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Review of Flux Synthesis Methods

by

Raymond E. Alcouffe

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REVIEW OF FLUX SYNTHESIS METHODS

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ABSTRACT

Flux synthesis techniques are reviewed with respect to the types of methods currently employed to obtain the detailed neutron flux from lower-order calculations. The areas considered are reactor statics, including the diffusion and transport equations, and reactor dynamics. Recommendations for the implementation and further development of synthesis methods are also included.

I. INTRODUCTION

The so-called synthesis method of numerical reactor analysis is an outgrowth of the idea of using a combination of lower-order solutions of the system of interest to yield a representation of a higher-order solution to the same system. An example is to perform one-dimensional diffusion calculations on a two-dimensional system and combine this information to yield the two-dimensional flux. To accomplish this, a method for the combination or synthesis must be devised. The most concise methods are based upon the indirect methods of the calculus of variations or, more generally, upon the weighted residual method.¹⁻⁴ In the latter method, the original problem is reformulated in a functional representation which is a weighted integral over all independent variables in the equations. For example, in a generalized operator notation, the governing equations of the system may be written as

$$H(x) \phi(x) = S(x), \quad (1)$$

where

$x \in \{x_1\}$ represents all independent variables,

$\phi(x)$ is some unknown vector function of x ,

$H(x)$ is a known linear operator, and

$S(x)$ is an inhomogeneous vector function.

A functional representation would be

$$\int dx W(x) [H(x) \phi(x) - S(x)] = 0, \quad (2)$$

where $W(x)$ is some arbitrary weighting function, and $W(x) \neq 0$ for the entire range of x . Equation (2) is a more convenient form than Eq. (1) from which to derive approximate equations for the solution $\phi(x)$. A variety of methods result from the choice of the weighting function in order to give an estimate of some integral parameter of the system with low-order sensitivity to errors in the estimate.

This report concentrates on methods that emphasize the synthesis approach for obtaining the detailed higher-order solution to the problem of interest. If one desires an accurate approximation to the function $\phi(x)$ for all $x \in \{x_1\}$ and not just some integral of $\phi(x)$ over x , the procedure is to assume a form for the solution $\phi(x)$ which contains both known and unknown functions of some, but not all, of the variables $x \in \{x_1\}$. This allows some of the integrals of Eq. (2) to be performed over the known functions. The resulting functional is termed the reduced functional, from which equations for the unknown functions may be determined. These equations are deduced from the reduced functional by extremizing with respect to the weighting function, as in the calculus of variations or by minimizing the integral residual between the approximate and true solutions.² Mathematically, this process may be visualized as follows.

1. Choose a representation of the solution

$$\phi(x) = \sum_k \psi_k(x_1) a_k(x_2), \quad (3)$$

where

x_1 is some subset of x ,

x_2 is another subset of x , with x_1 plus x_2 containing all of the $\{x\}$,

$\psi_k(x_1)$ is a known function of x_1 , and

$a_k(x_2)$ is an unknown function of x_2 .

2. Likewise, represent the weighting function

$$W(x) = \sum_k \chi_k(x_1) b_k(x_2). \quad (4)$$

3. Substitute into Eq. (2), yielding

$$\int dx_1 \int dx_2 \sum_k \sum_{k'} \chi_k(x_1) b_{k'}(x_2) \cdot \left[H(x) \psi_{k'}(x_1) \cdot a_k(x_2) - S(x) \right] = 0. \quad (5)$$

4. Derive the reduced functional

$$\int dx_2 \sum_k \sum_{k'} b_{k'}(x_2) [G_{kk'}(x_2) a_k(x_2) - S_k(x_2)] = 0, \quad (6)$$

where

$$G_{kk'}(x_2) = \int dx_1 \chi_k(x_1) H(x) \psi_{k'}(x_1)$$

$$S_k(x_2) = \int dx_1 \chi_k(x_1) S(x).$$

5. Determine the approximation equation for the a_k by extremizing with respect to $b_{k'}(x_2)$ yielding

$$\sum_{k'} G_{kk'}(x_2) a_{k'}(x_2) = S_k(x_2) \quad (7)$$

for all k . Equation (7) may be viewed as an equation that selects the quantities a_k consistent with the information given by the quantities ψ_k and by Eq. (1) to yield a valid representation for the solution $\phi(x)$ by the prescription of Eq. (3).

