 10 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

$$A\underline{\phi} = \frac{1}{k} B\underline{\phi}, \quad k_1 = 1, \quad \underline{\phi}_1 \begin{bmatrix} 1 \\ 1 \\ 8 \end{bmatrix}.$$

If the matrix T is chosen as

$$T = \begin{bmatrix} 1 & 0 \\ 0 & 1 \\ 0 & a \end{bmatrix},$$

where a is a free parameter, than one has for the coarse mesh rebalancing method the following relations:

$$W = \begin{bmatrix} 1 & 0 \\ 0 & 1 \\ 0 & 1 \end{bmatrix}, \quad (W^{*}AT)\underline{d} = \frac{1}{\lambda}(W^{*}BT)\underline{d}$$

$$\begin{bmatrix} 80 & 0 \\ -72 & 8(1+a) \end{bmatrix} \underline{d} = \frac{1}{\lambda} \begin{bmatrix} 0 & 10a \\ 0 & 0 \end{bmatrix} \underline{d}$$

or

$$\lambda(a) = \frac{9a}{8(1+a)}, \quad \underline{d} = \begin{bmatrix} 1+a \\ 9 \end{bmatrix}, \quad \underline{\phi} = \begin{bmatrix} 1+a \\ 9 \\ 9a \end{bmatrix}.$$

For the coarse mesh Galerkin method the following results are obtained:

$$(T^{*}AT)\underline{d} = \frac{1}{\lambda}\,(T^{*}BT)\underline{d}$$

$$\begin{bmatrix} 80 & 0 \\ -72 & 72+8a^2-64a \end{bmatrix} \underline{d} = \frac{1}{\lambda} \begin{bmatrix} 0 & 10a \\ 0 & 0 \end{bmatrix} \underline{d}$$

or

$$\lambda(a) = \frac{9a}{8(a-4-\sqrt{7})\,(a-4+\sqrt{7})} \quad ,$$

$$\underline{d} = \begin{bmatrix} a^2-8a+9 \\ 9 \end{bmatrix} \quad , \quad \underline{\phi} = \begin{bmatrix} a^2-8a+9 \\ 9 \\ 9a \end{bmatrix} \quad .$$

In Figure 1 the largest eigenvalue λ is plotted as a function of the parameter "a" for the rebalancing and the Galerkin method. For the rebalancing method the function shows a rather smooth behavior for positive parameters "a". For the Galerkin method the function $\lambda(a)$ has two singularities and one of these singularities, i.e. at $a = 4+\sqrt{7}$ causes an anomalus behavior for some positive "a" not too far from $a = 8$, which gives the exact solution. For example, $\lambda(7) = 3.9375$ and $\lambda(6) = -6.75$.

The state of the art for flux synthesis methods has been summarized on Tables IV and V. THEORY means the status of theoretical foundation. If the entry says COMPLETE, than the synthesis equations have the existence and positivity properties (P) mentioned above. EXPERIENCE is an abbreviation for numerical experience and the corresponding entry should indicate whether or not difficulties have occurred and how much numerical experience has been gained.

On Table IV the coarse mesh methods are considered. One observes that the coarse mesh rebalancing method has a complete theoretical foundation and the numerical experience is good for all physics situations, including upscattering problems and group collapsing. Due to this fact, coarse mesh rebalancing methods are very well suited for nonlinear convergence acceleration of iterative solution techniques for fine mesh difference equations. This is accomplished by periodically interrupting the fine mesh iterations and by applying coarse mesh rebalancing to the results.

For coarse mesh Galerkin methods the situation is different. This method can lead to difficulties in case of group collapsing or for problems with a full scattering matrix; but a simple additional condition guarantees the important existence and positivity properties.

On Table V the blending methods have been considered. Galerkin blending methods have been successfully applied to light water reactor problems. These problems had downscattering only, and methods without group collapsing were applied. No real anomalies have been observed, but a rigorous theoretical foundation is still lacking. V. LUCO /59/ discovered an anomaly for such problems in case of adjoint weighting. The notation NEGATIVE FLUX POSSIBLE should indicate that the synthesized flux can be partly negative. For fast reactor calculations flux synthesis blending methods with group collapsing have been successfully applied by skilled researchers using various weighting

schemes /60,61/, but serious anomalies have been discovered (see Example 5). Serious difficulties can also occur for problems with up- and downscattering in case of no group collapsing. Practically useful sufficient criteria for avoiding anomalies in case of blending methods are desperately needed.

4.3 The Finite Element Methods

The finite element methods were originally developed for the numerical solution of structural mechanics problems, see for example /62/ and /63/. A short survey directed to mathematicians has been published by FELIPPA and CLOUGH /64/. During the last two or three years the method has also been applied to the neutron transport and diffusion equations; see for example /65,66,67,68/. It is not our intention here to give a survey of these applications; instead, only a few remarks about the status of the theoretical foundation of these methods will be made.

The finite element methods can be regarded as special variational or synthesis methods, were the trial and weight functions are chosen as polynomials in each finite element or coarse mesh. For flux synthesis techniques described in Section 4.2, the basic trial functions are obtained by lower dimensional calculations (e.g. two dimensional calculations for a three dimensional synthesis) or by approximate calculations. The choice of polynomials for each finite element or coarse mesh has the great advantage that the results of the approximation theory can be applied, see /43,69/, and in this way the finite element methods are not that much dependent on the ingenuity of the user as for example flux synthesis methods are. Recently, BABUSKA and KELLOGG /31,68/ have derived very important results for the order of convergence of finite element methods with respect to mesh refinements in case of the diffusion equation. These results were obtained for heterogeneous problems and for various norms. For heterogeneous problems the solution of the diffusion equation may have singularities at the cornerpoints between different materials. BABUSKA and KELLOGG discuss especially how the order of convergence depends on these singularities. They also discuss possibilities of enriching the space of trial functions by singular functions in order to improve the order of convergence.

Another important problem for the finite element methods has received very little attention up to now: What are the properties of the socalled "stiffness equations" - these were called synthesis equations in the previous Section 4.2 and how well conditioned are the matrices involved ?

Let us apply - for example - the finite element method to a multigroup diffusion problem in two or three dimensions. The resulting equations for the coefficients of the basic polynomials constitute an eigenvalue problem for a linear system of equations. It is not known, whether or not this problem has certain positivity properties, especially it is not known whether or not this problem will have a largest positive eigenvalue.

This situation is typical for more sophisticated methods in multidimensional reactor statics: The properties of the matrices involved cannot easily be analized. It should only be mentioned here that almost nothing appears to be known about the matrices of the linear systems of equations which result from collission probability methods.

5. Physics Properties of Various Reactor Types and their Relevance to Computational Difficulties

The various types of fast and thermal power reactors have quite different physics properties. In Table VI the core averaged power densities and the characteristic diffusion lengths are presented. The energy dependent diffusion lengths L^g are defined as follows

$$L^g = \sqrt{\frac{D^g}{\Sigma^g}}, \tag{16}$$

where D^g is the diffusion constant for energy group g and Σ^g is the removal cross section for energy group g. The characteristic diffusion lengths in Table VI are rough one group values. The information is given for high temperature gas cooled reactors (HTGRs), boiling water reactors (BWRs), pressurized water reactors (BWRs), gas cooled fast reactors (GCFRs), and for liquid metal cooled fast breeder reactors (LMFBRs). The numbers presented may be disputable in detail but they should be sufficient for the following more qualitative considerations. It is interesting to note that HTGRs have extremely low power densities, thermal light water reactors have power densities approximately 10 times higher, and the power densities of fast reactors are up to 70 times higher than the power density of an HTGR. The characteristic diffusion lengths are extremely small for light water reactors and about six times larger for an HTGR. The diffusion length of fast reactors is somewhere in the middle.

The relevance of these properties to computational methods for the determination of flux and power distributions for the various reactor types will be investigated. The difference approximation methods for the multigroup diffusion equations will be considered in some detail, because these methods are still the most frequently used methods for calculating flux and power distributions in large and thermal power reactors.

In addition the discrete form of the transport equation will be considered and some characteristic computational difficulties will be discussed. These difficulties are partly quite different from the difficulties observed for the discrete form of the diffusion equation and they do depend also on different physics parameters.

5.1 On the Necessary Number of Meshpoints for the Discrete Form of the Multigroup Diffusion Equation

How many meshpoints are required to determine the flux and power distributions for the various reactor types with a certain accuracy ? This problem of the global discretization error, i.e. the difference between the exact solutions of the discrete and of the continuous multigroup diffusion problem, is a very difficult one. Most error bounds have been derived under simplifying assumptions, as, uniform meshes, constant coefficients, etc. But even under these assumptions the results are very often of limited practial value, because the error bounds do usually require the advance knowledge of bounds for the higher derivatives of the unknown exact solution for the continuous problem. See for example the recent publication by G. BIRKHOFF /43/.

Despite of many ingenious results derived by various mathematicians the author of this article must confess (after having done a survey of the recent literature) that there appears to be a lack of rigorous and at the same time practically useful methods for calculating reasonably sharp bounds for the global discretization error in case of a heterogeneous reactor problem. In order to try to assure a sufficiently accurate solution one does indeed almost entirely rely on the simple method of halving the meshlengths, i.e. solving the same physics problem twice by halving the meshes of a given meshgrid and comparing the two solutions. Certainly, this method has a number of pitfalls. By using the last method carefully for many large power reactor calculations some supporting evidence was obtained for various reactor types that one can calculate sufficiently accurate (within a few percent) flux and power distributions by using mesh lengths of 0.5 to 1.0 diffusion lengths.

Estimates of the necessary number of meshpoints for different reactor types can easily be made if the meshlength is assumed to be one diffusion length and the reactors are assumed to be homogeneous.

Based on the information contained in Table VI, and by assuming the reactors have the shape of a cube, the entries of Table VII can be easily calculated. The diameters of the 3000 megawatt (thermal) reactors are actually the sidelengths of the cube. The table shows that thermal light water reactors are extremely big if measured in diffusion lengths. Light water reactors require an exceptionally high number of space-meshpoints for multidimensional diffusion calculations.

Table VIII displays the final estimates for the necessary numbers of group-space meshpoints. It has been assumed that 4 energy groups are sufficient for thermal light water reactors, 7 energy groups are adequate for thermal high temperature reactors, and fast reactors can be calculated in ten energy groups. Even a 26 group treatment for fast reactors would not change the situation significantly: Group-space meshpoint requirements for thermal light water reactors are 10 to 50 times higher than for the other reactor types considered.

5.2 Dependence of Convergence Rates for the Iterative Solution of the Discrete Diffusion Equation on the Size of a Reactor and on the Meshspacings Used.

