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Abstract

This project is directed toward development of numerical methods suitable for the computer solution of problems in reactor dynamics and safety. Specific areas of research include methods of integration of the time-dependent diffusion equations by finite difference and finite element methods; representation of reactor properties by various homogenization procedures; application of synthesis methods; and development of response matrix techniques.

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I. INTRODUCTION

This report is a summary of research carried out under contract AT(11-1)-2262 during fiscal year 1975. The contract is for research in numerical methods for the analysis of time-dependent reactor dynamics. Work is centered upon developing methods for the effective and efficient computer simulation of reactor dynamics problems.

Our principal efforts can be divided into areas of:

1. numerical solution of time-dependent problems by finite difference and finite element methods;
2. application of the finite element method;
3. synthesis and similar methods; and
4. other methods.

Section 2 following is a review of work on finite difference and finite element time-dependent problems. Section 3 contains a discussion of the finite element work to date for multidimensional static problems. Section 4 is devoted to a discussion of synthesis methods, and section 5 is given to other methods.

2. METHODS FOR TIME-DEPENDENT PROBLEMS

2.1 The Checkerboard Alternating Direction Method

If a spatial finite difference approximation is imposed on the time dependent group diffusion equations, the resultant set of time-dependent algebraic equations may be written

$$\frac{\partial}{\partial t}[\phi] = [A][\phi] \quad (1)$$

where $[\phi]$ is the column vector of group fluxes and delayed precursor concentrations for all mesh cubes throughout the reactor.

Since solution of the spatial part of such finite difference representations (i.e., inversion of $[A]$) is very time-consuming, the investigation of methods for increasing the time interval between spatial solutions provides a potentially fruitful approach to reducing overall computing times for transient calculations.

One such method that appears to be attractive is a two-time-level scheme described - but not tested - by Werner several years ago⁽¹⁾.

During the past year we have studied this method, which we call the "checkerboard method". We were able to show that it was an alternating direction scheme involving a different splitting of the matrix $[A]$ than any of those examined by Reed⁽²⁾ or Ferguson⁽³⁾.

We then found it was a special case of a class known as "Hopscotch Methods" and investigated extensively (although not for reactor problems) by Gourlay⁽⁴⁾. Using Gourlay's mathematical approach we have been able to prove that the scheme is unconditionally stable. Moreover it is accurate through order $(\Delta t)^2$ in the time-step size.

A two-dimensional example in XY geometry will suffice to show the basic idea of the checkerboard method. We begin with the group diffusion equations and partition the XY plane into spatial mesh rectangles, deriving time-dependent finite difference equations of

the form (1) in the usual manner. The XY mesh layout is then itself partitioned like the red and black squares of a checkerboard such that a given mesh rectangle belonging to one class has, as its four nearest neighbors, mesh rectangles belonging to the other class. The solution of the time-dependent difference equations for a time step then proceeds in two half-steps. During the first half-step, of size $\Delta/2$, flux values in the black squares are advanced in time explicitly and those in red squares are advanced "implicitly". We write "implicitly" in quotes since the fluxes for the four adjacent black squares coupled to the flux of a given red square (which would be solved simultaneously with the flux in the central red square at time $t + \frac{1}{2}\Delta$ in a truly implicit procedure) are instead represented by the values just computed at $t + \frac{1}{2}\Delta$ through the initial explicit advancement of the black fluxes. Thus, mathematically, the advancement of the red fluxes is only superficially implicit. From the numerical point of view the matrices inverted are (for G groups) $G \times G$ block diagonal (just as in the explicit advancement) rather than 5-stripe block $G \times G$ as in a truly implicit inversion. The same procedure is carried out during the second half-step, except that the fluxes in the red squares are advanced first explicitly and then those in the black squares are advanced "implicitly".

Since the checkerboard scheme is an alternating-direction method it might be expected to have characteristics quite similar to the alternating-direction methods investigated by Ferguson and Hansen⁽³⁾. However we have not found that to be the case.

The most notable example of this failure to obey the usual pattern concerns the use of the so-called "frequency transformation"⁽²⁾⁽³⁾. The essential idea of this transformation is to

estimate frequencies, ω_{ij}^g , such that, during time step Δ , the group-g flux $\phi_{ij}^g(t)$ at mesh point (ij) will behave as $e^{i\omega_{ij}^g \Delta}$. The ω_{ij}^g are predicted from the flux behavior during the previous time interval or from the basic time-dependent matrix equations themselves. Once the ω_{ij}^g are determined, the $\phi_{ij}^g(t)$ in the difference equations are replaced by transformed fluxes, $\psi_{ij}^g(t)$, defined by

$$\phi_{ij}^g(t) = e^{i\omega_{ij}^g \Delta} \psi_{ij}^g(t) \quad (2)$$

The $\psi_{ij}^g(t)$ are then advanced in time by the alternating-direction method. Since they vary in time more slowly than the $\phi_{ij}^g(t)$, larger time steps can be taken without loss in accuracy. It has been found that, for the conventional alternating-direction schemes, the time-step size can be increased by an order of magnitude with little loss in accuracy when the frequency transformation is applied.

A most attractive characteristic of the checkerboard method is the fact that it is as accurate without the frequency transformation as the conventional alternating-directional schemes are with that transformation. However the obvious hope that applying the frequency transformation to the checkerboard scheme will permit an additional increase in time-step size has not been realized. In fact, when the transformation was applied to the checkerboard equations in strict analogy with the way it is applied to the conventional alternating-direction equations, the transformed checkerboard equations (except for the one-group case) diverged unless the time-step size was substantially decreased. We spent much time in trying to understand and correct the behavior and finally discovered that

by going back and rederiving the checkerboard equations systematically, with the frequency transformation present from the start, we could obtain a set of difference equations that are stable. Unfortunately, although these transformed equations do not hurt accuracy, they do not appear to help it much. In this regard the checkerboard scheme appears to behave like iterative methods for solving the time-dependent diffusion equations without splitting the matrix $[A]$ of Eq. (1). Such schemes are time consuming because they are iterative. On the other hand, relatively large time steps can be taken without loss in accuracy. It has been found, however, that applying the frequency transformation, while it does not hurt the accuracy of iterative methods, improves it only a small amount.

Another characteristic of the checkerboard method that sets it apart from conventional finite element procedures concerns the sensitivity of solution to the values of the group velocities, v_g . In the conventional method, values of $\frac{1}{v_g}$ for groups higher than thermal may be set to zero with very little effect on the solution. If the $\frac{1}{v_g}$ are decreased for the checkerboard scheme, the solution begins to oscillate unless the time step size is reduced. We believe that this behavior is due to the nature of the time differencing approximations that are inherently a part of the alternating direction schemes. To use an analogy: we are trying to approximate $e^{\alpha\Delta}$ where α becomes a very large negative number. Conventional alternating direction schemes in effect represent $e^{\alpha\Delta}$ as $[1-\alpha\Delta]^{-1}$ which goes to zero as α becomes more more negative. The checkerboard scheme in effect represents $e^{\alpha\Delta}$ as $[1-\frac{1}{2}\alpha\Delta]^{-1}[1+\frac{1}{2}\alpha\Delta]$ which

unless Δ is continually decreased, approaches (-1) (and thus causes an oscillation in the solution) as α becomes more negative. We have circumvented this oscillatory tendency in the checkerboard scheme by setting all the v_g equal to the thermal velocity. Such an assumption introduces a small error in that it slows down adjustments in the neutron spectra. However, physically, such effects occur on a time scale comparable to that required for higher-order angular perturbations to die away. Thus the small errors introduced are of the same order as those already inherent in the diffusion theory approximation.

The study of the checkerboard method has led us to conclude that it is a satisfactory alternative to the conventional alternating direction schemes. For a given time step size it appears to have comparable accuracy, and, since it does not require a frequency transformation, it may be somewhat faster.

2.2 Improved Temporal Truncation Error

Much of the work on this project has been based upon various splitting methods for multidimensional problems. It has been shown in a number of cases that an exponential transformation provides a large reduction in truncation error. The exponential transformation, also called "frequency transformation", is a nonlinear transform and can, and often does, effect the stability of the various methods. Much effort has been spent in the past attempting to find simple, accurate, and stable means of selecting the frequencies. We have recently completed a study that has provided some improvement in the frequency selection method.

Alternating-direction explicit (ADE) methods have been proposed for the approximate solution of the space-dependent reactor kinetics equations^(2,3). Two such methods are the symmetric ADE (SADE) method and the nonsymmetric ADE (NSADE) method. The peculiarities of these splitting methods are:

- (a) The use of an exponential transformation of the dependent variables which allows for improved temporal truncation error.
- (b) Their computation ease; all matrix inversions required are simple back substitutions.

The NSADE method was shown to treat, with a reasonable size time step, a wide variety of test problems in two⁽²⁾ and three-dimensional⁽³⁾ rectangular geometry. The objective of this current study is to describe further improvements of the temporal truncation error, preserving computation ease.