This procedure can yield an enormous variety of approximations, depending upon the choice of the functions ψ and the weighting χ . The art of this approximation method is in the choice of these functions to yield an accurate approximate solution and to minimize computational effort. For example, the choice of the weighting function may yield approximations that are, or resemble, finite difference

equations or, on the other hand, modal equations. That is, the weighting function determines the physical form of the approximating equation. The choice of the ψ 's reflects the amount of information about the solution available from auxiliary calculations or other independent sources. The main weakness of the synthesis method is that it has not yet been proven mathematically that, given some particular choice of ψ 's, the synthesis procedure will give a good estimate of the function ϕ . The literature cites many attempts to verify empirically that it is possible to obtain a good representation of ϕ , given a class of ψ 's. Consequently, at this stage of development, experience with the synthesis method is required to yield valid approximations.

Another variable of the synthesis method is the choice of the best way to partition the independent variables. This is a crucial point and is reflected in this report in the way the synthesis method is applied to the equations of reactor physics. The following three sections cover (1) diffusion statics concerned with the partitioning of space and energy variables, (2) kinetics concerned with handling time dependence and hence the partitioning between time and space and/or energy variables, and (3) transport statics concerned with space-angle-energy partitioning. The main formulations of the synthesis method are outlined in each section for the particular aspect being examined, including the type of weighting and trial functions used and their apparent value and limitations. Section V summarizes developments at other laboratories in applying synthesis methods to fast breeder research. Recommendations for developments still necessary for the fast breeder programs are given in Sec. VI. The list of references, extracted from a large body of literature, covers what is necessary for this report. A more extensive bibliography is available (Ref. 5).

II. SYNTHESIS METHODS FOR THE STATIC NEUTRON DIFFUSION EQUATION

The flux synthesis method has been applied most extensively to the neutron diffusion equation. These applications may be broken down into two areas: (1) the multigroup diffusion equation whose flux is synthesized by utilizing trial functions composed of solutions to multigroup diffusion equations of fewer

spatial dimensions than the problem to be solved, and (2) the synthesizing of a multigroup, multidimensional solution from trial functions that are separable in the space and energy variables. The first method is by far the most successful and has been widely used in thermal reactor analysis. The second method has not been successful for any but the most simple applications in which reasonable trial spectra are easily computed for each region of the system. The main drawback of the second method is that accurate trial spectra are not easily obtained for realistic fast reactor configurations, which, therefore, obviates much of the possible utility of the method.

A. Synthesis Involving the Construction of a Multidimensional Flux from Lower-Dimensional Calculations

Synthesis methods by which lower space-dimensional calculations are used to construct an estimate of the multidimensional flux have been extensively researched for the few-group form of the diffusion equation.⁶⁻¹⁰ The applications have been successful in going from one-dimensional trial functions to two-dimensional results, and also from two to three dimensions. When trial solutions are properly computed and there are enough solutions to account for the variation in data in the synthesized dimension, the resultant synthesis solution is very accurate. This method is well suited for multidimensional computations in which the synthesized direction has very few regions, thus requiring few calculations to obtain trial functions. An efficient way to reduce the amount of coupling that results from the modal synthesis is to use a functional admitting discontinuous trial functions. In the simplest case, the resulting equations resemble matrix, one-dimensional, finite difference equations with coupling only between adjacent regions. This is a very effective use of the flux synthesis method.¹¹⁻¹⁶

To perform three-dimensional perturbation or survey-type calculations, this procedure may be carried further by partitioning the two-dimensional trial function regions into two-dimensional subregions.¹³ At the boundaries of each subregion, the trial function is allowed to be discontinuous. This additional degree of freedom makes it possible to perturb certain regions from their reference condition (that is, the state of the system for which

the trial functions were computed) and yet compute the flux for the perturbed case using the reference trial functions.