The discrete form of the multigroup diffusion equations is usually solved for two and three dimensions by a combination of so called outer and inner iterations. A third iterative scheme which may be required for converging problems with up- and downscattering, is neglected here. In this section a homogeneous one group model problem will be considered. The asymptotic convergence rates for the most frequently used outer iteration methods, i.e. the fission source iterations with and without convergence acceleration by the method of Chebyshev polynomials, will be analized for different reactor sizes and meshspacings. The same will then be done for various inner iteration methods.

5.2.1 Convergence Properties of the Outer Iterations

The one group diffusion equation

$$-D\Delta\Phi + \Sigma\Phi = \frac{1}{k}\,\nu\Sigma_f\Phi \qquad (17)$$

with constant coefficients is considered for a cube (interval or square for one or two dimensions) of sidelength H. $\Phi = 0$ is assumed on the outer surface of the cube. If there are N meshpoints in each coordinate direction (i.e. N-1 uniform mesh intervals in each direction) and one measures the sidelength H and the meshspacing h in diffusion lengths then one has

$$\bar{H} = H \cdot \sqrt{\frac{\Sigma}{D}} \quad , \quad h = \frac{H}{N-1} \quad , \quad \bar{h} = h\sqrt{\frac{\Sigma}{D}} . \tag{18}$$

The error reduction factor for the straightforward fission source iteration is equal to the dominance ratio $\sigma = |k_2/k_1|$, where k_1 is the fundamental eigenvalue (k-effective) and k_2 is the eigenvalue with the next-highest absolute value. The dominance ratio can be expressed as follows:

$$\sigma = \left|\frac{k_2}{k_1}\right| = \frac{2dD(1-\cos\frac{\pi}{N-1}) + \Sigma h^2}{2D\left[d-(d-1)\cos\frac{\pi}{N-1} - \cos\frac{2\pi}{N-1}\right] + \Sigma h^2} , \tag{19}$$

where d is the number of dimensions (d = 1,2,3) considered. By using (18) the dominance ratio can be expressed in the following form:

$$\sigma = \left|\frac{k_2}{k_1}\right| = \frac{2d(1-\cos\frac{\pi}{N-1}) + \bar{h}^2}{2\left[d-(d-1)\cos\frac{\pi}{N-1} - \cos\frac{2\pi}{N-1}\right] + \bar{h}^2} . \tag{20}$$

For N large compared to π one obtains the following approximate representation for the dominance ratio:

$$\sigma = \left|\frac{k_2}{k_1}\right| \approx \frac{1 + d\left(\frac{\pi}{\bar{H}}\right)^2}{1 + (d+3)\left(\frac{\pi}{\bar{H}}\right)^2} . \tag{21}$$

Finally, for $\bar{H}$ large compared to π one obtains:

$$\sigma = \left|\frac{k_2}{k_1}\right| \approx 1 - 3\left(\frac{\pi}{\bar{H}}\right)^2 . \tag{22}$$

This approximation shows that for $N \gg \pi$ and $\bar{H} \gg \pi$ the dominance ratio σ is strongly dependent on $\bar{H}$, the sidelength of the cube measured in diffusion lengths, but very weakly dependent on the meshsize $\bar{h}$ and on the dimension d.

If one uses symmetry conditions, i.e. only one octant of the cube (one half for d = 1, one quadrant for d = 2) one obtains for the dominance ratio of this problem

$$\sigma = \left|\frac{k_2}{k_1}\right| \approx 1 - 8\left(\frac{\pi}{\bar{H}}\right)^2 . \tag{23}$$

By using symmetry properties in reactor calculations one does not only have the benefit of a smaller number of meshpoints but one has in addition a considerable convergence improvement, as a comparison of Equations (22) and (23) indicates.

For $\bar{H}$ large, the dominance ratio gets very close to one and convergence acceleration, e.g. by Chebyshev polynomials, becomes very attractive. The asymptotic error reduction factor σ_{Ch} for the fission source iterations accelerated by the method of Chebyshev polynomials is

$$\sigma_{Ch} = \sqrt{\omega_b - 1} \quad , \quad \omega_b = \frac{2}{1+\sqrt{1-\sigma^2}} . \tag{24}$$

If $N_s(N_{Ch})$ is the number of iterations required for the straight source iterations (Chebyshev accelerated source iterations) to reduce the error by a factor 1000, then these numbers can be written

$$N_s = 0.24 \times (\bar{H})^2 \quad , \quad N_{Ch} = 0.59 \times \bar{H}. \tag{25}$$

Table IX displays these numbers for 3000 MW(th) reactors of different type. The extremely large number of necessary outer iterations for the light water reactors is due to the large size of these reactors measured in diffusion lengths.

5.2.2 Convergence Properties of the Inner Iterations

The one group model problem

$$-D\Delta\phi + \Sigma\phi = S \tag{26}$$

is considered for a cube (interval or square for one or two dimensions) of sidelength H. D and Σ are assumed constant, S may be spacedependent, and $\phi = 0$ is assumed on the outer surface of the cube. If one assumes a uniform mesh with N meshpoints in each coordinate direction and measures the sidelength H and the meshsize h in diffusion lengths (see also Equations (18)), then one obtains for the spectral radius ρ_{PJ} of the point Jacobi iterative method the following formula:

$$\rho_{PJ} = \frac{2d \cos \frac{\pi}{N-1}}{2d + \bar{h}^2} . \tag{27}$$

For the line Jacobi iterative method one obtains:

$$\rho_{LJ} = \frac{2(d-1) \cos \frac{\pi}{N-1}}{2(d-\cos \frac{\pi}{N-1}) + \bar{h}^2} . \tag{28}$$

For $N >> \pi$ and $\bar{h} \lesssim 1$ one obtains the following approximations:

$$\rho_{PJ} \approx \frac{1}{1 + \frac{\bar{h}^2}{2d}} \quad , \quad \rho_{LJ} \approx \frac{1}{1 + \frac{\bar{h}^2}{2(d-1)}} \; . \tag{29}$$

For $N >> \pi$ and $\bar{h} << 1$ one obtains the approximations:

$$\rho_{PJ} \approx 1 - \frac{1}{2}\left[\frac{1}{d} + \left(\frac{\pi}{\bar{H}}\right)^2\right] \bar{h}^2 \tag{30}$$

and

$$\rho_{LJ} \approx 1 - \frac{1}{2}\left[\frac{1}{d-1} + \frac{d}{d-1}\left(\frac{\pi}{\bar{H}}\right)^2\right] \bar{h}^2 \; . \tag{31}$$

The spectral radii of the Gauss-Seidel methods are the square of the spectral radii of the corresponding Jacobi methods. It is also wellknown that the spectral radii for the optimized point- and line-overrelaxation methods can be obtained as follows:

$$\rho_{PO} = \frac{1 - \sqrt{1 - \rho_{PJ}^2}}{1 + \sqrt{1 - \rho_{PJ}^2}} \quad , \quad \rho_{LO} = \frac{1 - \sqrt{1 - \rho_{LJ}^2}}{1 + \sqrt{1 - \rho_{LJ}^2}} \; . \tag{32}$$

If one introduces the asymptotic convergence rate $R = -\ln \rho$ as the inverse of the number of iterations required to reduce the error asymptotically by a factor of e, one obtains for the various iterative methods, under the assumption $N >> \pi$, $\bar{h} << 1$, and $\bar{H} >> \pi$, the convergence rates displayed in Table X.

One should not overestimate the importance of Table X because in practice (for large power reactors) one can hardly use small meshspacings $\bar{h}$. For $\bar{h} \approx 1$ one should use Equation (29) together with Equation (32). On the other hand, the spectral radii of the Jacobi methods for practical problems (heterogeneous material properties and/or non-uniform meshes) are much closer to one and convergence acceleration will be more beneficial than the model problem does indicate for $\bar{h} \approx 1$.

In summary one can say: The convergence rates of the inner iteration methods depend very weakly on the size of the reactor (for $\bar{H} >> \pi$). They depend strongly on the dimension of the calculation and on the used meshsize.

5.3 Estimates of Time Requirements for the Numerical Solution of the Discrete Multigroup Diffusion Equations

Time estimates for the solution of the discrete form of the multigroup diffusion equations for different reactor types can be obtained by combining the results of the two previous sections (5.1 and 5.2).

In Table XI time estimates for calculating static flux and power distribution of various 3000 MW(th) reactors are presented. The estimates are given for one, two, and three dimensions. It has been assumed that Chebyshev accelerated fission source iterations and line overrelaxation methods have been utilized and that the asymptotic convergence behavior for the outer and inner iterations of the one group model problem is also representative for the outer and inner iterations of the multigroup reactor problem. In addition it has been assumed that the execution time per group-space meshpoint is 24 µsec including overhead; this might be typical for fast computers as the CDC 6600. The necessary numbers of group-space meshpoints have been adopted from Table VIII.

The time estimates in Table XI indicate, that the use of three dimensional difference approximation methods for light water reactor static calculations appears to be unfeasible. One should also keep in mind that reactor depletion calculations require the execution of 20 to 100 static calculations. For fast reactors the use of three dimensional difference approximation methods for static calculations appears to be possible. The same is true for high temperature gas cooled thermal reactors. Depletion calculations for fast reactors based on three dimensional difference approximation methods are only possible on some of the fastest presently existing computers.

5.4 Computational Difficulties for the Numerical Solution of the Discrete Transport Equation

K.D. LATHROP, see for example /34/, has discussed several computational difficulties for solving the discrete form of the transport equation. Here several difficulties should only be mentioned and the situation should be compared with the situation for the discrete form of the diffusion equation.

1.) For the most popular discrete form of the transport equation the positivity of the solution cannot generally be guaranteed. This is quite different from the discrete form of the diffusion equation where for the most popular difference equations the positivity is always guaranteed. For practical transport problems negative angular fluxes and negative angle-integrated fluxes are indeed possible. For one dimensional plane geometry negative fluxes can be avoided if

$\Sigma_{total}\ \Delta x/2\mu_m < 1$ for all mesh-width Δx and all μ_m. For one dimensional problems, the necessary refinement of the mesh-widths is usually possible and no serious problem arises. For two dimensional problems the situation is more complicated. Strictly positive difference schemes have been developed, but unfortunately it has been observed that the positive schemes possess a higher discretization error than the popular diamond difference equations. For more details see /34/ and the references given there.

2.) Socalled "ray effects" have been observed for the discrete form of the transport equation. This phenomenon does not occur for the discrete diffusion equation. K.D. LATHROP /34/ has discussed several remedies for the ray effect. The use of finite element methods, especially spline approximations for the angular dependence, may have the greatest potential.

3.) For the iterative solution of the discrete transport equation usually inner and outer iterations are performed. The inner iterations are done to solve one group problems with an inhomogeneous source; the outer iterations are usually fission source iterations. For problems with up- and down-scattering a third iteration scheme may be required, but this will not be discussed here.