The semidiscrete form of the multigroup space-time diffusion equations are

$$\frac{d\underline{x}}{dt} = A\underline{x}, \quad (1)$$

where $\underline{x}$ is a column vector of the dependent variables (both group fluxes and precursor densities) at each mesh point and each group, and A is an essentially-positive square matrix⁽⁵⁾. The approximate solution to Eq. (1) for a time step $\Delta t = 2h$, can be written as⁽³⁾ $\underline{x}(2h) = \underline{x}^1 = B(h)\underline{x}^0$, with

$$B(h) = \exp(h\Omega) [I - h(A_4 - \alpha\Omega)]^{-1} [I + h(A_3 - \gamma\Omega)] [I - h(A_2 - \alpha\Omega)]^{-1} [I + h(A_1 - \gamma\Omega)] \exp(h\Omega), \quad (2)$$

where $\gamma = 1 - \alpha$, $A = A_1 + A_2 = A_3 + A_4$ and Ω is a diagonal matrix of free parameters. The exponential transformation $\underline{x}(t) = \exp(h\Omega)\phi(t)$ has been introduced into equation (1).

We consider two classes of splitting. For the symmetric methods (SADE) we let:

$$\begin{aligned} A_1 &= \gamma T + U + D_1; \\ A_2 &= \alpha T + L + D_2; \\ A_3 &= \gamma T + L + D_2; \\ A_4 &= \alpha T + U + D_1. \end{aligned} \quad (3)$$

For the nonsymmetric methods (NSADE):

$$\begin{aligned}
 A_1 &= \gamma T + U + D_1; \\
 A_2 &= \alpha T + L + D_2; \\
 A_3 &= \gamma T + U + D_2; \\
 A_4 &= \alpha T + L + D_1.
 \end{aligned}
 \tag{4}$$

All these matrices have been previously defined⁽³⁾; we recall that T is diagonal and contains the net group production. In the references ^(2,3) the SADE method is defined by splitting (3) with $\alpha = .5$ and the NSADE method by splittings (4) with $\alpha = 1$. Moreover, it has been suggested that the Ω values to be used at each point j , ω_j^N , for the time step $(N\Delta t, (N+1)\Delta t)$ may be successfully evaluated by

$$\omega_j^N = \frac{1}{\Delta t} \ln \frac{x_{\bar{g},j}^N}{x_{\bar{g},j}^{N-1}}
 \tag{5}$$

The group $\bar{g}$ to be used in equation (5) is the thermal group in thermal reactor problems and a representative fast group in fast reactor problems.

Numerical experiments have been performed with the MITKIN code⁽²⁾ to test the behavior of the NSADE method with respect to h and α . We present the results for a two-dimensional simple case, (the test case 1 of Ref. (2)) which can be solved exactly. Thermal flux values at the reactor center are quoted in Table 1. The results show that $\alpha = .5$ is better than $\alpha = 1$ for $\omega_j^N = 0$; however the error is completely unacceptable. Using the exponential transformation and evaluating ω_j^N by means of

equation (5), then for $\alpha = .5$ instability effects appear as h increases. To avoid this unpleasant effect, we have tried to smooth the values of the frequencies ω_j^N using the following interpolation formula:

$$\omega_j^N = \frac{1}{2} [\omega_j^{N-1} + \frac{1}{h} \ln \frac{x_{g_j}^N}{x_{g_j}^{N-1}}]$$

with $\omega_j^0 = 0$. The results obtained are an improvement over previous methods; for $\alpha = .5$ the maximum error is less than .5% for $h = .002$ and less than 1.5% for $h = .004$.

Table 1. Thermal Flux at Reactor Center

Time	h=.004		h=.002		h=.001		h=.0005		EXACT	ω_j^N
(sec.)	$\alpha=.5$	$\alpha=1.$	$\alpha=.5$	$\alpha=1.$	$\alpha=.5$	$\alpha=1.$	$\alpha=.5$	$\alpha=1.$		
0.00									.382	$\omega_j^N = 0$
0.08	.529	.420	.539	.447	.542	.482	.546	.520	.613	
0.16	.677	.457	.685	.509	.688	.576	.696	.649	.816	
0.24	.813	.495	.819	.569	.823	.666	.833	.768	.997	
0.32	.938	.529	.944	.627	.949	.752	.960	.880	1.158	
0.40	1.055	.564	1.060	.684	1.065	.833	1.070	.985	1.303	
0.00									.382	$\omega_j^N = \frac{1}{\Delta t} \ln \frac{x_{2j}^N}{x_{2j}^{N-1}}$
0.08		.526	.610	.596	.612	.610	.613	.612	.613	
0.16		.773	.815	.815	.816	.816	.817	.816	.816	
0.24		1.008	.999	1.004	.997	.999	.997	.997	.997	
0.32		1.205	1.248	1.170	1.159	1.161	1.159	1.159	1.158	
0.40		1.370		1.318	1.304	1.307	1.304	1.304	1.303	
0.00									.382	$\omega_j^N = \frac{1}{2} \left[\omega_j^{N-1} + \frac{1}{\Delta t} \ln \frac{x_{2j}^N}{x_{2j}^{N-1}} \right]$
0.08	.604	.483	.607	.570	.610	.605	.612	.611	.613	
0.16	.813	.685	.815	.806	.816	.816	.816	.816	.816	
0.24	.998	.934	.998	1.009	.998	1.001	.998	.998	.997	
0.32	1.163	1.182	1.161	1.183	1.160	1.164	1.159	1.159	1.158	
0.40	1.323	1.401	1.307	1.335	1.305	1.311	1.304	1.305	1.303	

2.3 Finite Element Point Kinetics

The principal goal of using the Finite Element Method to describe a reactor transient is to reduce the number of unknowns per time step, and the number of time steps required to describe a given transient, thus reducing the computing time, while still retaining accuracy and providing relatively detailed information about the time-dependent behavior of the reactor core. The method has been applied successfully to a number of transient problems⁽⁶⁾, and comparison of the results of these calculations to those obtained using more conventional Finite Difference Techniques has shown that the Finite Element Method is a high-order accurate procedure that is indeed capable of achieving the desired goals of accuracy and computational speed.

Some additional work in Point Kinetics beyond that described in Reference 6 has been performed.

This work has focused on two areas:

1. The use of a cubic approximation for the flux in the precursors-integrated form of the Point Kinetics Equations.
2. The use of a finite element approximation for the neutron density combined with a simple finite difference treatment of the delayed neutron precursors.

The so-called Hermite Method⁽⁶⁾ has been used, rather than the standard Ritz-Galerkin finite element approach, to approximate time-dependent behavior. In the Hermite Method, once a polynomial approximation has been made for the time dependence of the neutron density, (and possible precursor concentration) the resulting equations are integrated directly over a time interval $[t_n, t_{n+1}]$, rather than first weighting the equations by a trial function and then integrating as is done in the standard Ritz-Galerkin finite element approach.

2.3.1 Time-Integrated Point Kinetics

The time integrated form of the point kinetics equations is given by

$$\frac{d}{dt} n(t) = \frac{\rho(t) - \beta}{\Lambda} n(t) + \sum_{i=1}^I \lambda_i \{ c_{i0} e^{-\lambda_i t} + \frac{\beta_i}{\Lambda} \int_0^t n(s) e^{-\lambda_i (t-s)} ds \} \quad (1a)$$

$$n(0) = n_0; c_{i0} = c_i(0) \quad (1b)$$

The neutron density in a time interval between t_n and t_{n+1} is approximated by

$$n(t) \approx \hat{n}(t) = \sum_{p=0}^{m-1} \{ \hat{n}_n^{(p)} u_n^{p+}(t) + n_{n+1}^{(p)} u_{n+1}^{p-}(t) \} \quad t \in [t_n, t_{n+1}] \quad (2)$$

where for a cubic approximation, $m=2$. It is assumed that $\hat{n}_j^{(1)}$ satisfies

$$\hat{n}_j^{(1)} = \frac{d}{dt} \hat{n}(t) \big|_{t_j} \quad j=n, n+1 \quad (3)$$

Substitution of (2) into (1a), and integration over the time interval of interest leads to

$$\hat{n}_{n+1} - \hat{n}_n = \int_{t_n}^{t_{n+1}} \frac{\rho(t) - \beta}{\Lambda} \hat{n}(t) dt + \sum_{i=1}^I \int_{t_n}^{t_{n+1}} \lambda_i \{ c_{i0} e^{-\lambda_i t} + \frac{\beta_i}{\Lambda} \int_0^t n(s) e^{-\lambda_i (t-s)} ds \} dt \quad (4)$$

$$\hat{n}_j^{(1)} = \left\{ \frac{\rho(t) - \beta}{\Lambda} \hat{n}(t) + \sum_{i=1}^I \lambda_i \left\{ c_{i0} e^{-\lambda_i t} + \frac{\beta_i}{\Lambda} \int_0^t \hat{n}(s) e^{-\lambda_i (t-s)} ds \right\} \right\} \big|_{t_j} \quad j=n, n+1 \quad (5)$$

Equations (4) and (5), with $m=2$ in equation (2) were used to solve for the results of two transients:

Case 1 - 6 delayed neutron group (see Table 1)

$$\Lambda = 5 \times 10^{-4} \text{ sec.}$$

$$n(0) = 1.0$$

$$0 \leq t \leq 2 \text{ sec.}$$

$$\rho(t) = \frac{\beta}{2} t;$$

Case 2 - 6 delayed neutron groups (see Table 1)

$$\Lambda = 10^{-7} \text{ sec.}$$

$$n(0) = 1.0$$

$$0 \leq t \leq 2 \text{ sec.}$$

$$\rho(t) = \frac{\beta}{2} t;$$

Note that the first integral in (4) allows this ramp behavior of the reactivity to be treated explicitly whereas a finite difference approach would require some approximation to the true ramp such as series of steps or some average reactivity, over a time interval.