B. Synthesis of Multigroup Flux from Separable Flux (Energy-Space) Trial Functions¹⁷⁻²¹

The energy-space separable method, called the overlapping-group method, consists of constructing trial functions that are linear combinations of space and energy functions. Reduced equations are then obtained either for the space or energy functions. This method has been shown to be reasonably accurate when accurate trial spectra can be obtained,¹⁷⁻¹⁹ usually when adjacent regions differ little in their composition and are large enough to allow an asymptotic spectrum. In this case, there is a decoupling of the energy and space variables in most of the spatial region. The transient region may therefore be reasonably approximated by a linear combination of spectra from the two regions. In the more general case of two greatly different regions, this is not true. First, the flux may not be reasonably represented by a linear combination of two space and energy functions where the energy functions are obtained from auxiliary calculations. Second, because the regions are greatly different, the dominant spectrum in each, if there is one, may not be the asymptotic spectrum for each composition. It is thus difficult to compute good trial spectra. The problem is alleviated if one of the regions dominates in the sense that it is the source of most of the neutrons. In this case, a spectrum for the second region may be computed by using the leakage spectrum of the dominant spectrum region as a source.¹⁹ Whether or not these conditions exist in a typical fast breeder design has not yet been definitively answered.

At present, the application of the overlapping-group method in fast reactor configurations has been limited. One promising use is cell calculations in the resonance region. However, before the method can be used routinely, it must be demonstrated that the results are more accurate than heterogeneous-cell calculations based upon zero-dimensional calculations and conventional multigroup computations based upon a few groups.

III. REACTOR KINETICS

The synthesis method has been applied to reactor kinetics in a variety of ways, particularly to

the time-dependent neutron diffusion equation. There are two main formulations which may be broken down roughly into two categories: (1) modal synthesis where a linear combination of computed global shapes is used to approximate the flux at any time, and (2) nodal synthesis where the reactor system is visualized as consisting of discrete regions coupled to one another by computed neutron fluxes. Both methods may be derived from the same functional method. However, the final equations are sufficiently different to merit separate consideration.

A. Modal Synthesis Applied to Multidimensional, Multigroup Diffusion Equation

1. Space-Time Synthesis Where the Unknown Quantities Are Functions of Time Only.²²⁻³² This formulation is accurate for problems in which the spatial shapes may be computed *a priori*, as in programmed rod motion. The situation is less certain when delayed neutrons are involved. Complications arise in the case of feedback terms, and the analysis may not be very accurate when feedback effects are large. Very few analyses using precomputed shapes have been attempted on feedback neutronics, and the value of the method remains to be demonstrated in this case.

2. Space-Time Synthesis Where the Unknown Quantities are Functions of Both Space and Time.³³⁻³⁵ This formulation is useful in going from two-dimensional trial functions to three-dimensional, time-dependent problems, particularly when one of the space dimensions is relatively homogeneous. In this case, few two-dimensional trial functions are needed. A necessary concept for this method, which aids in the formulation of the problem and also limits the trial function coupling in the one spatial dimension, is the use of discontinuous trial functions.

Because the method obviates the necessity of three-dimensional, multigroup calculations for the trial functions, it is preferred over method (1) above, even though it may be less accurate. The procedure should work for a multigroup problem, although few results are applicable to fast reactors.

B. Synthesis Which Utilizes Trial Functions Computed During the Course of the Transient^{32,37-39}

When the effects of delayed neutrons and temperature feedback need to be considered, it is not practical to use precomputed spatial shapes because, with feedback, the problem is nonlinear and,

therefore, it is not possible to take into account temperature effects upon the flux *a priori*. It is convenient, then, to account for these changes by computing trial functions during the course of the transient to allow trial-function information to be supplied from the state of the system at that time. A synthesis method may then be formulated that allows trial functions to be computed from the dynamic state of the system, allowing for the resultant discontinuities in time. One such method is the quasi-static method³⁰ where only one trial function is used for each large time interval. Methods have been formulated and used for two or three trial functions, one of which accounts for programmed motion of control rods or fuel and the others handle feedback effects.³⁷ This is the most promising use of modal methods for handling feedback problems.