The convergence properties of the outer iterations (fission source iterations) should be very similar to the convergence properties of the fission source iterations for the discrete multigroup diffusion equations. The convergence rate for reactor calculations should be dependent predominantly on the size of the assembly measured in mean free paths; or more precisely on the dominance ratio, i.e. the absolute value of the ratio of the second largest to the largest eigenvalue, of the problem. For convergence acceleration Chebyshev polynomial methods or coarse mesh rebalancing methods in the space-energy domain can be used, see for example /7o/.

The convergence properties of the inner iterations to solve a one group inhomogeneous problem for the discrete transport equation are quite different from the convergence properties of the inner iterations for the one group inhomogeneous discrete diffusion problem. For the discrete transport problem the convergence (error reduction factor) will be proportional to the ratio of within-group scattering sources divided by all losses. For thick homogeneous zones this ratio will approach the within-group scattering cross section divided by the total cross section. In other words, the more absorbing and "leaky" a group is, the faster it will converge. This error reduction factor can be very close to one for thermal reactor cell problems and it will cause extremely bad convergence. But it is important to notice that the convergence rate is completely insensitive to the meshsize used in space and angle. Also extremely small local meshspacings do not lead to bad convergence or even semi-convergence as has been observed for the discrete diffusion equation /5/.

6. Advantages and Difficulties of Various Numerical Methods

It cannot be the goal of this Section to review in detail the various numerical methods which have been invented for multidimensional reactor statics calculations. Instead, the advantages and difficulties for the various methods will be compared and reviewed from a somewhat more general point of view for thermal and fast power reactor calculations.

Let us first list some of the methods and techniques which have been invented:

(1) Analytical Methods
(2) Finite Difference Methods
(3) Finite Element Methods
(4) Flux Synthesis Methods
(5) Nodal Methods
(6) Collission Probability and Integral Transport Theory Methods
(7) Combined Methods
(8) Monte Carlo Methods

The methods listed have a certain amount of overlap; for example, finite element methods could be considered as special synthesis methods, etc.

In addition some of the more or less well-known review criteria for numerical computer methods are listed:

(a) Theoretical Foundation
(b) Possibility of an Error Analysis
(c) Convergence to Exact Solution
(d) Reliability
(e) Flexibility
(f) Simplicity of Programming and of Program Test
(g) Computer Independence
(h) Simplicity of Usage
(i) Effectivity

The criteria listed have important correlations and some criteria do include a few of the others.

In the following subsections it will be attempted to review some of the advantages and difficulties for the various numerical methods. Naturally, such a review must be incomplete and one cannot avoid introducing a considerable amount of personal judgement and preference. It is also attempted to list some of the more recent literature and to refer the reader to more detailed review articles for some of the methods listed above. The few numerical results presented in this section were partly supplied to the author most recently by several researchers in this field. These results are partly unpublished and they are included here with the permission of the originators. Results, which are easily available in the literature, are not reproduced here and may sometimes not even be mentioned.

6.1 Analytical Methods

Major advantages of analytical methods, see for example /22/, are their good theoretical foundation, reliability, and the possibility to provide an error analysis. The main difficulty with such analytical methods is that their flexibility and applicability to realistic problems is severely limited.

Analytical methods for the transport and the diffusion equation are indeed almost useless for practical reactor calculations, but they are very important for checking more flexible numerical solution procedures; i.e. for providing benchmark problem solutions. A text book concentrating on all possible analytical solutions of the transport and diffusion equation would be highly desirable for the methods analyst (and also from an educational point of view !).

6.2 Discretization Methods

In the field of numerical analysis, the derivation of discrete approximations to boundary value problems from the associated variational principles has been accomplished by two different methods:

1. The derivatives appearing in the integrand of the variational functional are replaced by finite differences of mesh point function values; then the integrals are approximated by well-known integration formulas over simple mesh regions. By setting the variations with respect to the function values equal to zero the "finite difference equations" are obtained, see for example /71/. This approach is called the finite difference method (FDM).

2. The functions appearing in the integrand of the variational functional are chosen as sets of "polynomial patch functions". The polynomial patch functions are defined as follows: The entire domain is subdivided into subregions, the finite element meshes, and the polynomials are defined over the subregions only, rather than over the entire domain. These polynomials are called "piecewise polynomials" for obvious reasons. The so defined trial function set depends linearly on certain parameters and the functions and their derivatives fulfill certain continuity conditions. Then the integration is performed and by setting the variations with respect to the free parameters equal to zero the "finite element discretization" is obtained. Usually, the free parameters are chosen as the mesh point function values and/or as the mesh point values of the derivatives by using suitable interpolation formulas. This second approach is called the finite element method (FEM).

One does observe an interesting relationship of both approaches; but one has to realize that there is a basic difference in the method of obtaining the discretization. The first procedure is a variational method for setting up difference equations and it shares some of the basic advantages of the FEM over the classical procedures to derive finite difference approximations. But one has to be aware that the first procedure is not a form of the Ritz-Galerkin method. The second procedure is based on the Ritz-Galerkin variational method; in addition the theory of spline-approximation contributed, as another powerful mathematical tool , to the rapid development of the FEM.

For dicretizing a problem many other methods have been used. For example the socalled "box integration" methods, i.e. approximating the divergence form of the diffusion equation /43/, have been used by several authors.

For the neutron transport equation a variety of difference approximations have been suggested, which were partly based on physical intuition. The theoretical understanding of these difference equations is still limited.

The next four sections will be devoted to the FDMs and the FEMs as applied to the transport equation and to the diffusion equation.

6.3 Finite Difference Methods for the Neutron Transport Equation

Finite difference methods for the transport equation have been reviewed in some detail by K.D. LATHROP, see for example and for more references /34,36/. These methods do have a sound basis for most applications; but from a more theoretical point of view one should be aware, that there are many open problems, e.g. positivity properties, convergence properties, etc.; see also the remarks in Sections 3 and 4. These finite difference methods (S_N-methods) have a high flexibility and the programs developed are strongly user oriented, computer independent, and efficient. The major difficulties are: negative fluxes may occur for larger spatial meshsizes and for higher dimensions; ray effects may occur for low order angular approximations, see for example K.D. LATHROP's /72/ discussion of the various remedies of ray effects. Difference equations with positivity properties have been derived, but these encounter higher discretization errors than the well-known diamond difference equations.

The difference equations are usually solved by iterative techniques. In Section 5 a few remarks have been made about convergence properties of inner and outer iterations. Especially for thermal reactor and cell problems a bad convergence behavior of the inner iterations can occur. Several convergence acceleration procedures have been applied. Chebyshew acceleration of the inner iterations works well for one dimensional problems but failed when applied in one two dimensional program /73/. Several other methods have been used for convergence acceleration of the inner iterations with mixed success. The most promising methods appear to be the coarse mesh rebalancing methods /7o,74,75/ and the synthetic methods /7o,76,77,78/. Both methods are related to each other as has been shown by REED /7o/.

The synthetic acceleration method for the iterative solution of the inhomogeneous transport equation is based on the following principle: A low order approximation to the transport equation is solved repeatedly for the residuals of a high order approximation of the transport equation. In this way the high order approximation can be solved under certain additional conditions which assure the convergence of the process, see for example /7o/. If one uses the inhomogeneous diffusion equation as the low order approximation, then the synthetic acceleration method has an interesting property: GELBARD and HAGEMAN /77,78/ have shown, that this acceleration method converges for a model problem with a theoretical error reduction factor $\rho \leq 0.23\ c$, where c is the ratio of the within-group scattering cross section to the total cross section. This is a remarkable property, because the error reduction factor for the ordinary iteration is equal c, which could be very close to one.

V.I. LEBEDEV and G.I. MARCHUK /79,8o/ have considered the socalled KP-method. It can be shown /81/, that the KP-method is a slight generalization of the wellknown synthetic acceleration method. LEBEDEV /8o/ reports also very good convergence properties for the KP method for c close to one if the diffusion equation is used as the low order approximation.

The exact solution of the transport equation has certain singularities, especially in case of discontinuous material properties, see also Section 3. These singularities have some relevance to the difference approximations and their convergence to the exact solution, see for example /32/. This problem requires further investigation.

6.4 Finite Difference Methods for the Diffusion Equation

Finite difference methods for the multigroup diffusion equation have a good theoretical foundation, see also Section 4.1. The diffusion theory computer programs are very flexible and they have been used for large power reactor calculations. An error analysis is usually attempted by the primitive method of mesh-halving. The iterative solution techniques have been discussed by several authors /44,45/. Semi convergence has been reported in /1/ for extremely non-uniform mesh spacings and/or drastically changing material properties. It has also been shown /1/ that good convergence could be achieved by applying coarse mesh rebalancing acceleration techniques. The problem of computer dependence of the large production codes was discussed in /5/. Programming of large diffusion theory codes, based on difference approximations, could be difficult because of the data handling problems involved; but testing is simple and can be done for model problems and by appropriate reduction to lower dimensional problems.

An interesting method should be mentioned here which was developed and analized by Z. WOZNICKI /46,47/. The method is a two sweep iterative method with some similarity to the "forward elimination and backward substitution technique" which was used for one dimensional problems. One specific method, the socalled EWA-II method has been described in /46/. During the last years several variants have been developed, which will be described in the dissertation of Z. WOZNICKI /47/. In Table XII some of the unpublished results of /47/ are presented with the permission of the author. The heterogeneous test example set up by VARGA /45, Appendix B/ was chosen. These two sweep methods may have a good potential for large diffusion theory production codes. They do perform very well for problems with extremely non-uniform mesh-spacings. One slight difficulty is the estimation of the best overrelaxation factor.

Another very promising iterative method for the solution of large difference equation systems is the socalled "strongly implicit iterative procedure", which was developed by H.L. STONE and others /82,83,84/. STONE /83/ did an extensive comparison of the efficiency of this new method with other methods. Four different test problems were chosen. The first and simplest one being a rectangular region in which the differential equation coefficients were uniform. The fourth and most difficult one was an irregularly shaped region with highly variable coefficients. Problems two and three were of intermediate irregularity and difficulty. - Of the previous methods tested, ADI (Alternating Direction Iteration) was found to be by far the most effective. Table XIII summarizes the comparison of the ADI to the Strongly Implicit Procedure (SIP) for the four test problems. Since the computational work per iteration is very nearly the same for ADI and SIP, the number of iterations is proportional to the computational work required.

During the last years direct inversion techniques for large systems of linear equations with sparse coefficient matrices have gained more interest. These methods have been used for stress analysis problems, and they are based on automatic reordering techniques which should minimize the number of operations during the elimination process. D'AMICO /85/ reported considerable success with certain semi-empirical minimizing procedures.