The results are summarized in Tables 2 and 3 for Cases 1 and 2 respectively. Also presented are the results obtained using a linear approximation for the neutron density in (4) (i.e., $m=1$ in (2)), and results from solving the neutron and precursor equations, (6) and (7), simultaneously using a cubic approximation for both the neutron density and the precursor concentrations. Point-wise errors, based on the converged solution, are also given.

The results show:

Case 1 - (1) The order of convergence for the time-integrated method is essentially the same as that for the method

where the neutron and precursor equations are solved simultaneously.

(2) The pointwise errors are also essentially the same for the two methods.

Case 2 - (1) At $T=1.0$, the time integrated method appears to be generally more accurate than the "simultaneous" method, however, the order of convergence is lower than expected.

(2) At $T=2.0$, uniform convergence is not observed for any of the methods, and the flux actually becomes negative for large time-step sizes with the time-integrated method.

2.3.2 Mixed Finite Element-Finite Difference Treatment

The standard form of the point kinetics equations is:

$$\frac{d}{dt} n(t) = \frac{\rho(t) - \beta}{\Lambda} n(t) + \sum_{i=1}^I \lambda_i C_i(t) \quad (6)$$

$$\frac{d}{dt} C_i(t) = \frac{\beta_i}{\Lambda} n(t) - \lambda_i C_i(t) \quad i=1, \dots, I \quad (7)$$

$$n(0) = n_0; C_i(0) = C_{i0}$$

Applying the Hermite method to (6) leads to

$$\hat{n}_{n+1} - \hat{n}_n = \int_{t_n}^{t_{n+1}} \frac{\rho(t) - \beta}{\Lambda} n(t) dt + \sum_{i=1}^I \lambda_i \int_{t_n}^{t_{n+1}} C_i(t) dt \quad (8)$$

It was thought that as long as the first integral in (8) was treated according to the Hermite method, more accurate solutions would be obtained than if finite difference techniques were used. It was also expected that the solution would be more sensitive to the order of the approximation for $n(t)$ than to variations in the treatment of the precursor contributions. Therefore, in this phase of the study the effect on accuracy and order of convergence of using a finite element approximation for the neutron density, and a finite difference approximation to the precursor behavior, was examined.

Linear ($m=1$ in eq. (2)) and cubic ($m=2$ in eq. (2)) approximations to the neutron density were used. The precursor term in equation (8) was approximated by

$$\int_{t_n}^{t_{n+1}} C_i(t) dt = \{ \theta_1 C_{n+1}^i + \theta_2 C_n^i \} (t_{n+1} - t_n) \quad \theta_2 = 1 - \theta_1 \quad (9)$$

A similar finite difference approach was used on (7) to yield

$$\frac{C_{n+1}^i - C_n^i}{t_{n+1} - t_n} = \theta_3 \frac{\beta_i}{\Lambda} \hat{n}_{n+1} + \theta_4 \frac{\beta_i}{\Lambda} \hat{n}_n - \theta_5 \lambda_i C_{n+1}^i - \theta_6 \lambda_i C_n^i \quad (10)$$

$$\theta_4 \equiv 1 - \theta_3; \theta_6 \equiv 1 - \theta_5$$

The two transients described in the previous section were solved for three combinations of θ 's.

(1) Implicit (all odd θ 's = 1.0, all even θ 's = 0.0) - the solution at t_{n+1} depends only on information at t_{n+1} .

(2) Semi-Implicit (all θ 's = 0.5) - the solution at t_{n+1} depends equally on information at t_n and at t_{n+1} .

(3) Explicit (all even θ 's = 1.0, all odd θ 's = 0.0) - the solution at t_{n+1} depends only on information at t_n .

The results of these calculations are summarized in Tables 4 and 5, where a linear ($m=1$) approximation for $n(t)$ has been used in solving cases 1 and 2 respectively, and Tables 6 and 7 where a cubic approximation for $n(t)$ has been used. For comparison, results from Reference 1 are presented where the same cases were solved using linear and cubic approximations to the time dependence of both $n(t)$ and $C_i(t)$. Errors based on these "converged" solutions are also given.

The results show:

Case 1 - (1) For the case of a linear approximation to $n(t)$

(a) Treating the precursors via a finite difference scheme reduced the order of convergence from ~ 2 to ~ 1 . (In this situation the semi-implicit and full

Hermite approaches are identical.)

(b) The error for time steps up to .1 sec. is $\sim 10\%$ and in this range of time steps is roughly the same magnitude for both the fully implicit and the fully explicit treatments.

(2) For the case of a cubic approximation to $n(t)$

(a) The semi-implicit approach is roughly comparable, in terms of magnitude of error and order of convergence, to the full linear Hermite solution.

(b) The use of a higher order approximation to $n(t)$ has no effect on the accuracy of the solution or on the order of convergence if the precursors are treated in a fully explicit or implicit manner.

Case 2 - (1) For $T=1.0$, similar results to those mentioned for Case 1 were observed.

(2) For $T=2.0$, the mixed methods generally have huge errors.

The general conclusion from these results is that mixed methods of this type have nothing to offer if solutions on the order of 1% accuracy are sought.

It should be noted that Case 2 is considered to be very unrealistic, and there is therefore not much concern over the problems encountered in its solution.

Table 1Delayed Neutron Constants

<u>Group</u>	<u>β_i</u>	<u>λ_i</u>
1	0.285×10^{-3}	0.127×10^{-1}
2	0.15975×10^{-2}	0.317×10^{-1}
3	0.141×10^{-2}	0.115
4	0.30525×10^{-2}	0.311
5	0.96×10^{-3}	0.14×10^1
6	0.195×10^{-3}	0.387×10^1

$$\beta = \sum \beta_i = .0075$$

Table 2

Point Kinetics Problem - Case 1
n(t)

T	Δt	Hermite Method		
		$m=2^+$	$m=1(\text{time-integ})^+$	$m=2(\text{time-integ})$
1.0	0.5	1.9465955 (0.17)*	1.9046032 (2.33)*	1.9525556 (0.131)*
	0.1	1.9499962 (0.13x10 ⁻³)	1.9476481 (0.12)	1.9500020 (0.169x10 ⁻³)
	0.05	1.9499987 (0.0)	1.9494094 (0.30x10 ⁻¹)	1.9499989 (0.103x10 ⁻⁴)
	0.01	1.9499987 (0.0)	1.9499751 (0.12x10 ⁻²)	1.9499987 (0.0)
	0.005	1.9499987 (0.0)	1.9499928 (0.30x10 ⁻³)	1.9499987 (0.0)
	Order of Conv.* 4.48 2.08 4.09			
	0.5	10.943181 (2.54)*	10.925652 (2.70)*	11.251728 (0.208)*
	0.1	11.227962 (0.37x10 ⁻²)	11.219269 (0.81x10 ⁻¹)	11.228399 (0.240x10 ⁻³)
	0.05	11.228356 (0.14x10 ⁻³)	11.226118 (0.20x10 ⁻¹)	11.228373 (0.891x10 ⁻⁵)
	0.01	11.228372 (0.0)	11.228282 (0.80x10 ⁻³)	11.228372 (0.0)
	0.05	11.228372 (0.0)	11.228349 (0.20x10 ⁻³)	11.228372 (0.0)
	Order of Conv.* 4.36 2.09 4.48			

* Order of Convergence and %|error| (given in ()) are based on
n(1.0)=1.9499987; n(2.0)=11.228372

+ From Ref. 6

Table 3

Point Kinetics Problem - Case 2
n(t)

T	Δt	Hermite Method		
		m=2 ⁺	m=1(time-integ) ⁺	m=2(time-integ)
1.0	0.5	2.1453451 (6.24)*	2.1770162 (4.86)*	2.2899769 (0.774x10 ⁻¹)*
	0.1	2.2761511 (0.53)	2.2823753 (0.25)	2.2882851 (0.349x10 ⁻²)
	0.05	2.2873140 (0.39x10 ⁻¹)	2.2867310 (0.64x10 ⁻¹)	2.2882338 (0.125x10 ⁻²)
	0.01	2.2881994 (0.25x10 ⁻³)	2.2881894 (0.69x10 ⁻³)	2.2882071 (0.83x10 ⁻⁴)
	0.005	2.2882052 (0.0)	2.2881461 (0.26x10 ⁻²)	2.2882054 (0.874x10 ⁻⁵)
	Order of Conv.*	3.75	1.90	
2.0	0.5	0.13191022x10 ⁵ (36.15)*	0.10859238x10 ³ (99.47)*	-0.30170372x10 ³ (101.46)*
	0.1	0.63665597x10 ⁴ (69.18)	0.26780006x10 ⁴ (87.03)	-0.16594721x10 ⁵ (180.3)
	0.05	0.67090612x10 ⁴ (67.52)	0.30757093x10 ⁴ (60.91)	0.44913107x10 ⁵ (117.42)
	0.01	0.18399171x10 ⁵ (10.93)	0.20823698x10 ⁵ (0.81)	0.21043545x10 ⁵ (1.87)
	0.005	0.20657232x10 ⁵ (0.0)	0.20264628x10 ⁵ (1.90)	0.20952349x10 ⁵ (1.43)
	Order of Conv.			