This idea may be used to extend either of the above methods to practical multidimensional kinetics problems involving both delayed neutrons and feedback effects.

C. Nodal Synthesis Applied to Time-Dependent Multidimensional, Multigroup Diffusion Theory

1. Multichannel Methods.³⁴⁻³⁶ The multichannel methods are developed by partitioning the reactor system into a number of contiguous regions. Trial functions are written for each region and a functional is developed to allow for discontinuities in the trial functions at the boundaries of the regions. Normally, these trial functions take the form of precomputed shapes that are blended, as in the case of modal synthesis. However, an extra degree of freedom is given by allowing the discontinuous forms. In this case, the final synthesized solution is not as sensitive to the trial functions as the continuous method, and, hence, trial solutions may not have to be computed for every dynamic analysis. This method may also be effectively used in conjunction with quasi-static methods to synthesize transients with feedback effects.

2. Nodal Synthesis Based on Finite Difference Methods.⁴⁰

A generalization of both the multichannel method and the straight finite difference techniques efficiently uses a trial solution without the need for a discontinuous functional. It is possible to use this nodal synthesis based on finite difference methods, together with the quasi-static method to generate a synthesized solution to the problem.

D. Formulation for Other Problems

The synthesis method for neutron kinetics has been formulated and applied mainly to the diffusion equation. Time synthesis formulations for the transport equation exist, but their application or necessity has not yet been investigated. It appears, however, that these techniques would be expensive in computer utilization to apply to fast reactor analysis because there is as yet no space-time formulation based upon the transport equation. Another area that has been investigated very little is the energy-time synthesis where the main dynamic effects are expected to come from spectral changes rather than from spatial changes. This concept would be more applicable to small, fast systems rather than to the large breeders and would be useful for kinetics analysis of the small systems.

IV. TRANSPORT SYNTHESIS⁴¹⁻⁴⁹

Synthesis methods applied to the neutron transport equation have been mainly an attempt to represent the angular flux as a linear combination of space-angle separable terms. Most of such attempts have been unsuccessful because of the inability to estimate angular or spatial shapes for any but simple geometries. Useful applications have been made in deriving finite difference equations for space-angle systems that contain both P_n - and S_n -type trial solutions.⁴⁷ A method analogous to the diffusion equation that utilizes one-dimensional calculations to yield accurate two-dimensional results for the flux has yet to be developed. This problem is difficult because of the number of independent variables involved.

A. Modal Space-Angle Synthesis

In modal space-angle synthesis, the angular flux is represented as a trial function consisting of a linear combination of space functions and angle functions.^{43,45,46} In one case, the angular functions are estimated and P_n -type equations are derived for the space functions. In the alternative case, the space functions are estimated and integral equations are derived for the angular functions. The main difficulty is in choosing accurate trial functions for either dimension to accurately represent the flux by the linear expansion, as in simple cases where there is some rationale for choosing angular functions. However, when the situation is complicated by adding regions in which the

angular behavior is not easily predicted, the method probably does no better than the unbiased P_n , and could do worse.

B. Spatial Flux Synthesis

The intent of spatial flux synthesis is to synthesize the multidimensional flux from lower-dimensional transport calculations by (1) deriving a one-dimensional transport equation based upon one-dimensional transport calculations in the other dimension to produce a two-dimensional angular flux, or (2) deriving diffusion-type equations that utilize transport information to determine the parameters of the equation. The first method is the most general and is likely to lead to the most accurate results for an arbitrary, multidimensional transport calculation. However, the method is difficult to formulate consistently because of the angle-space coupling in each dimension. It is also difficult to solve the reduced equations when the problem contains many spatial regions.

The second method is attractive because of the simplicity of the final form of the synthesis equations and because it can be made compatible with existing diffusion codes.^{44,48} However, the accuracy of the technique has not been thoroughly investigated so that its usefulness cannot be assessed.