In conclusion it should be mentioned that a detailed comparison of various solution methods of large difference equation systems for a set of suitable multidimensional reactor benchmark problems would be highly desirable. This would be especially beneficial for an reliable evaluation of some of the newer methods.

6.5 Finite Element Methods

In Section 6.2 the finite element method has been characterized as a specific Ritz-Galerkin method. The trial functions are socalled piecewise polynomials, which can yield high accuracy approximations for the functions and their derivatives.

For practical calculations the piecewise polynomials provide some convenient features which polynomials defined over the entire domain lack /65/. For example, the piecewise polynomials permit flexibility in imposing certain continuity or jump conditions at the interfaces and corners between subregions; convenient piecewise polynomial basis functions can be found, such that the expansion coefficients are directly related to the values of the functions and of their derivatives at mesh points.

Another advantage is the high degree of flexibility in selecting the appropriate shape for the subregions, i.e. the finite element meshes: Rectangular meshes, triangular meshes, or even curved mesh shapes are easily possible. For example, this flexibility is important for finding the neutron flux near round fuel or control rods in a square or hexagonal cell.

6.5.1 Finite Element Methods for the Multigroup Diffusion Equation

The finite element method has been applied to the diffusion equation by several authors, see for example /65,67,86-92/. It is not intended here to review these and other papers in detail, instead some typical results will be presented and the more general advantages and difficulties will be considered.

KANG /65/ considers an eigenvalues problem for the two group diffusion equation in two dimensions. The model consists of a fuel region and of a reflector as shown in Figure 2. For this problem bilinear (m = 1) and bicubic (m = 2) basis functions have been used. At the singular point, i.e. the corner $(\frac{L}{2}, \frac{L}{2})$, three different sets of bicubic basis functions have been applied: The two basis functions of set A fulfill all the continuity conditions for flux and current at the corner; the four basis functions of set B are continuous but the continuity of the currents at the singular corner point is relaxed; the six basis functions of set C are continuous but the coupling of the derivatives at the singular corner point is even further relaxed. For the precise details see /65, page 97/. Table XIV summarizes the results for the eigenvalues obtained by the finite difference method and by the finite element method using bilinear and bicubic piecewise polynomials. It should be noted that bicubic polynomials for $\Delta x = \Delta y = L/2$ yield accuracies comparable to that of the finite difference scheme for $\Delta x = \Delta y = L/2o$. The order of convergence is approximately one for set A but approximately equal to three for sets B and C. It is interesting to note that although set A has low-order convergence, it gives quite accurate eigenvalues for large meshspacings.

This example shows that the finite element approach is quite promising for reactors with large homogeneous zones.

The major advantage of the finite element method is its flexibility with respect to mesh-shapes and order of approximation. The finite element method has also a good theoretical foundation; especially, the convergence to the exact solution has been proved, see for example /65,31,68,93/. The latter

problem and the accurance of singularities has already been discussed in Section 4.3. The price one has to pay for the higher order accuracy of the finite element methods is that the matrices of the stiffness equations (synthesis equations) have more nonzero elements and some of the nice properties, as for example diagonal dominance, are usually lost. This makes the solution of these stiffness equations more complicated. Also, one does not know, whether or not certain positivity properties still hold. Programming of finite element methods is somewhat more complicated than of usual finite difference methods; but this is again the price one has to pay for the greater flexibility of the mesh-shapes.

Another interesting variant of the finite element methods is W.J. GORDON's eextrapolation procedure /94/. The application of this method to multidimensional diffusion problems will be discussed by J.P. HENNART /95/.

6.5.2 Finite Element Methods for the Multigroup Transport Equation

The finite element methods have been applied to the transport equation in one and two dimensions /65,66,96-101/. The results reported look very promising.

Major advantages appear to be the high order accuracy and the great flexibility for the mesh-shapes. In addition the ray effect is considerably decreased.

The difficulties are again connected with the different nature of the stiffness or synthesis equations as compared to the ordinary discrete ordinates equations. The solution procedures, e.g. the Cholesky reduction used in /96/, might show a different sensitivity with respect to extremely fine or nonuniform meshes than the usual iterative solution procedure for the discrete ordinates equations, see also Section 5.4. In summary, the properties of the matrices appearing in the stiffness equations have not been studied in detail up to now.

6.6 Flux Synthesis Methods

Flux synthesis methods have been reviewed in detail for the multigroup diffusion equation by W.M. STACEY /102,103/. The status of the theoretical foundation of flux synthesis methods has been discussed in Section 4.2. Therefore the advantages and difficulties will be summarized very briefly in this Section.

Flux synthesis methods are very flexible and efficient for large power reactor calculations. Large computer codes, especially for light water reactor burnup studies, and for fast reactor applications /4,104/ have been developed. No serious anomalies have been reported for those applications. Unfortunately, serious anomalies have been found for group collapsing and energy synthesis methods. Practically useful criteria for avoiding these anomalies are highly desirable. Another difficulty is that it appears to be very difficult to estimate the accuracy of a flux synthesis solution; one possibility was discussed by J.B. YASINSKY /105/.

W.O. OLSON and A.H. ROBINSON /106/ will contribute to spectral flux synthesis for one and two dimensional problems.

Very little attention has been given to flux synthesis methods for the neutron transport equation, see for example /1o7/.

6.7 Nodal Methods for the Few Group Diffusion Equation

Nodal methods for the group-diffusion equations have been reviewed recently by A.F. HENRY /1o8/. One very promising method has been developed by S. BØRRESEN /1o9,11o/.

The advantages of coarse mesh nodal methods are: Short computer running times for large power reactor applications with reasonable accuracy for the nodal fluxes and powers, i.e. the coarse mesh averaged fluxes and power distributions. Tuning of these methods by comparison with experiments or fine mesh calculations appears to be possible but is also somewhat questionable.

The major difficulties are: Frequently occurance of insufficient accuracy for the nodal fluxes; inavailability of detailed power distributions; the mathematical properties of the nodal equations have not been throughly investigated. The first difficulty is based on the fact that it is very hard to obtain accurate nodal coupling coefficients without doing a corresponding fine mesh calculation.

The first and the second difficulty has been overcome for several test examples by a very interesting and promising combined nodal-flux synthesis approach, which is presently under development by M. WAGNER /111/. More detailed information about this approach will be provided in Section 6.9.

6.8 Collision Probability Methods

J.R. ASKEW /112/ has recently given a review of the status of collision probability methods (CPM). Collision probability methods have been applied successfully to complicated geometric situations, especially rod clusters and cell problems. The methods are very powerful where a modest accuracy is acceptable and approximate evaluation of the probabilities is adequate. ASKEW has, however, shown that as greater accuracy and refinement is demanded, and a finer mesh imposed, it will eventually be preferable to use "differential" methods.

The subject of collision probability methods will be discussed at this topical meeting by several authors /113,114,115,116/. Here only two specific applications will be mentioned:

Recently, a very efficient spectrum code for calculating homogenized group constants has been developed by P. WÄLTI /117/. This code is based on a collision probability approach including anisotropic scattering /118,119/ and on a synthetic kernel method for the scattering processes /12o/. This code is extremely efficient for calculating fast and thermal reactor group constants.

During the last two or three years several authors /121-124/ have applied collision probability methods in whole core three dimensional reactor calculations. Several of these methods were quite successful, especially M. WAGNER and A. MÜLLER /123,124/ developed highly efficient production codes for light water reactor applications. The application of response matrix methods to whole core reactor calculations will be discussed by R.J. PRYOR et al. /114/

and H.S. BAILEY /115/ during this topical meeting.

Let us briefly summarize some of the advantages and difficulties for collision probability methods: Some of the advantages: For moderate accuracy requirements CPMs are very efficient and flexible methods. Complicated geometrical structures can be treated successfully. The methods are applicable to cell, subassembly, and whole core reactor calculations; they are reliable and computer independent.

Some of the difficulties: The accurate calculation of the collision probabilities is difficult. Collision probability methods with an approximate evaluation of the collision probabilities (e.g. escape and transmission probabilities) have the drawback that they do not converge to the exact solution in case of mesh refinements; in fact, the results could be worse for a refined mesh. This will be demonstrated by D. EMENDÖRFER /113/. The mathematical properties of the resulting equations have not been investigated in detail for the collision probability methods.

6.9 Combined Methods

Combined methods have been discussed by several authors, see for example /1,5,34,125,126/. Fine mesh difference equation methods for the multigroup transport equation and for the multigroup diffusion equation have been combined with flux synthesis techniques, e.g. coarse mesh rebalancing techniques, to accelerate the convergence of the iterative solution techniques. One possible procedure has been sketched in the schematic flow diagram displayed in Figure 3.

Coarse mesh rebalancing methods have also been used to accelerate very successfully the convergence of iterative solution techniques for collision probability methods /123,124/.

S. NAKAMURA /127/ will discuss the effect of weighting functions on coarse mesh rebalancing acceleration, a difficult mathematical problem, which had attracted very little attention up to now. A successful analysis of this problem could be of great practical value.

Recently, M. WAGNER /111/ has developed a socalled nodal synthesis approach. The motivation for this approach is to overcome two of the basic drawbacks of most nodal methods currently in use. These drawbacks are:
a) Accurate nodal coupling coefficients have been calculated by corresponding off-line fine-mesh calculations.
b) Coarse mesh nodal calculations have provided the average fluxes for each coarse mesh only; the detailed space dependent fluxes (and the power) cannot easily be generated.

The new nodal synthesis technique combines the features of the multi-channel synthesis approach with the features of the conventional nodal methods. In each coarse mesh cell (or node) it is assumed that the flux is separable into the product of one dimensional fluxes. Use is made of one dimensional fine mesh diffusion calculations through nodal channels, where the cross coupling is described by transverse bucklings. In this way self-generated nodal coupling coefficients are calculated. The local fine mesh flux shapes normal to the interfaces between nodes are taken into account explicitly. The method works by alternating between nodal solutions and complete one dimensional multichannel sweeps which update the set of coupling coefficients. In this way a rapidly converging procedure is obtained. The method is self-consistent in the sense that both the spatial coupling coefficients and the

fine mesh fluxes (seperable in each node) are automatically generated during the iterational process. The smoothing of the small flux discontinuities at the nodal interfaces requires special attention.

An important property of the nodal synthesis technique is the fact that the fine mesh fluxes need not be stored. Only the coarse mesh variables, including transverse bucklings, must be kept in storage. The fine mesh flux distributions may be calculated selectively at the users option.