* Order of Convergence and %|error| (given in ()) are based on
n(1.0)=2.2882052; n(2.0)=.20657232+5

⁺ From Ref. 6

Table 4

Point Kinetics Problem - Case 1
 $n(t)$
 $M=1$ (Linear) for Neutron Density; FD for Precursors

T	Δt	Full Hermite ⁺ ≡Semi-Implicit	Implicit	Explicit
1.0	0.5	1.9144400	2.1479482	1.7754011
		(1.83)*	(10.15)*	(8.95)*
	0.1	1.9482021	1.9921449	1.9101654
		(0.92x10 ⁻¹)	(2.16)	(2.04)
	0.05	1.9495497	1.9707917	1.9297985
		(0.23x10 ⁻¹)	(1.07)	(1.04)
	0.01	1.9499808	1.9541094	1.9459119
		(0.92x10 ⁻³)	(0.21)	(0.21)
	0.005	1.9499942	1.9520510	1.9479523
		(0.23x10 ⁻³)	(0.11)	(0.10)
Order of Conv.*		1.92	.997	.97
2.0	0.5	11.145270	21.018435	7.6123162
		(0.74)*	(87.19)*	(32.20)*
	0.1	11.243498	12.699173	10.157455
		(0.13)	(13.10)	(9.54)
	0.05	11.232274	11.902347	10.653920
		(0.35x10 ⁻¹)	(6.00)	(5.12)
	0.01	11.228529	11.354416	11.106293
		(0.14x10 ⁻²)	(1.12)	(1.09)
	0.005	11.228411	11.290886	11.166849
		(0.35x10 ⁻³)	(0.56)	(0.55)
Order of Conv.*		1.97	1.09	.90

* Order of Convergence and % |error| (given in ()) are based on
 $n(1.0)=1.9499987$; $n(2.0)=11.228372$

⁺ From Ref. 6

Table 5

Point Kinetics Problem - Case 2
n(t)

M=1(Linear) for Neutron Density; FD for Precursors

T	Δt	Full Hermite=Semi-Implicit ⁺	Implicit	Explicit
1.0	0.5	2.1903963	2.6256727	1.9428203
		(4.27)*	(14.75)*	(15.09)*
	0.1	2.2835253	2.3722375	2.2097630
		(0.20)	(3.67)	(3.43)
	0.05	2.2870330	2.3296300	2.2982941
		(0.51x10 ⁻¹)	(1.81)	(1.74)
	0.01	2.2881595	2.2963724	2.2801140
		(0.20x10 ⁻²)	(0.36)	(0.35)
	0.005	2.2881928	2.2922787	2.2841495
		(0.54x10 ⁻³)	(0.18)	(0.18)
Order of Conv.*		1.93	.97	.97
2.0	0.5	0.62508242x10 ²	0.27909426x10 ³	0.21326204x10 ²
		(99.70)*	(98.65)*	(99.90)*
	0.1	0.11526595x10 ⁴	0.80050560x10 ⁵	0.24323692x10 ³
		(94.42)	(287.52)	(98.82)
	0.05	0.39038912x10 ⁴	0.36657699x10 ⁶	0.74559161x10 ³
		(81.10)	(1674.57)	(96.39)
	0.01	0.21227155x10 ⁵	0.53092938x10 ⁶	0.63243625x10 ⁴
		(12.76)	(2470.19)	(69.38)
	0.005	0.21803225x10 ⁵	0.79686518x10 ⁵	0.10266357x10 ⁵
		(5.55)	(285.76)	(50.3)

* Order of Convergence and % |error| (given in ()) are based on
n(1.0)=2.2882052; n(2.0)=.20657232x10⁵

⁺ Ref. 6

Table 6

Point Kinetics Problem - Case 1
 $n(t)$
 $M=2$ (Cubic) for Neutron Density; FD for Precursors

T	Δt	Full Hermite ⁺	Implicit	Semi-Implicit	Explicit
1.0	0.5	1.9465955 (0.17)*	2.2079878 (13.23)*	1.9899512 (2.05)*	1.8490971 (5.17)*
	0.1	1.9499962 (0.13 $\times 10^{-3}$)	1.9959034 (2.35)	1.9519581 (0.10)	1.9138850 (1.85)
	0.05	1.9499987 (0.0)	1.9717352 (1.11)	1.9504913 (0.25 $\times 10^{-1}$)	1.9307361 (0.99)
	0.01	1.9499987 (0.0)	1.9541471 (0.21)	1.9500184 (0.10 $\times 10^{-2}$)	1.9459496 (0.21)
	0.005	1.9499987 (0.0)	1.9520605 (0.11)	1.9500036 (0.25 $\times 10^{-3}$)	1.9479618 (0.10)
	Order of Conv.*	4.48	1.05	1.97	.88
2.0	0.5	10.943181 (2.54)*	25.854762 (130.26)*	13.234390 (17.87)*	8.6228581 (23.20)*
	0.1	11.227962 (0.37 $\times 10^{-2}$)	12.778000 (13.80)	11.307765 (0.71)	10.211200 (9.06)
	0.05	11.228356 (0.14 $\times 10^{-3}$)	11.919855 (6.16)	11.248138 (0.18)	10.668391 (4.99)
	0.01	11.228372 (0.0)	11.355060 (1.13)	11.229161 (0.70 $\times 10^{-2}$)	11.106913 (1.08)
	0.005	11.228372 (0.0)	11.291045 (0.56)	11.228569 (0.18 $\times 10^{-2}$)	11.167005 (0.55)
	Order of Conv.*	4.36	1.16	2.00	.85

* Order of Convergence and % |error| (given in ()) are based on
 $n(1.0)=1.9499987$; $n(2.0)=11.228372$

⁺ Ref. 6

Table 7

Point Kinetics Problem - Case 2
 $n(t)$
 $M=2$ (Cubic) for Neutron Density; FD for Precursors

T	Δt	Full Hermite	Implicit	Semi-Implicit	Explicit
1.0	0.5	2.1453451 (6.24)*	2.4244997 (5.96)*	2.2948969 (0.29)*	2.1450074 (6.26)*
	0.1	2.2761511 (0.53)	2.3232530 (1.53)	2.2890604 (0.37x10 ⁻¹)	2.2546922 (1.46)
	0.05	2.2873140 (0.39x10 ⁻¹)	2.3064402 (0.80)	2.2884836 (0.12x10 ⁻¹)	2.2706237 (0.77)
	0.01	2.2881994 (0.25x10 ⁻³)	2.2940801 (0.26)	2.2882354 (0.13x10 ⁻²)	2.2824656 (0.25)
	0.005	2.2882052 (0.0)	2.2918767 (0.16)	2.2882149 (0.42x10 ⁻³)	2.2845856 (0.16)
	Order of Conv.*	3.75	.79	1.48	.80
	2.0	0.1319022x10 ⁵ (36.15)*	0.73236911x10 ⁸ (10 ⁵)*	0.34279729x10 ⁸ (10 ⁵)*	0.24676399x10 ⁵ (19.46)*
	0.1	0.63665597x10 ⁴ (69.18)	0.41426641x10 ⁷ (10 ⁴)	0.12312410x10 ⁷ (10 ³)	0.13256804x10 ⁵ (35.82)
	0.05	0.67090612x10 ⁴ (67.52)	0.13569333x10 ⁷ (10 ³)	0.31303009x10 ⁶ (10 ³)	0.10820359x10 ⁵ (47.62)
	0.01	0.18399171x10 ⁵ (10.93)	0.92936221x10 ⁶ (10 ³)	0.34288457x10 ⁵ (65.99)	0.88134413x10 ⁴ (57.33)
	0.005	0.20657232x10 ⁵ (0.0)	0.90899705x10 ⁵ (340)	0.24314648x10 ⁵ (17.71)	0.11169770x10 ⁵ (45.93)
	Order of Conv.*		1.837	1.98	

* Order of Convergence and % |error| (given in ()) are based on
 $n(1.0)=2.2882052$; $n(2.0)=.20657232 \times 10^5$

+ Ref. 6

3. FINITE ELEMENT METHODS

3.1 Two-Dimensional Finite Element Methods

In the period of time covered by this report, further work has been carried out on the application of higher-order finite elements to rectangular geometry. The objectives of this work have been twofold: (1) to develop a faster, more generalized, production-oriented version of the cubic Hermite finite element computer code CHD developed recently at M.I.T., and (2) to make use of the extended capabilities of the newer code to assess the performance of cubic Hermite finite elements in comparison with linear Hermite finite elements and lower-order finite differences for realistic reactor problems.