Another variation of the second method makes use of transport trial functions of the same spatial dimensionality as the synthesizing diffusion equation.⁴⁹ That is, a diffusion equation is derived as the result of "angle collapsing" the transport equation by using a reference transport flux calculation. Its usefulness is in studying perturbations about a reference system while taking into account scalar flux and current perturbations. Consequently, the method yields accurate results beyond those possible with conventional perturbation theory.

The above method is advantageous only for perturbation-type studies because it requires trial functions that have as many space dimensions as the problem to be solved. This method can theoretically be made useful for general application by utilizing lower dimension trial functions. For example, one-dimensional calculations can be made on the system in both dimensions, and the results can be combined to form two-dimensional trial functions for the two-dimensional diffusion equation. This method has

yet to be tested. (An example of this with no trial function is given in Ref. 47.)

V. DEVELOPMENTS UNDER DIVISION OF REACTOR DEVELOPMENT AND TECHNOLOGY PROGRAMS

Synthesis methods are currently being developed and implemented under the Division of Reactor Development and Technology Programs at various installations. The main emphasis is to generate and assess methods and codes applicable to fast breeder analysis and design. The following is a brief synopsis of the efforts at each installation.

A. Pacific Northwest Laboratory

A code is being developed to synthesize the three-dimensional, multigroup diffusion flux from two-dimensional trial functions. The synthesis code is RSYN and uses ZDB to generate the trial functions. As such, it is limited to slowing-down problems and is capable of yielding X-Y-Z, R- θ -Z, and hexagonal-Z fluxes, where the synthesis is performed in the Z direction. The code does not presently employ discontinuous trial functions; it is still being tested and documented.

B. Brookhaven National Laboratory

The effort at the Brookhaven National Laboratory is mainly in developing techniques of space-energy synthesis¹⁸ in which one-dimensional transport S_n calculations perform the spatial computation. The energy trial spectra are generated in several ways to search for a reliable and efficient method to obtain accurate trial spectra to produce accurate synthesis results. This effort was discontinued on July 1, 1970.

C. Oak Ridge National Laboratory

The synthesis work at the Oak Ridge National Laboratory is in developing a two-dimensional transport synthesis that uses one-dimensional S_n calculations in one spatial direction to formulate, in general, coupled S_n equations in the other direction. This technique eliminates one of the spatial variables in the synthesis and retains the angle. This is a variation of the space-angle synthesis where the known spatial modes come from the spatial part of the S_n calculation. An experimental code to perform the synthesis has been developed and test cases have been run that demonstrate the accuracy and application of the technique.

D. General Electric - Sunnyvale, California

The synthesis effort at General Electric, Sunnyvale, California, is to develop and use the two-dimensional synthesis code BISYN.⁵⁰ The code synthesizes one-dimensional, multigroup diffusion calculations on the system to produce two-dimensional fluxes. The technique assumes separability in each dimension in each region of the system with no coupling between regions except through the synthesis equations. This procedure applied to fast breeders has been found satisfactory for all but final design calculations.

E. Argonne National Laboratory

The synthesis work at the Argonne National Laboratory is mainly in two areas: space-time kinetics and diffusion statics.

1. Kinetics. In order to implement synthesis methods for time-dependent problems, effort has been directed toward perfecting the quasi-static method for solving space-energy-dependent kinetics.³⁰ The quasi-static method can be viewed as a synthesis method in which one trial function is used for a large time step and is computed from the state of the system at the beginning of that time step. This trial or shape function may itself be computed from the static synthesis methods mentioned in Sec. II, although this has not been employed at present. A code has been developed for one-dimensional, multigroup diffusion kinetics with feedback and delayed neutrons (QX1). A similar code is being developed for two-dimensional problems.

A kinetics synthesis has also been developed that yields space-time-dependent equations by using separable trial functions in energy and space-time. This is analogous to the overlapping-group method except that the time dependence is also considered.

2. Statics. The effort in static synthesis is directed toward the development of a code to synthesize two-dimensional multigroup diffusion fluxes from one-dimensional calculations. The synthesis technique involves the use of discontinuous trial functions in the spatial direction being synthesized and requires coupling between adjacent regions only. The code is presently operational and will be documented soon.