The method has been evaluated for two twodimensional test examples:

The first test example is the difficult IAEA benchmark problem for a medium-sized light water reactor in a two group representation. The results of a comparison of the new nodal synthesis method with the usual finite difference methods and the collision probability method used in the code MEDIUM /123/ are displayed in Figure 4. The finite difference method (FDM) uses a fine meshsize of approximately 2 centimeters and a rather coarse mesh-size of 1o centimeters; MEDIUM uses boxes of 10 cm sidelength; and the nodal synthesis method uses also nodes (coarse mesh cells) of 1o cm sidelength and in addition a fine mesh of one centimeter for the onedimensional multichannel calculations. The keff values for the fine mesh FDM shows very good agreement with the $k_{effective}$ of the nodal synthesis method. The computing time (in CDC-6600 central processor seconds) is considerably smaller for the new method. The coarse mesh FDM shows large discrepancies for $k_{effective}$ and for the power distribution. The nodal synthesis method needs roughly 3 times more computing time (in the 10 second range !) than MEDIUM, but shows a remarkable improvement in accuracy. The wellknown EQUIPOISE code was used to obtain the FDM results.

The second test example is the two dimensional two group, heterogeneous reactor problem presented by KANG /65, page 98/. The model used and the inverse k_{eff} results are displayed in Figure 5. The nodal synthesis method performs again very well. It should be mentioned that the nodal synthesis method used the given meshspacings Δx as the nodal meshlengths; the fine-mesh spacing was smaller by a factor 4 to 16, where 4 corresponded to $\Delta x = L/20$ and 16 to $\Delta x = L/2$. Again the computing time for the nodal synthesis is given. In Figure 6 the thermal flux traverse for $y = 0$ is displayed for the different methods. The description in Figures 4, 5,6 is given in German, but no translation appears to be necessary.

The examples presented demonstrate the power of the combined methods. It is the opinion of this author, that combined methods must be used for multi-dimensional reactor calculations. One of the great advantages of the two combined methods

(1) finite difference fine mesh iterational methods combined with coarse mesh rebalancing acceleration,

(2) coarse mesh nodal methods combined with fine mesh synthesis,

is their convergence to the exact solution of the diffusion equation for mesh refinements.

6.1o Monte Carlo Methods

Monte Carlo methods have been reviewed by several authors in the past, see for example /128,129/. During the last topical conference on new developments in reactor mathematics and applications (1971) two sessions were devoted to Monte Carlo methods. Here, only some advantages and difficulties of Monte Carlo

methods (MCMs) will be listed.

Some advantages: MCMs are very flexible; they can provide benchmark solutions for other numerical methods because they are rigorous in a certain sense; they do provide error bounds for a desired confidence level, what very few other methods do; they are especially suited for geometrically complicated situations in two and three dimensions.

Some difficulties: MCM are well suited only for the determination of integral quantities; the determination of flux- or power-distributions is time-consuming; eigenvalue problems provide specific complications; sophisticated biasing techniques have dangerous pitfalls; non-linear problems are difficult to treat; the test of Monte Carlo computer programs could be difficult.

7. Summary of Some Outstanding Problems for Reactor Calculations; Conclusions

Whilst it is true, that there are many difficult and interesting problems partly of a fundamental nature still remaining in multidimensional reactor calculations, such problems can hardly be considered as problems of prime importance[1]. All the efforts towards the solution of the remaining problems must be justified on economic grounds or, if one desires, by some of the other motivations mentioned in Section 2. One should, on the other hand, not underestimate those economic reasons, because the break through of a new reactor type or the survival of a reactor concept in a competitive market will strongly, if not entirely, depend on economic reasons.

Before the outstanding mathematical and computational problems will be summarized and briefly discussed, which is the main goal of this topical conference, some of the remaining practical neutron physics problems should be listed first.

1. Some physics problems of specific interest for fast reactors:

- control rod worths and shadowing effects;
- heterogeneity effects, especially for control rod followers;
- power prediction in and near blankets;
- sodium void effects for LMFBRs;
- streaming effects for GCFRs;
- reactivity effects during burnup.

2. Some physics problems of specific interest for thermal reactors:

- prediction of power distributions in large power reactors;
- improved homogenization methods for fuel pin and fuel subassemblies;
- determination of neutron fluxes in fuel pins near water holes, control rods, and plutonium loaded rods;
- resonance shielding in the presence of plutonium and fission products;
- boron worth for LWRs;
- temperature coefficient for HTGRs;
- doubly heterogeneous fuel element structure of HTGRs.

1) A reactor problem is defined as one of "prime importance", if the technical realization and safe operation of a certain reactor depends entirely on the solution of that problem.

It is interesting to note that the prediction of whole core power distributions for fast reactors is not listed explicitly, because the accurate prediction of power distributions for fast reactors is much simpler than the corresponding task for light water reactors (see also Section 5.3).

Outstanding problems in numerical reactor calculations have been discussed at various occasions, see for example /130/. It is attempted here, to summarize and list some of the outstanding mathematical, numerical, and computational problems for multidimensional reactor statics calculations. The order of presentation has nothing to do with their priority, instead the more theoretical problems are listed first and the more practical problems are listed last.

Some of the Outstanding Mathematical, Numerical, and Computational Problems in Multidimensional Reactor Statics

(1) Mathematical properties of the exact solutions of the transport and diffusion equations; especially, singularities of the solutions for problems with regionwise constant nuclear parameters and influence of boundary conditions.

(2) Positivity, reality, existence, and unity properties for the eigenvalues and eigenfunctions of the homogeneous transport- and diffusion equations (spectral theory). The properties of the higher eigenfunctions, e.g. the number and form of the positivity and negativity regions, are almost unknown in more than one dimension.

(3) Completeness of the system of eigenfunctions for the transport- and diffusion equations.

(4) Mathematical analysis of homogenization methods. A more rigorous analysis of this problem will possibly result in practically useful homogenization techniques and new recipes for getting the appropriate homogenized nuclear parameters.

(5) Order of convergence for the finite difference solutions and the finite element solutions to the exact solution of the transport or diffusion equations in case of mesh-refinement. Dependence of the order of convergence on singularities. Relevance of these results to realistic two- and three-dimensional calculations.

(6) Positive difference equations with low discretization error for the neutron transport equation. Development of methods for avoiding ray effects, e.g. finite element methods in the angular phase space.

(7) Development of good quadrature schemes for functions on the sphere to be used in multidimensional transport methods.

(8) Development of new iterative methods for solving the discretized transport and diffusion equations. The methods should overcome convergence difficulties for non-uniform meshspacings, for c close to one ($c = \Sigma_s/\Sigma_{total}$), for strongly heterogeneous material properties, etc. Convergence acceleration by synthetic methods, coarse mesh methods, Chebyshev polynomial methods, etc.

(9) Development of discretization methods (FDMs and FEMs) for nonrectangular geometries.

(10) Mathematical properties (positivity, condition numbers, etc.) of the stiffness equations (synthesis equations) for the finite element methods.

(11) Convergence Properties for the iterative solution methods of the FEM stiffness equations and dependence on the size of the reactor, the mesh-

size, the parameter c (Σ_s/Σ_{total}), etc.

(12) Theoretical foundation for flux synthesis methods. For example: Proof of positivity properties for blending methods in case of downscattering only and no group collapsing; derivation of sufficient conditions for avoiding anomalies in case of spectral synthesis and up- and down-scattering problems, taking into account various weighting schemes.

(13) Development of methods and recipes for selecting basic trial functions for flux synthesis methods.

(14) Error analysis for the flux synthesis solutions, finite difference solutions, finite element solutions, etc. Avoidance of semi-convergent behavior for iterative solution methods.

(15) Development of collision probability methods which include anisotropy effects.

(16) Development of accurate methods for calculating fuel subassemblies.

(17) Development of accurate and efficient methods for calculating space dependent few and multigroup constants, e.g. by using collision probability methods and synthetic kernel methods, and by using flux or bilinear weighting.

(18) Development of accurate and efficient methods for calculating power distributions for large power reactors, e.g. nodal methods, FDMs or FEMs accelerated by coarse mesh rebalancing methods, nodal synthesis methods, etc.

(19) Convergence properties of non-linear acceleration techniques, e.g. coarse mesh rebalancing. Effect of weighting functions on coarse mesh acceleration methods.

(20) Systematic development of benchmark problems for testing accuracy and efficiency of calculational methods. Analysis of model problems for numerical techniques.

(21) Adaption of computer programs to new computer hardware and new operation systems, e.g. new storage devices and concepts, multiprogramming environment, etc.

(22) Development of modular code systems to increase the efficiency and reliability of doing complex calculations.

(23) Standardization of program module interfaces, data files, etc.

(24) Increase of the reliability and efficiency of computational methods by cross-checking of input data, graphic display, and automatic selection of problem dependent parameters, e.g. mesh-spacings, etc.

(25) Development of new numerical methods applicable to computers with parallel processing.

The great emphasis put on theoretical analysis of methods is based on the following reason: The methods have reached a degree of sophistication which makes a good understanding of the mathematical properties necessary for the development of efficient and reliable improvements. A similar statement could be made for computational techniques on modern high speed computers.

The discussion of current problems in multidimensional reactor calculations has been restricted to static problems in this paper. In addition the attention has been focussed on neutron-physics calculations only. Thermal hydraulics calculations and stress analysis calculations have not been discussed. This omission is a serious drawback of the review-paper presented here. For example, the interplay between neutron physics and thermal hydraulics has a strong

computational relevance for some reactor types. In addition, the experts do realize today that the economy of the fuel cycle in large power reactors, i.e. a high fuel burnup rate, does depend very much on the close cooperation of the neutron physicist and the fuel and cladding specialist. An accurate prediction of the local power histories and of the stress analysis behavior for cladded fuel pins are the two major essentials here.

One should remember that a thorough investigation of steady state problems is usually the first step for treating time dependent, i.e. dynamics problems.

The accuracy requirements in dynamics calculations can be much higher, e.g. for the reactivities, than for steady state calculations. This point is demonstrated in a forthcoming paper by W.B. TERNEY and R. SRIVENKATESAN /131/ for the few group treatment of fast reactor transients.

The number of outstanding problems for multidimensional reactor calculations is indeed very impressive. But one should not forget that sizeable improvements are very hard to obtain at this advanced stage of methods development. On the other hand one should be aware that even small improvements, e.g. for the fuel cycle cost of reactors, could have a great economic incentive within a fast growing reactor industry.

8. Acknowledgements

The author would like to express his thanks to C.M. Kang, E.E. Lewis, M. Wagner, and Zb. Woznicki for making partly unpublished material available, for discussing several details of the methods, and for giving the permission to include selected results into this review paper. The author does also express his sincerest thanks to Mrs. J. Lott for typing this paper under time pressure with almost indefinite patience and great skill.