3.1.1 Finite Element Code Development

The first objective involved extensive revisions and numerous additions to a code developed here for a Nuclear Engineer's Thesis (7). The major limitations of the original code which were addressed by this work are as follows:

- a) All fissions led to neutrons being born in the highest energy group (group 1). Any number of energy groups could be used, but all fission neutrons would always be born in group 1. The generalized version of the code allows for an arbitrary distribution of the fission neutrons in the multigroup structure. The input routines were revised to permit the reading of the fission spectrum.
- b) All outscattering led to the energy group immediately below, i.e. only downscattering from a group to the

adjacent group below was possible. The generalized version of the code allows for arbitrary group-to-group downscatter, i.e., group "jumping" is permitted to any depth in the group structure. The input routines were modified to permit the reading of any combination of downscatter iron-sections.

- c) The calculation of region-wise reaction rates and average fluxes could only be done over each finite element. There was no provision for specifying an edit region within an element. Since cubic Hermite elements have the potential for providing very coarse meshes which give reasonably accurate results, the ability to obtain reaction rates and average flux edits within an element (e.g., edits for each assembly within a coarse-mesh element covering several assemblies) is needed to assess the accuracy of assembly powers and assembly-averaged-to-core-averaged power ratios produced by various coarse mesh cubic Hermite element sizes and arrangements. The new version of the code has the provision for specifying arbitrary region edits within any size element.
- d) The power iteration method used by the code for solving the coupled multigroup equations did not incorporate any acceleration technique to reduce the number of outer iterations required for convergence. The new version of the code applies a Chebyshev acceleration strategy to the fission source vector to reduce the number of outer iterations. In one large quarter-core

reactor problem, for instance, the number of outer iterations was reduced from 136 to 42. In another problem, the outer iterations were reduced from 134 to 33. These numbers were obtained for an eigenvalue and point-wise flux convergence interim of 10^{-4} , and the machine was an IBM 370/168.

Details on the solution strategy and use of the code, along with results of several problems, will be presented in a forthcoming AEC/MIT report (8).

3.1.2 Coarse-mesh Test Problems

The second objective of the work involved the analysis of several large generator-core reactor problems using various coarse mesh element arrangements. The three problems for which results are presented here are (1) the IAEA 2-D, quarter-core benchmark problem, (2) the Maine Yankee 2-D, quarter-core problem, and (3) the Zion 1 2-D, quarter-core problem. All of these problems were analyzed with three different coarse mesh arrangements, ranging from a mesh where there is one assembly per element to a mesh where there are as many as 9 or 16 of the innermost assemblies in an element. All of the problems were analyzed using a two-group representative of the energy structure.

3.1.2.1 IAEA 2-D Benchmark

The quarter-core layout of the IAEA 2-D Benchmark problem is illustrated in Figure 1. There are four material compositions, and there is no baffle between the fuel assemblies and the water reflector region.

One core was run with one assembly per element. The coarse mesh element patterns for the other two cases are shown in

Figures 2 and 3.

On the basis of results presented in Ref: (1), derivative continuity was used for any singular point completely surrounded by fuel elements, and first derivatives were uncoupled otherwise.

A comparison between the assembly power fractions obtained with a PDQ 16 x 16 mesh (per assembly) and the three CHD coarse meshes is shown in Figure 4. The percent errors in the CHD power fractions relative to the power fractions obtained with the PDQ 16 x 16 mesh are given in Figure 5. Considering the degree of difficulty of this problem and coarseness of the meshes, the CHD results are impressive.

A comparison of the eigenvalues, number of unknowns per group, number of outer iterations, and the job run times are given in Table I.

A comparison of the percent errors in assembly power fractions from cubic Hermite (CHD) and linear Hermite (9) finite element run is given in Figure 6. The results show the cubic Hermite elements, one per assembly, to be superior to the linear Hermite elements, 4 x 4 per assembly.

3.1.2.2 Maine Yankee 2-D Problem

The quarter-core layout of the Maine Yankee two-dimensional problem is illustrated in Figure 7. There are nine material compositions, and offset fuel assemblies are used in the core pattern. A baffle surrounds the core at a distance of 2.597 inches from the edge of the outermost assemblies.

One core was run with one assembly per element, except for the offset boxes which were treated as shown in Figure 8.

The coarse mesh element patterns for the other two cases are shown in Figures 9 and 10.

In all the runs the baffle was implicitly accounted for as a subregion of an overall baffle-moderator expansion element. It was shown in Reference (7) that current continuity across the fuel-baffle interface is expected to introduce large distortions of the flux shape. Therefore, the first derivatives of the solution at all these interface points were uncoupled. For any singular point completely surrounded by fuel elements, derivative continuity was used. Otherwise, first derivatives were uncoupled.

A comparison between the assembly power fractions obtained with a PDQ 16 x 16 mesh (per assembly) and the three CHD coarse meshes is shown in Figure 11. The per cent errors in the CHD power fractions relative to the power fractions obtained with the PDQ 16 x 16 mesh are given in Figure 12. In view of the coarseness of the meshes, the performance of the cubic Hermite elements is quite good.

A comparison of the eigenvalues, number of unknowns per group, number of outer iterations, and the job run times are given in Table II.

3.1.2.3 Zion 1 2-D Problem

The quarter-core layout of the Zion 1 two-dimensional problem is illustrated in Figure 13. There are five material compositions. A baffle surrounds the core at a distance of 2.86 inches from the edge of the outermost assemblies.

One core was run with one assembly per element. The coarse mesh element patterns for the other two cases are shown in Figures 14 and 15.

In all the runs the baffle was implicitly accounted for as in the Maine Yankee problem. The solution continuity conditions were also treated the same as in the Maine Yankee cases.

A comparison of the assembly power fractions obtained with the three CHD coarse meshes is shown in Figure 16.

A comparison of the assembly-averaged-to-core-averaged power ratios obtained with a PDQ-5 44 x 44 mesh (7) and the three CHD coarse meshes is shown in Figure 17. The PDQ-5 run was made with a point-wise flux convergence criterion of 4×10^{-4} . In view of this less stringent convergence criterion, coupled with the fact that a 44 x 44 finite difference mesh is relatively coarse for this problem, the PDQ results were not considered to be "truth" for a comparison with the CHD results. For this reason a chart was not compiled for the percent error in the CHD results relative to the PDQ-5 results.

A comparison of the eigenvalues, number of unknowns per group, number of outer iterations, and the job run times are given in Table III.

The results of these three test problems are quite encouraging for the potential of cubic Hermite elements to offer a substantial reduction in the number of unknowns with little loss of accuracy.

Table I
Data for IAEA 2-D Benchmark Analysis

	Eigenvalue	No. Unknowns Per Group	No. Outer Iterations	Total Job Run Time (Total CPU%)
PDQ (16 x 16 per assembly)	1.02951			
CHD (10 x 10)	1.02973	324	42*	2.318 min. (88%)**
CHD (8 x 8)	1.02933	212	43*	1.690 min. (83%)**
CHD (7 x 7)	1.02815	162	44*	1.424 min. (80%)**

CHD Eigenvalue convergence criterion = 1×10^{-4}

CHD Point-wise flux convergence criterion = 1×10^{-4}

* - with Chebyshev acceleration

** - For IBM 370/168

Table II
Data for Maine Yankee Analysis

	Eigenvalue	No. Unknowns Per Group	No. Outer Iterations	Total Job Run Time (total CPU%)
PDQ (16 x 16 per assembly)	0.99926			
CHD (11 x 11)	0.99856	436	51*	3.927 min. (93%)**
CHD (8 x 8)	0.99799	248	41*	2.243 min. (88%)**
CHD (7 x 7)	0.99351	174	51*	1.768 min. (84%)**

* - with Chebyshev acceleration

** - For IBM 370/168

Table III

Data for Zion 1 Analyses

	Eigenvalue	No. Unknowns Per Group	No. Outer Iterations	Total Job Run Time/ (Total CPU %)
PDQ-5(44x44)	1.2749***	1936		
CHD (10x10)	1.27462	348	45*	2.690 min.(89%)**
CHD (7x7)	1.27467	190	45*	1.808 min.(84%)**
CHD (6x6)	1.27533	128	33*	1.317 min.(79%)**

* - with Chebyshev acceleration

** - for IBM 370/168

*** - Point-wise flux convergence criterion= 4×10^{-4}

Figure 1. Core Layout for IAEA Benchmark*

* - Numbers Refer to Material Composition

Comp.	Description
1	high enrichment fuel
2	low enrichment fuel
3	rodded assemblies
4	reflector