Another use of the synthesis method is in the collapse of energy-group cross sections for a medium of variable composition. Spectrum calculations are performed for the extreme compositions, and the spectrum for an intermediate composition is synthesized by using the previous spectra as trial functions. Approximate group constants are computed from the synthesized spectrum.

F. Los Alamos Scientific Laboratory

The main effort at the Los Alamos Scientific Laboratory in the development of synthesis methods is formulation and use of S_n transport synthesis, whereby one-dimensional transport calculations can be used to give two-dimensional transport results. The aim is to formulate a generalized two-dimensional S_2 equation that utilizes trial function information. Two-dimensional trial functions are then formulated from one-dimensional calculations and are synthesized by the two-dimensional S_2 equation. Two-dimensional S_n trial functions can also be used to compute the flux resulting from perturbations on a reference system. This aspect of the synthesis has been used to calculate perturbation of some simple systems and found to work satisfactorily. A code is presently being developed to accomplish the synthesis.

VI. RECOMMENDATIONS

Because the main testing of the synthesis method has been on thermal systems, there is abundant experience in the synthesis of the spatial flux. The application to fast reactors has been minimal, especially in the area of spectral effects important to fast systems. However, it appears that multigroup spatial synthesis will be successful based upon knowledge thus far obtained. Certain aspects of fast reactor kinetics can be readily handled by this method, but application of synthesis to the transport equation and to the space-energy problem, both of which are important for fast breeder analysis, has either been not particularly successful or is nonexistent. On the whole, the synthesis method is very attractive in that it makes effective use of the information available from lower-order calculations to yield an estimate of the solution to a higher-order system. This is helpful in that it is possible to use the computer economically without sacrificing accuracy. The development of these methods should continue and

greater effort should be put into producing codes to gain more experience in using the synthesis techniques.

To make the synthesis method more applicable to fast breeder analysis, the following recommendations are made.

1. Multigroup flux synthesis. An experimental multigroup diffusion synthesis code that incorporates all available synthesis techniques is needed. This code would then allow the assessment of the accuracy and desirability of these techniques to perform fast reactor calculations. The code being developed at ANL comes the closest to meeting this need; however, it lacks the ability to do a multi-channel analysis. It was pointed out in Sec. II.A that this extra degree of freedom may be desirable when performing survey-type calculations.

2. Overlapping-group method (space-energy synthesis). The overlapping-group method should be useful in fast reactor analysis where spectral effects call for detailed computations with many groups (>100) and with spatial effects. It has been shown that, if the trial spectra used are a good representation of the true spectra in each spatial region, the method yields accurate flux results. This technique needs further development in the generation of trial spectra for realistic fast breeder configurations. Also, there is a need to show that the results are applicable when more than one spatial dimension is used.

3. Kinetics. The chief requirement in kinetics is to develop a code that incorporates the useful aspects of the synthesis method. The code should be able to demonstrate that spectral effects can be handled accurately and that delayed neutron and feedback effects may also be effectively treated. This has been demonstrated by using the quasi-static method, but this method, at its current stage, is limited in that detailed trial functions need to be computed each time the system's spatial or spectral configuration changes significantly. This can be expensive for multidimensional and/or transport computations. The code should therefore build on this type of method with the following additional characteristics.

- a. Space-time synthesis in which only two-dimensional trial functions are required for a three-dimensional calculation with synthesis in the other dimension and time.

- b. Allowance for a nodal approach in the space dimensions utilizing either the discontinuous trial function approach or the generalized finite difference method. This yields a greater degree of freedom and helps to reduce the number of trial function calculations during the transient.

4. Transport synthesis. The effort in applying the synthesis method to the transport equation has yet to produce a practical method for space synthesis. Such a method is needed for fast reactor analysis where a multigroup treatment is required because conventional multidimensional transport codes are expensive to use. Because transport synthesis is the weakest area of all synthesis applications, it appears that most of the synthesis development work should be concentrated in this area.

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