TABLE I

ESTIMATED POWER REACTOR BURNUP PHYSICS
ACCURACY FOR THERMAL REACTORS

(Extracted from the Conclusions of the IAEA Panel on
Reactor Burn-Up Physics, Vienna 1971)

Quantity	Predictive Accuracy in %			
	Capabilities (1971)		Target Values	
	LWR	GCR/HWR	LWR	GCR/HWR
Steady State Reactivity				
Initial k_{eff} (U fueled)	± 1	± 1	± 0.25-0.5	± 0.25-0.5
Initial k_{eff} (Pu fueled)	somewhat worse		± 0.25-0.5	± 0.25-0.5
Reactivity Lifetime	± 2-5	± 13	± 2-5	± 5
Steady State Power Distribution*				
Within a fuel pin	± 10-20		± 5	
Fuel pin relative to assembly	± 3- 5		± 2	
Axial, within an assembly	± 6-10		± 3-5	
Radial, between assemblies	± 3- 8		± 1-3	
Overall, pellet to average	± 8-13		± 3-5	
Fuel Burnup				
Peak pellet	± 5		± 3	
Fuel assembly	± 4		± 2	
Discharge batch	± 3		± 2	

*Best methods give ± 5 % accuracy remote from singularities, but up to a factor 2 worse than this near control rods, reflectors, etc.

TABLE - II. Uncertainties of LMFBR Physics Parameters*

(One Standard Deviation, in Percent)

Quantity	SNR 300			SNR 2000	
	1969 Capabilities	1972 Capabilities	1974 Targets	1972 Capabilities	1976 Targets
keff (2 % Average Burnup)	± 2	± 1	± 0.8	± 1.5	± 0.9
Peak to Average Core Power	± 5	± 3	± 1.5	± 3	± 2.5
Average Power in Blankets	—	± 12	± 9	± 20	± 9
Breeding Ratio	± 10	± 6	± 3.5	± 6	± 3
Control Rod Worth	± 11	± 10	± 5	± 15	± 6
Doppler Coefficient	± 15	± 10	± 10	± 15	± 10
Na-Void Effect	± 30	± 20	± 12	± 20	± 12

*) Extracted from: Küsters, H. et al. "Progress in Fast Reactor Physics in the Federal Republic of Germany", KFK-1632, (1973).

Wintzer, D. et al. "Unsicherheiten bei der Voraussage wichtiger neutronenphysikalischer Parameter des SNR 300 und großer Leistungsbrüter und Reduzierung dieser Unsicherheiten durch SNEAK-Experimente", To be presented at the KTG annual meeting in Karlsruhe, 1973.

TABLE - III. Uncertainties of HTR Physics Parameters and Cost Benefit from Improvements of the Predictive Accuracy of these Parameters

Uncertainties for HTR Parameters (One Standard Deviation)

Quantity	1969	November 1972	Target
Temperature Coefficient	$\pm$ 1 to 1.5 mN/°C	$\pm$ 0.7 mN/°C	$\pm$ 0.5 mN/°C
Maximum to Average of Axial Power Distribution	$\pm$ 10 %	$\pm$ 7 %	$\pm$ 3 to 5 %

Remark: $1\ mN = 10^{-5}\ \frac{\Delta k}{k}$

Cost Benefit from Improvements

Quantity	Improvement of Accuracy	Cost Benefit for 1000 MW(e) Reactor
Temperature Coefficient	From $\pm$ 1 mN/°C to $\pm$ 0.5 mN/°C	\$ 10^6
Maximum to Average of Axial Power Distribution	From $\pm$ 10 % to $\pm$ 5 %	\$ 5.10^5
Overall Formfactor	From $\pm$ 10 % to $\pm$ 5 %	\$ 10^6

Extracted from: Jonstone, I. and J. A. Scott: "Objectives for an HTR R&D Physics Programme", presented at Topical Meeting on Requirements and Status of the Prediction of Physics Parameters for Thermal and Fast Reactors, Jülich, Germany, 23-25 January, 1973.

TABLE IV

THEORY AND EXPERIENCE FOR COARSE MESH TECHNIQUES

PROBLEM TYPE		COARSE MESH TECHNIQUES	
		REBALANCING	GALERKIN
ONE GROUP	THEORY	COMPLETE	COMPLETE
	EXPERIENCE	GOOD	GOOD
DOWN SCATTERING NO GROUP COLLAPSING	THEORY	COMPLETE	COMPLETE
	EXPERIENCE	GOOD	GOOD
DOWN SCATTERING WITH GROUP COLLAPSING	THEORY	COMPLETE	NEG. EIGENVALUE POSSIBLE, BUT $A\underline{\phi}_a \geqq 0$ IS SUFFICIENT.
	EXPERIENCE	GOOD	PARTLY BAD
UP AND DOWN SCATTERING NO GROUP COLLAPSING	THEORY	COMPLETE	NEG. EIGENVALUE POSSIBLE, BUT $A\underline{\phi}_a \geqq 0$ IS SUFFICIENT.
	EXPERIENCE	GOOD	LIMITED
UP AND DOWN SCATTERING WITH GROUP COLLAPSING	THEORY	COMPLETE	NEG. EIGENVALUE POSSIBLE, BUT $A\underline{\phi}_a \geqq 0$ IS SUFFICIENT.
	EXPERIENCE	GOOD	LIMITED

TABLE V

THEORY AND NUMERICAL EXPERIENCE FOR BETTIS TYPE BLENDING METHODS

PROBLEM TYPE		BETTIS TYPE BLENDING	
		GALERKIN	ADJOINT
ONE GROUP	THEORY	LARGEST POSITIVE EIGENVALUE NEG. FLUX POSSIBLE	LARGEST POSITIVE EIGENVALUE NEG. FLUX POSSIBLE
	EXPERIENCE	GOOD	GOOD
DOWN SCATTERING NO GROUP COLLAPSING	THEORY	LARGEST POSITIVE EIGENVALUE ? NEG. FLUX POSSIBLE	NEG. EIGENVALUE POSSIBLE NEG. FLUX POSSIBLE
	EXPERIENCE	GOOD	GOOD
DOWN SCATTERING WITH GROUP COLLAPSING	THEORY	NEG. EIGENVALUE POSSIBLE NEG. FLUX POSSIBLE	NEG. EIGENVALUE POSSIBLE NEG. FLUX POSSIBLE
	EXPERIENCE	PARTLY BAD	BAD
UP AND DOWN SCATTERING NO GROUP COLLAPSING	THEORY	NEG. EIGENVALUE POSSIBLE NEG. FLUX POSSIBLE	NEG. EIGENVALUE POSSIBLE NEG. FLUX POSSIBLE
	EXPERIENCE	LIMITED	LIMITED
UP AND DOWN SCATTERING WITH GROUP COLLAPSING	THEORY	NEG. EIGENVALUE POSSIBLE NEG. FLUX POSSIBLE	NEG. EIGENVALUE POSSIBLE NEG. FLUX POSSIBLE
	EXPERIENCE	LIMITED	LIMITED

TABLE VI

POWER DENSITIES AND DIFFUSION LENGTHS FOR DIFFERENT REACTOR TYPES

REACTOR TYPE	DESCRIPTION	CORE AVERAGED POWER DENSITY $\left[\frac{\text{watt}}{\text{cm}^3}\right]$	CHARACTERISTIC DIFFUSION LENGTH [cm]
HTGR	GRAPHITE MODERATED, He COOLED REACTOR	7.0	12.0
BWR	BOILING LIGHT WATER REACTOR	50.0	2.2
PWR	PRESSURIZED LIGHT WATER REACTOR	75.0	1.8
GCFR	GAS (He) COOLED FAST BREEDER REACTOR	280.0	6.6
LMFBR	SODIUM COOLED FAST BREEDER REACTOR	530.0	5.0

TABLE VII

SPACE MESHPOINT REQUIREMENTS FOR DIFFERENT 3000 MW(t) REACTOR TYPES

REACTOR TYPE	VOLUME OF 3000 MW(t) REACTOR [m^3]	DIAMETER OF 3000 MW(t) REACTOR IN DIFFUSION LENGTH	NECESSARY NUMBER OF MESH POINTS (ONE PER DIFFUSION LENGTH)	
			2 DIMENSIONS	3 DIMENSIONS
HTGR	428.6	62.8	3 947	247 969
BWR	60.0	178.0	31 666	5 635 001
PWR	40.0	190.0	36 100	6 859 000
GCFR	10.7	33.4	1 115	37 253
LMFBR	5.7	35.6	1 270	45 270

TABLE VIII

GROUP-SPACE MESHPOINT REQUIREMENTS FOR DIFFERENT 3000 MW(t) REACTOR TYPES

REACTOR TYPE	NUMBER OF GROUPS (THERMAL GROUPS)	NECESSARY NUMBER OF GROUP-SPACE MESHPOINTS (ONE PER DIFFUSION LENGTH)		
		1 DIMENSION	2 DIMENSIONS	3 DIMENSIONS
HTGR	7 (4)	441	27 629	1 735 783
BWR	4 (1)	712	126 664	22 540 004
PWR	4 (1)	760	144 400	27 436 000
GCFR	10 (0)	330	11 150	372 530
LMFBR	10 (0)	360	12 700	452 700

TABLE IX

NECESSARY NUMBER OF OUTER ITERATIONS FOR 3000 MW(t) MODEL PROBLEMS

(AN ERROR REDUCTION BY A FACTOR 1000 HAS BEEN ASSUMED)

REACTOR TYPE	STRAIGHT SOURCE ITERATIONS	CHEBYSHEV ACCELERATED SOURCE ITERATIONS
HTGR	940	38
BWR	7 550	105
PWR	8 650	112
GCFR	278	20
LMFBR	311	21

TABLE X Asymptotic Convergence Rates for the Model Problem ($N \gg \pi$, $\bar{H} \gg \pi$, and $\bar{h} \ll 1$)

Iterative Method	Dimension	Convergence Rate
Point Jacobi	1	$\bar{h}^2/2$
	2	$\bar{h}^2/4$
	3	$\bar{h}^2/6$
Line Jacobi	1	∞
	2	$\bar{h}^2/2$
	3	$\bar{h}^2/4$
Point Gauss-Seidel	1	$\bar{h}^2$
	2	$\bar{h}^2/2$
	3	$\bar{h}^2/3$
Line Gauss-Seidel	1	∞
	2	$\bar{h}^2$
	3	$\bar{h}/2$
Point Overrelaxation	1	$2\bar{h}$
	2	$\sqrt{2}\,\bar{h}$
	3	$2\bar{h}/\sqrt{3}$
Line Overrelaxation	1	∞
	2	$2\bar{h}$
	3	$\sqrt{2}\,\bar{h}$