Figure 2. CHD 8x8 Mesh for IAEA Benchmark

Figure 3. CHD 7x7 Mesh for IAEA Benchmark

+ 0.3 + 2.7 -15.0	+ 0.5 + 2.4 - 2.1	+ 3.1 + 7.1 +20.3					
- 0.9 + 0.8 + 0.3	- 0.6 + 0.5 + 4.7	- 0.1 + 0.4 + 3.1	+ 1.5 + 5.6 +10.8	+ 3.7 + 5.8 + 8.7			
- 1.3 - 1.1 - 1.2	- 0.8 - 0.7 - 1.8	- 0.5 + 0.2 + 2.5	- 0.6 0.0 + 2.6	- 0.6 + 0.4 + 2.2	+ 3.9 + 6.1 + 8.9		
+ 0.3 + 3.0 +11.0	- 0.7 - 2.6 -13.5	- 0.5 - 1.4 + 3.6	- 1.0 - 1.8 - 2.5	+ 1.1 + 3.7 + 7.3			
- 0.5 - 2.7 - 5.9	- 0.3 - 1.8 - 6.3	- 0.3 - 1.2 - 1.0	- 0.6 - 1.2 - 1.4				
+ 0.1 - 2.2 - 2.1	+ 0.1 - 1.5 - 3.2	- 0.1 - 1.2 - 3.6					
+ 0.1 - 3.2 -15.4	+ 0.2 - 2.1 -12.2						
+ 0.7 + 3.4 +13.6							

XX
XX
XX

CHD 10X10 Mesh
CHD 8X8 Mesh
CHD 7X7 Mesh

Figure 5. Percent Error in Assembly Powers
for IAEA Benchmark*

*-CHD (cubic Hermite) - 10X10 Mesh (1 assembly per element)
 - 8X8 Mesh (2X2 & 2X1 assemblies per element)
 - 7X7 Mesh (3X3, 3X2, & 3X1 assemblies per element)

*-Reference = PDQ (16X16 mesh per assembly)

+0.3	+0.5	+3.1							
3.3	3.6	5.8							
-0.9	-0.6	-0.1	+1.5	+3.7					
0.4	0.5	1.0	3.5	6.2					
-1.3	-0.8	-0.5	-0.6	-0.6	+3.9				
-1.1	-0.8	-0.3	0.2	0.9	5.9				
+0.3	-0.7	-0.5	-1.0	+1.1					
0.5	-1.8	-1.1	-1.2	2.0					
-0.5	-0.3	-0.3	-0.6						
-2.1	-1.8	-1.5	-1.4						
+0.1	+0.1	-0.1							
-1.7	-1.7	-1.6							
+0.1	+0.2								
-2.1	-1.9								
+0.7									
-0.1									

X X	CHD (1x1)
X X	Linear Hermite (4x4)

Figure 6. Comparison of Percent Error in Assembly Powers with Cubic Hermite and Linear Hermite Elements for IAEA Benchmark*

* - CHD (cubic Hermite) - 1x1 per assembly
 Linear Hermite - 4x4 per assembly

Eigenvalues: PDQ - 1.02951
 CHD - 1.02973
 Linear - 1.02982

* - Reference = PDQ (16x16 per assembly)

Figure 9. CHD 8x8 Mesh for Maine Yankee

Figure 10. CHD 7x7 Mesh for Maine Yankee

.1462-1	.1671-1
.1403-1	.1620-1
.1459-1	.1650-1
.1501-1	.1757-1

1/4 assembly

for Maine Yankee

X	X	CHD 11 x 11 mesh
X	X	CHD 8 x 8 mesh
X	X	CHD 7 x 7 mesh

-4.0	-3.1
-0.2	-1.3
+2.7	+5.1

			-3.9	-2.5	-2.2	-1.8	-1.5
			-2.6	-0.3	-0.3	-0.5	+0.3
			+1.0	+9.7	+0.1	-0.2	+10.9
		-4.3	-2.6	-2.3	-1.8	-0.5	-1.0
		-4.0	+2.8	-1.8	-0.6	+1.1	-1.3
		+1.4	+3.5	+8.1	-8.3	+8.7	-3.6
		-2.7	-2.5	-4.2	-0.2	-0.1	+0.4
		-0.7	-3.0	-0.02	-0.06	-0.5	+2.0
		-0.3	-2.2	+4.0	-2.6	-7.9	+12.7
			-1.5	+0.1	+0.2	+1.5	+0.9
			-0.6	+0.07	-0.4	+1.9	-1.2
			-7.2	+5.2	-10.3	+6.1	-5.7
				+0.6	+2.0	+1.5	+2.2
				-0.6	+1.7	-0.5	+2.0
				-8.9	+5.8	-7.9	+6.4
					+1.6	+2.8	+2.1
					-3.0	+1.6	-1.3
					-7.8	+6.1	-8.0
						+2.4	+3.1
						-0.8	+1.7
						-7.8	+6.3
							+2.5
							-2.0
							-7.4

Fig. 12 Per Cent Error in Assembly Power for Maine Yankee*

- *CHD (Cubic Hermite) - 11 x 11 Mesh (1 assembly per element)
 - 8 x 8 Mesh (2 x 2 & 2 x 1 assemblies per element)
 - 7 x 7 Mesh (4 x 4, 4 x 2, 4 x 1, 2 x 2, 2 x 1
 assemblies per element)

* Reference = PDQ (16 x 16 Mesh per assembly)

Figure 13. Core Layout for Zion 1

* - Numbers Refer to Material Composition

Comp.	Description
1	baffle
2	low enrichment fuel
3	medium enrichment fuel
4	high enrichment fuel
5	water reflector

Figure 14. CHD 7x7 Mesh for Zion 1

Figure 15. CHD 6x6 Mesh for Zion 1

.86373-2	.18924-1	.16186-1	.16557-1	.13081-1	.12137-1	.81502-2	.50333-2
.86033-2	.19081-1	.16151-1	.16681-1	.13038-1	.1222-1	.80999-2	.50674-2
.82708-2	.19269-1	.15549-1	.16883-1	.12602-1	.12525-1	.77702-2	.50876-2
	.33460-1	.35520-1	.29278-1	.28685-1	.21360-1	.18971-1	.97239-2
	.33448-1	.35688-1	.29263-1	.28782-1	.21322-1	.19079-1	.96752-2
	.32087-1	.36174-1	.28157-1	.29390-1	.20796-1	.20356-1	.99730-2
		.30382-1	.31166-1	.24540-1	.22470-1	.14610-1	.86935-2
		.30390-1	.31250-1	.24490-1	.22483-1	.14507-1	.87151-2
		.29167-1	.31873-1	.23754-1	.23268-1	.14184-1	.88534-2
			.25870-1	.25339-1	.18304-1	.14589-1	.60163-2
			.25854-1	.25301-1	.18247-1	.14524-1	.58641-2
			.24959-1	.25773-1	.17930-1	.15013-1	.59639-2
				.22194-1	.17293-1	.10359-1	
				.22258-1	.17106-1	.10444-1	
				.21990-1	.17471-1	.10344-1	
					.13337-1	.60815-2	
					.13466-1	.59063-2	
					.13411-1	.61032-2	

X	X
X	X
X	X

CHD 10x10 mesh

CHD 7x7 mesh

CHD 6x6 mesh

Figure 16 Assembly Power Fraction Comparison for Zion 1

1.6361	1.8002	1.5387	1.5856	1.2560	1.1758	0.7904	0.4954
1.6670	1.8262	1.5619	1.5978	1.2623	1.1712	0.7865	0.4857
1.6604	1.8413	1.5586	1.6097	1.2582	1.1792	0.7816	0.4890
1.5963	1.8595	1.5005	1.6292	1.2161	1.2087	0.7498	0.4910
	1.5873	1.6051	1.3990	1.3818	1.0318	0.9230	0.4786
	1.6144	1.7138	1.4127	1.3841	1.0306	0.9154	0.4692
	1.6139	1.7219	1.4119	1.3887	1.0293	0.9206	0.4668
	1.5482	1.7454	1.3586	1.4181	1.0034	0.9822	0.4812
		1.4490	1.4966	1.1813	1.0903	0.7092	0.4285
		1.4659	1.5038	1.1841	1.0842	0.7049	0.4195
		1.4663	1.5078	1.1816	1.0848	0.7000	0.4205
		1.4073	1.5379	1.1461	1.1227	0.6844	0.4272
			1.2439	1.2255	0.8872	0.7123	0.3013
			1.2482	1.2226	0.8832	0.7039	0.2903
			1.2475	1.2208	0.8804	0.7008	0.2829
			1.2043	1.2435	0.8651	0.7244	0.2878
				1.0749	0.8401	0.5104	
				1.0709	0.8344	0.4998	
				1.0739	0.8254	0.5039	
				1.0610	0.8430	0.4991	
					0.6516	0.3042	
					0.6435	0.2934	
					0.6497	0.2850	
					0.6471	0.2945	

X	X
X	X
X	X
X	X

PDQ-5 44x44 mesh
CHD 10x10 mesh
CHD 7x7 mesh
CHD 6x6 mesh

Figure 17. Assembly-Averaged-to-Core-Averaged
Power Ratios for Zion 1

3.2 Finite Element Method for Hexagonal Geometry

We have been investigating the application of the FEM to problems in hexagonal geometry, which is characteristic of the LMFBR or an HTGR. The work is now complete and a project report is forthcoming. In this report we will review some of the principle results of the study.

The particular objective of the study was to try and find appropriate element functions for hexagonal geometries. The appropriate element functions are those that permit high accuracy with little computing cost. Almost always computing cost increases with the number of unknowns, hence to seek low computing cost is synonymous with seeking representations with few unknowns. A standard finite difference code for use on hexagonal-geometry cores is the GA code BUGTRI. The mesh can be refined to very small spacings with BUGTRI. Much production analysis of HTGR's is done with a finite difference code GAUGE, which uses a fixed triangular mesh of the form shown in Fig. 1. GAUGE is reasonably accurate for analysis of an HTGR and any attempt to find improved methods must be superior to GAUGE. On the average GAUGE uses 3 unknowns/hex and this, then, is the practical upper limit to the number of unknowns that a higher-order method should require. Experience at GA indicates that GAUGE results are generally accurate to about $\pm 1/2\%$ in k_{eff} , and $\pm 7\%$ in power peaking factors. Thus, the constraints on the number of unknowns, and acceptable error limits define a narrow region in which to define element functions for a FEM.

One of the first considerations of the work was the shape of the region of definition of the element functions. There appear to be two logical contenders for use in hexagonal geometry. In Figure 2 we show a plausible shape for an element function which we call a "physical mesh". Note that the boundaries of the region are parallel to the physical boundaries of the hexagons. Further, within each of the elementary triangles making up to overall shape there are only two regions. Thus, if we were interested in putting detailed structure within a triangle, we would have only 1 interior interface. In Figure 3 we show another possible hexagonal region of definition which we call the "mathematical mesh". Note that the interior of each elementary triangle has 3 regions for this case.

Our initial experimentation with the physical mesh has indicated that it is not acceptable for use in reactor problems. All of the results reported subsequently are for the mathematical mesh.

The element functions to be constructed on the mathematical mesh are bivariate polynomials defined over triangles, and joined by continuity conditions at the interfaces between triangles. In general the continuity conditions alone are not sufficient to completely define the element function. The single exception to this statement is for the linear element, where the function is linear over each triangle, unity at the center and zero on the edges, and continuous at the interface.

For quadratic functions on triangles there are 6 coefficients.

The function continuity conditions yield only 5 coefficients and some additional constraint must be imposed. An example might be the constraint of zero current across the outer edge of the triangle. However, when an additional constraint is imposed then the element function may not be complete in the space of quadratic functions. The constraints on the number of unknowns per hexagon leads to a choice between low-order complete polynomial spaces and high-order incomplete spaces. We have done considerable experimenting with various types of spaces and we present some results below.

A number of incomplete cubic sets have been studied which have the property that they are also incomplete in the quadratic and linear spaces. Results obtained with these "totally" incomplete sets are compared with sets that are complete, which we term "shell" sets. The shell sets C_R are constructed so that C_1 is complete in the linear space, $C_1 + C_2$ are complete in the quadratic space, $C_1 + C_2 + C_3$ are complete in the cubic space, etc. The results are given in Table 1. It is apparent that, for this problem, it is far more important to retain completeness in a space, even a low-order space, than to use high-order incomplete polynomials.

The benchmark problem used in the test calculations corresponded to a small HTGR as shown in Figure 4. Each of the numbered segments in the figure is a set of 7 basic hexagons. The shaded outer region is the reflector. The fueled regions were uniform, except for the central hex of each segment which

had a control rod inserted. The power shapes within each segment are quite complex, and the problem is a severe test of any method.

It should be noted that the finite difference and finite element solutions in table 1 used slightly different outer boundary conditions, and hence the converged k_{eff} is slightly different for the two cases. In table 2 we show some further results where the boundary conditions were treated the same for both the finite difference and finite element methods. We also include some GAUGE results, as this is the competitive method.

The GAUGE calculation uses an average of 3 unknowns per hex whereas the C_1 shell set uses 1 and the $C_1 + C_2$ shell set uses 2. It is evident that the GAUGE results are better than either FEM result. In order for the FEM to compete it would be necessary to use a finer mesh, and hence more unknowns.

The conclusion from this particular study is that coarse mesh finite element methods are not better than finite difference methods for problems with detailed flux shape changes.

Table 1 Coarse Mesh Hexagonal FEM Results

Calculation Type	k_{eff}
1. BUGTRI Reference Solution	0.7708
2. C_1 Shell Set	0.7702
3. $C_1 + C_2$ Shell Set	0.7743
4. 1-element incomplete cubic set	0.6704
5. 2-element incomplete cubic set	0.6918
6. 3-element incomplete cubic set	0.6975

Table 2 FEM and GAUGE Hexagonal Results

Calculation Type	k_{eff}
1. BUGTRI Reference	0.7708
2. GAUGE-Fine Mesh	0.7690
3. FEM C_1 Shell Set	0.7595
4. FEM $C_1 + C_2$ Shell Set	0.7598

Figure 1 Gauge Finite Difference Mesh

Figure 2 Physical Mesh

Figure 3 Mathematical Mesh

Fig. 4 Small HTGR Core

3.3 Three Dimensional Finite Element Methods

The work on the Finite Element Method has been concentrated upon two-dimensional problems. In the past year we have begun work on a three-dimensional test code. The previous work has been convincing in demonstrating the use of Hermite cubic elements in 2D, rectangular geometries. We will continue to use such elements for the axial direction. The initial results are for linear elements, further tests with cubic Hermite and Spline elements for the axial dimension are under development.

The strategy used for solving the 3D problem is straightforward. A fission-source iteration method used with a simple Gauss-Seidel iteration in the z-direction. Within each plane, and energy group, the planar solution is obtained by a direct inversion. Other alternatives are possible and will be investigated in the future.

Two test problems have been used to test the program, and the use of linear elements. The axial profile of the assembly is shown in Figure 1. The FEM mesh is also shown on the Figure. A total of 16 unknowns are used in each axial plane. The reactor core was 90 cm high and a 20 cm reflector was added on the top and bottom. The mesh spacing axially was 10 cm and albedo boundary conditions were used at the top and bottom. The computed and analytic values of k_{eff} are shown in table 1.

A slight variation of the problem was also considered. In this test the reflectors were removed, but the material properties were varied linearly with the axial dimension.

A core height of 80 cms was used and a mesh spacing of 10 cms.

The resulting k_{eff} calculation is given in Table 2.

Table 1 k_{eff} Calculation for Reflected Homogeneous Problem

$$k_{\text{eff}} \text{ analytic} = 0.95069$$

$$k_{\text{eff}} \text{ computed} = 0.95106$$

Table 2 k_{eff} Calculation for Bare Homogeneous Problem

$$k_{\text{eff}} \text{ analytic} = 0.935887$$

$$k_{\text{eff}} \text{ computed} = 0.935877$$

cubic Hermite

Linear - 10 plane
albedo B.C.

Computed $k_{\text{eff}} = .951058$

Analytic $k_{\text{eff}} = .950715$

Figure 1. Horizontal and Vertical Profiles of Top & Bottom Reflected Reactor

4. SYNTHESIS METHODS

We have completed an analysis of the so-called "cell stitching synthesis technique" (10,11) for a two-dimensional, two-group model. The rather extreme case of a light water moderated and reflected reactor composed of assemblies containing cross-shaped control rods or water-holes (see Fig. 1) was examined. The results, some of which are given below, are encouraging.

The basic idea of the cell stitching technique is to express the group-g flux, $\phi_g(x,y)$, within each subassembly making up the reactor (see Fig. 1) as the product of a precomputed shape function $\psi_g^{(a)}(x,y)$ for the assembly and a finite element shape $U_g(x,y)$ having support only at the corners of the subassembly. To keep the complexity of the programming within bounds we have restricted attention to linear finite element shapes. Thus, for subassembly (i,j) occupying the area $h_x^i h_y^j \equiv (x_{i+1} - x_i)(y_{j+1} - y_j)$, $U_g(x,y)$ is written

$$U_g(x,y) = \phi_g^{(i,j)} \left(\frac{x_{i+1} - x}{h_x^i} \right) \left(\frac{y_{j+1} - y}{h_y^j} \right) + \phi_g^{(i+1,j)} \left(\frac{x - x_i}{h_x^i} \right) \left(\frac{y_{j+1} - y}{h_y^j} \right) \\ + \phi_g^{(i,j+1)} \left(\frac{x_{i+1} - x}{h_x^i} \right) \left(\frac{y - y_j}{h_y^j} \right) + \phi_g^{(i+1,j+1)} \left(\frac{x - x_i}{h_x^i} \right) \left(\frac{y - y_j}{h_y^j} \right) \quad (1)$$

With the shape functions (normalized to unity at the corner points) determined by a fine mesh, finite-difference solution for the subassembly alone (employing zero-net-current boundary conditions on the subassembly surface) the flux for group-g is then approximated by

$$\phi_g(x,y) = U_g(x,y) \psi_g^{(a)}(x,y) \quad (2)$$

Figure 1

Equations relating the $\phi_g^{(ij)}$'s are found by using expressions (2) in a variational principle ⁽¹²⁾ made stationary by the solution to the P-1 equations in energy group form and admitting of discontinuous trial and weight functions for both flux and current and for the corresponding weight functions. To simplify, we have used as current trial functions $-D_g \nabla \phi_g(x,y)$ where the $\phi_g(x,y)$ are approximated by Eq. (2). For weight functions we have used both the $\phi_g(x,y)$ themselves (Galerkin weighting) and adjoint quantities

$$\begin{aligned}\phi_g^*(x,y) &= U_g^*(x,y) \psi_g^{(a)*}(x,y) \\ J_g^*(x,y) &= D \nabla [U_g^*(x,y) \psi_g^{(a)*}(x,y)]\end{aligned}\tag{3}$$

where $\psi_g^{(a)*}(x,y)$ are solutions of the adjoint group-equations for the subassembly, and $U_g^*(x,y)$ is defined by (1) with the $\phi_g^{(ij)}$'s replaced by independent coefficients $\phi_g^{(ij)*}$.