TABLE XI

TIME ESTIMATES FOR THE ITERATIVE SOLUTION OF DIFFERENCE EQUATIONS FOR VARIOUS 3000 MW(t) REACTORS

REACTOR TYPE	TIME ESTIMATES		
	ONE DIMENSION [SECONDS]	TWO DIMENSIONS [MINUTES]	THREE DIMENSIONS [HOURS]
HTGR	0.40	2.0	1.8
BWR	1.80	22.0	66.0
PWR	2.20	26.0	85.0
GCFR	0.16	0.4	0.2
LMFBR	0.2	0.4	0.2

TABLE XII

Results obtained by Z. WOŽNICKI [47] for VARGA's Test Example [45, Appendix B]

Method	Without Overrelaxation (ω=1)	Overrelaxation Method			
	Number of Iterations	Number of Iterations	ω	Arithmetical Operations per Meshpoint and Iteration	
				Additions	Multiplications
Point SOR	5010	139	1.9177	6	6
EWA-II Single SOR	564	404	1.17	7	8
EWA-II Double SOR	564	380	1.09	9	10
AGA-II-A Single SOR	371	36	1.485	8	9
AGA-II-B Single SOR	189	100	1.23	11	10
AGA-II-C Single SOR	305	32	1.356	12	13
AGA-II-D Single SOR	120	21	1.296	15	14

TABLE XIII

Numbers of Iterations Required for STONE's Method and Comparison with the Alternating Direction Iteration Method

Method	Numbers of Iterations Required			
	Problem 1	Problem 2	Problem 3	Problem 4
Strongly Implicit Procedure (SIP)	22	16	30	34
Alternating Direction Iteration (ADI)	16	50	80	127
Ratio ADI/SIP	0.7	3.1	2.6	3.7

TABLE XIV

Eigenvalues 1/k for Two-Dimensional, Two Group, Two Region Reactor Test Problem

Δx=Δy	Hermite FEM				FDM
	m=1	m=2			
		A	B	C	
L/ 2	1.0802150	1.1157980	1.1081760	1.1082321	1.0783013
L/ 4	1.0962251	1.1153879	1.1134294	1.1134916	1.0797120
L/ 6	1.1040456	1.1149521	1.1140668	1.1140943	1.0895577
L/20	-	-	-	-	1.1105031
	Order of Convergence				
	1.4	0.95	3.2	3.2	0.8

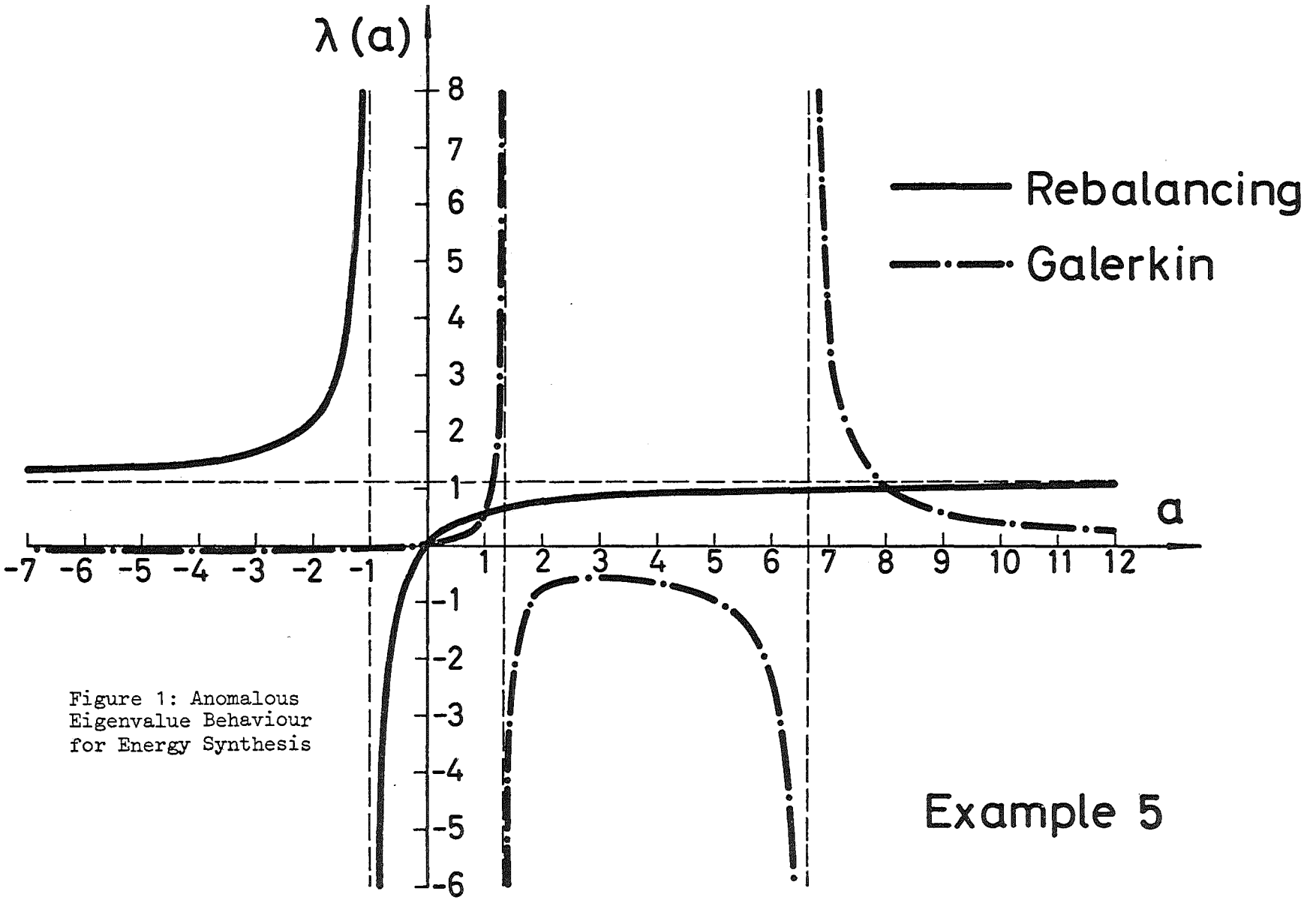
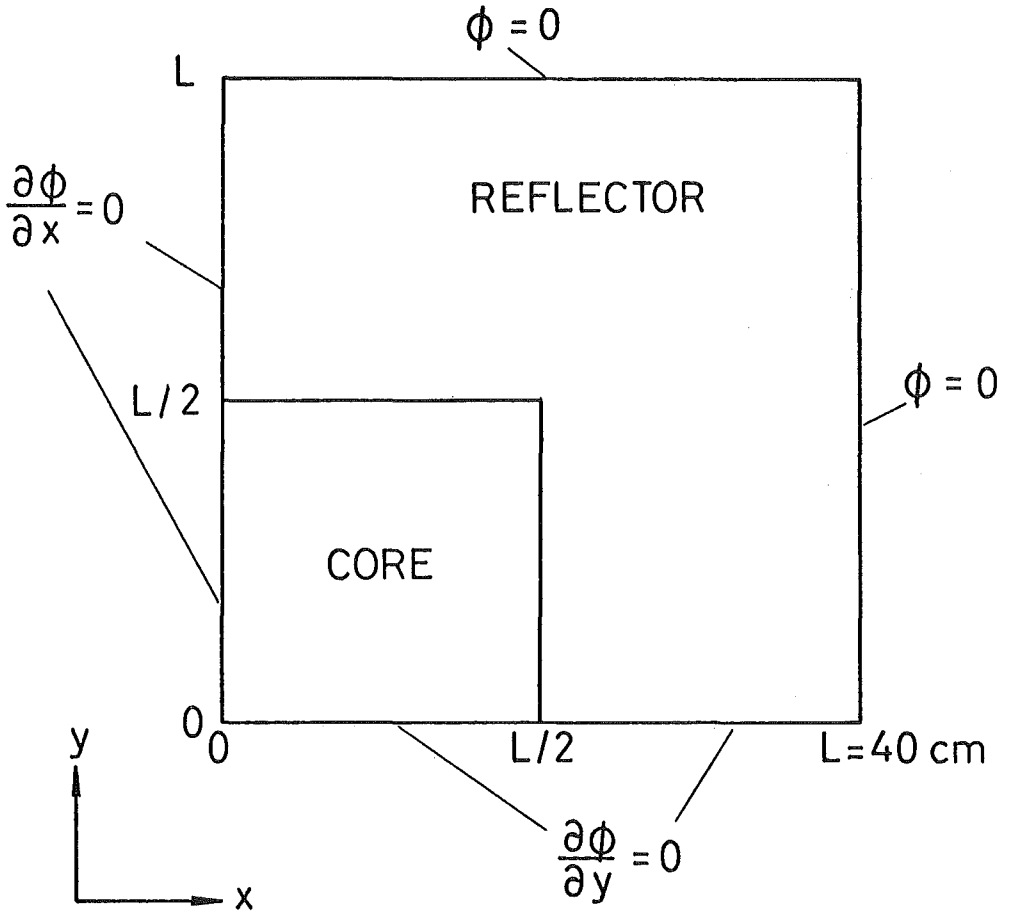


Figure 1: Anomalous Eigenvalue Behaviour for Energy Synthesis

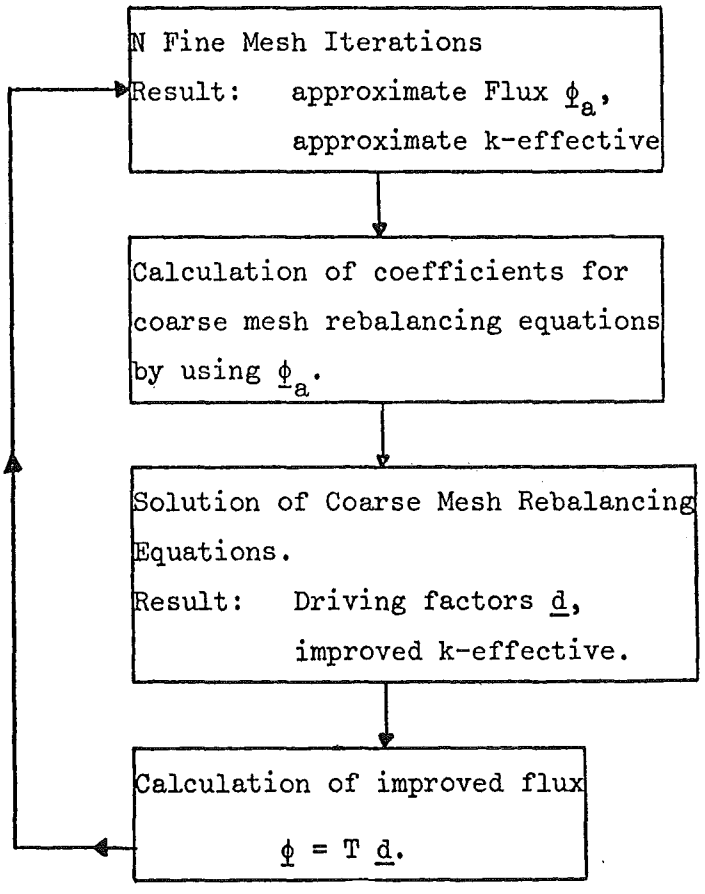
Figure 2
Reactor Configuration and
Nuclear Parameters

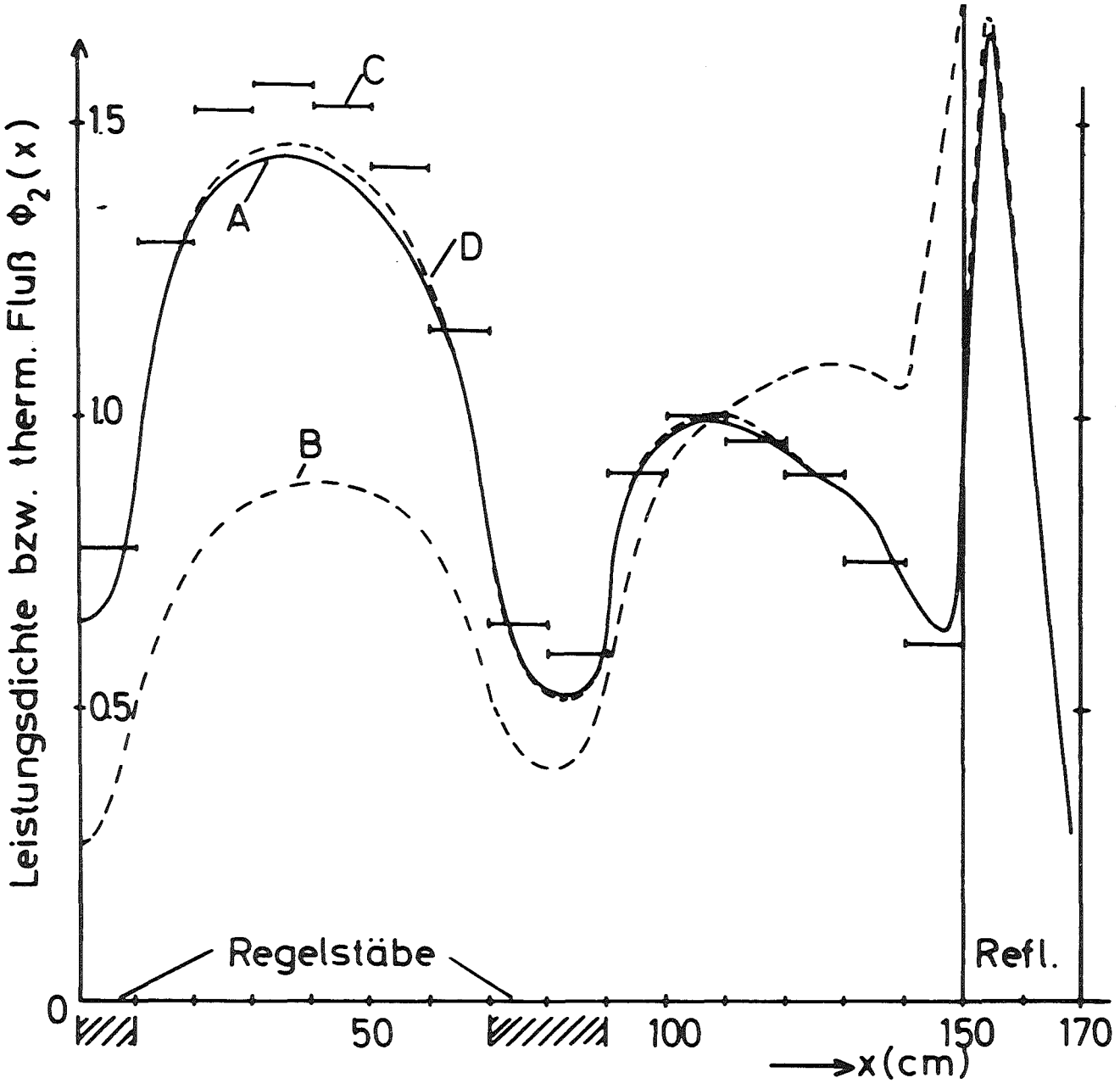


PARAMETER	CORE	REFLECTOR
D^1	1.5	1.2
D^2	0.4	0.15
Σ_R^1	0.0623	0.101
Σ_R^2	0.2	0.02
$\Sigma_S^{1\rightarrow 2}$	0.06	0.1
$\Sigma_S^{2\rightarrow 1}$	0	0
$\nu\Sigma_f^1$	0	0
$\nu\Sigma_f^2$	0.218	0
χ^1	1.0	1.0
χ^2	0	0

Figure 3

Convergence Improvement of Fine Mesh Iterative Solution Methods by Coarse Mesh Rebalancing Techniques





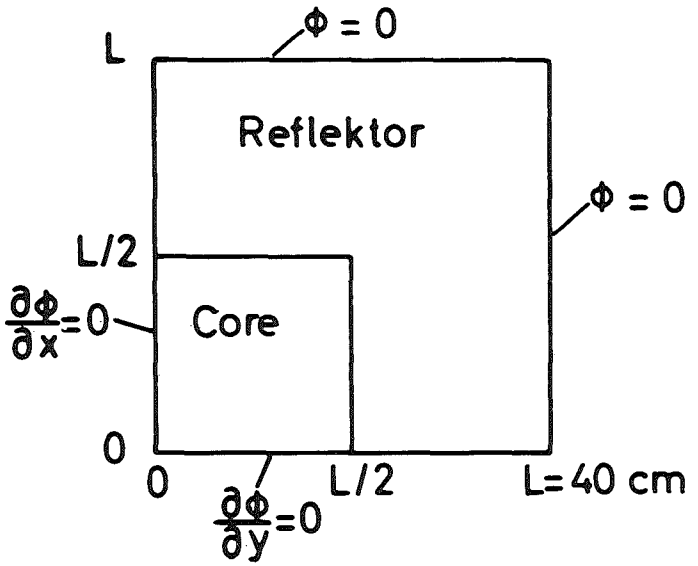
	METHODE	h(cm)
A	FDM	~2
B	"	10
C	MEDIUM	10
D	Nodale Synth.	10/1

	k_{eff}	CP-Sek.
A	1.02998	1000
B	1.03285	61
C	1.02922	5.6
D	1.02989	16.1

M.R. Wagner , paper 109
Reaktortagung
Karlsruhe , April 1973

Figure 4

2D IAEA Benchmark Problem , Radiale Traverse (y = 5)

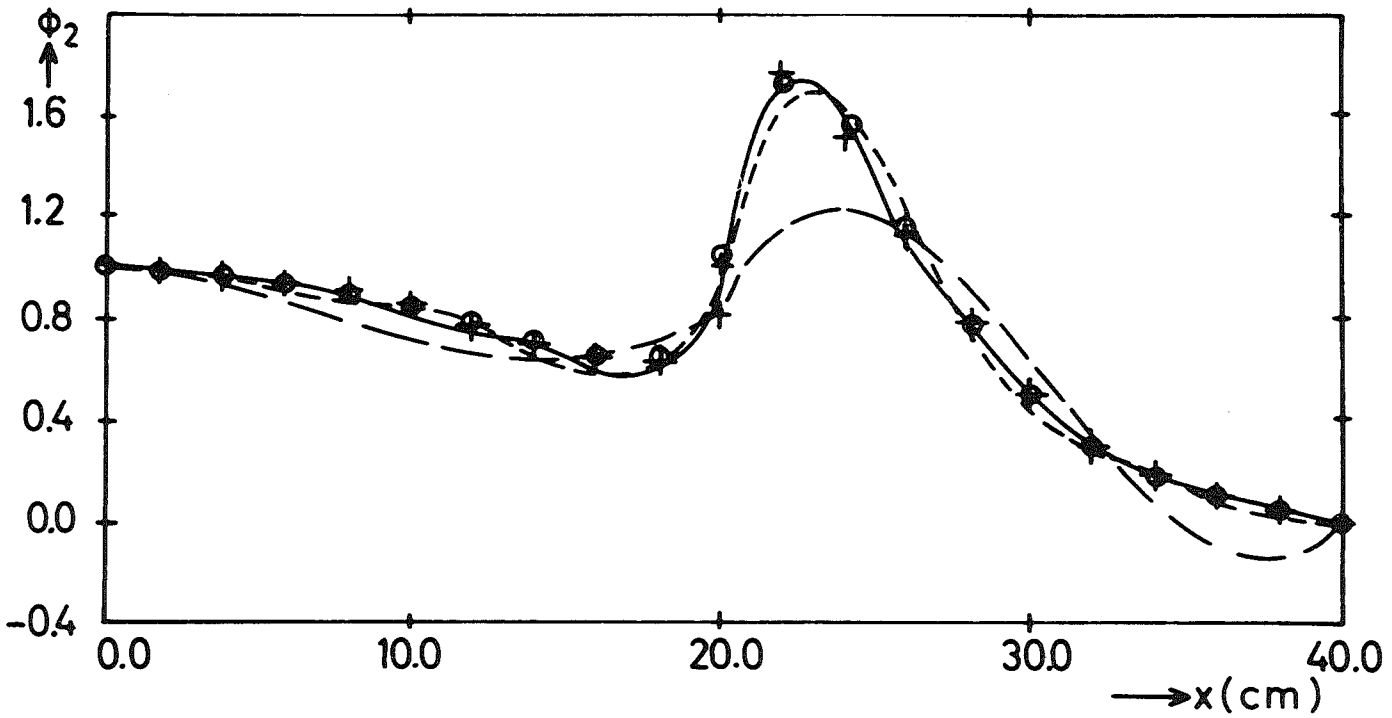


× Nodale Synthese,
M.R. Wagner, KWU Erlangen,
RT 11

Reziproker Eigenwert $1/\lambda$

Δx	FDM	FEM Kang, Set C	Nodale Synth.×	CP-Sek.
L / 2	1.078310		1.115852	0.30
L / 4	1.079712	1.113492	1.114769	1.5
L / 6	1.089558	1.114094		
L / 8			1.114159	3.4
L / 20	1.110503		1.114000	10.4

Figure 5 Kangs 2D Eigenwertproblem



FEM : —— —— Δx = L / 2 Nodale Synthese + Δx = L / 2
------ Δx = L / 3
——— Δx = L / 6 FDM o Δx = L / 20

FEM : Kang, bikubische Hermitesche Polynome , Set C
Fig. 4.5 , MIT-Thesis , 30. Nov. 1971

Figure 6 Kangs 2D Eigenwertproblem
Traverse y = 0 , Thermischer Neutronenfluß

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