For the reactor model shown in Figure (1) (having two group parameters for the three types of assembly as given in Table 1)

	Material (1)	Material (2)	Material (3)
D_1	1.436	1.092	1.545
Σ_1	0.02647	0.003185	0.028824
$\nu \Sigma_{f1}$	0.007293	0.0	0.0
Σ_{21}	0.01596	0.0	0.02838
χ_1	1.0	---	---
D_2	0.3868	0.3507	0.3126
Σ_2	0.1018	0.4021	0.008736
$\nu \Sigma_{f2}$	0.1531	0.0	0.0
χ_2	0.0	---	---

Table 1: Reactor Model Used to Test Stitching Method

Figures (2) and (3) show thermal flux traverses at $y=27$ cm and $y=63$ cm. These fluxes were obtained using shape functions $\psi_g^{(a)}(x,y)$ for the reflector boxes (pure water) taken from the full two-dimensional solution. This procedure was found to improve accuracy over what is obtained if completely flat values of the $\psi_g^{(a)}(x,y)$ are used. (Zero current boundary conditions lead to flat shapes for homogeneous material.) Such two-dimensional shapes would not of course generally be available if one were to analyse the problem by the cell synthesis method alone. However, one-dimensional shapes would serve just as well, or the whole reflector could be represented by a homogeneous boundary condition at the core-reflector interface (13).

In Figures (2) and (3) the solid curves are full core, fine mesh finite difference results. The dashed line is the linear finite element solution (i.e., all $\psi_g^{(a)}(x,y)=1$); the open circles are stitched solutions weighted by subassembly adjoint weight functions Eq. (3). The dots are stitched solutions with the expansion functions themselves used as weight functions (Galerkin weighting). The eigenvalues k_{eff} for the reactor for these four cases are respectively: 1.043, 1.040, 1.032, and 1.038.

The agreement in eigenvalue and flux shape for this very severe test of the method is encouraging, especially when it is recognized that the detailed finite difference result involved solving a 2401 mesh point problem whereas the cell-stitched solution (Galerkin weighted) required only two 225 point detailed subassembly solutions followed by a 49 point finite element solution. The figures show that the linear finite element solution for this

Figure 2: Thermal Flux at $y=27$ cm (Modified)

Figure 3: Thermal Flux at $y=63$ cm (Modified)

problem with 18 cm mesh spacings is extremely inaccurate. One dimensional results⁽¹⁾ suggest that a cubic Hermite finite element approximation would be little better for this highly heterogeneous case. Thus the cell stitching method appears to be an economical and accurate alternative for providing detailed flux shapes for certain classes of problems not amenable to economical finite difference or finite element analysis.

5. OTHER METHODS

5.1 Response Matrix Techniques

a) Static Studies

The response matrix technique described in last year's progress report ⁽¹⁾ has been programmed and investigated for two-group situations. Because of limited computing budget and computer code availability we have limited our study to the diffusion theory model for computing response matrices. This is somewhat unfair to the response matrix method since its potential for dealing with complicated spatial, angular or energy neutron behavior is thereby neglected. Nevertheless, since both the response matrices and the full core "truth" problem are analysed by the same diffusion theory model and are solved by the finite difference technique employing the same spatial mesh sizes, a fairly unambiguous evaluation can be made of one essential approximation of the response matrix technique. Specifically, errors arising from the fact that the partial currents entering and leaving the faces of a node must be assumed to have some simple shape (flat, linear, piecewise flat, quadratic, etc.) over those faces can be evaluated.

Various assumptions about the spatial shape of incoming and outgoing partial currents were studied for a reactor model essentially the same as that shown in Figure (1) (the only difference being that the control rods were assumed to be thinner and blacker). Assuming that partial currents have a linear shape on the nodal surfaces led to the results shown in Table (1).

Table (1)

Power Fractions Predicted by Response Matrix Technique
assuming linear partial current shape on nodal surfaces

Assembly # (see Fig. 1)	Group	Power Fraction	
		<u>Full Core Finite Difference</u>	<u>Response Matrix Technique</u>
9	1	.004279	.004321
9	2	.01648	.01670
10	1	.007124	.007230
10	2	.03017	.03079
11	1	.007835	.007864
11	2	.02863	.02644
17	1	.01111	.01108
17	2	.03289	.03171
18	1	.01299	.01307
18	2	.04902	.04900
25	1	.01432	.01425
25	2	.04239	.04089

The k_{eff} for the core was computed to be 1.044 by finite difference method and 1.039 by the response matrix technique. The agreement is encouraging and suggests that the linear shape approximation for partial currents on the nodal surfaces is adequate for light water moderated reactors of the PWR-BWR type.

b) Dynamic Studies

Extending the response matrix technique to the analysis of transient situations is not a trivial problem. To understand some of the difficulties it is only necessary to consider a simple one-group reactor model in slab geometry. If we partition the

reactor into nodes extending from x_i to x_{i+1} , $i=1,2,\dots,(I-1)$, the appropriate time-dependent response matrix equations for node (i) are

$$\left. \begin{aligned} J_i^-(t) &= \int_{-\infty}^t R_i^+(t,\tau) J_i^+(\tau) d\tau + \int_{-\infty}^t T_{i+1}^-(t,\tau) J_{i+1}^-(\tau) d\tau \\ J_{i+1}^+(t) &= \int_{-\infty}^t T_i^+(t,\tau) J_i^+(\tau) d\tau + \int_{-\infty}^t R_{i+1}^-(t,\tau) J_{i+1}^-(\tau) d\tau \end{aligned} \right\} \quad (4)$$

where the $J_i^\pm(t)$ are the partial currents in the (+) and (-) directions across the nodal surface at $x=x_i$. The $R_i^+(t,\tau)$ and $R_i^-(t,\tau)$ are reflection "matrices" (scalars in the one group problem) defined as the partial current at $x=x_i$ in the (-) or (+) directions at time, t , due to unit input partial currents at $x=x_i$ in the (+) or (-) direction at time, τ . Finally $T_i^+(t,\tau)$ and $T_{i+1}^-(t,\tau)$ are transmission matrices defined as the partial currents at time, t , in the (+) and (-) directions at $x=x_{i+1}$ and $x=x_i$ due to unit input currents at time τ in the (+) direction at $x=x_i$ or the (-) direction at $x=x_{i+1}$. These reflection and transmission matrices are defined with the slab material between x_i and x_{i+1} located in a vacuum.

By finding the response matrices (R's and T's) for all nodes making up the reactor and solving simultaneously equations similar to (4) for all nodes the $J_i^\pm(t)$'s can be determined, and by finding auxiliary response matrices specifying the power level in node (i) at time t due to unit currents entering its faces at time τ , the power histories of all the nodes can then be determined.

Conceptually this procedure is straightforward. However a number of practical difficulties arise in implementing it. First

of all, because the nodes in general contain fissionable material, the response matrices must account for both prompt and delayed neutron effects. Thus they have a significant magnitude for values of $(t-\tau)$ up to minutes in length. Secondly, they must account for feedback effects the magnitude of which are unknown until the problem unfolds. Thus it appears that the response matrices cannot be computed a priori. Finally, the response matrices are not separable functions of t and τ . (They cannot even be written as functions of $(t-\tau)$ - i.e., as displacement kernels.) Thus to advance the solution of (4) from t to $t+\Delta t$ it appears necessary to use values of $J_i^+(\tau)$ for all past times.

During the past year we have investigated these difficulties and, we believe, largely resolved them. The key to the resolution is to separate prompt and delayed neutron effects. Thus we create auxiliary response matrices specifying the creation rate of delayed neutron precursors due to unit input currents on the nodal surfaces. We assume this creation rate is essentially instantaneous and that the distribution of precursors so created is spatially flat. We also define matrices specifying the rates at which neutrons escape from the nodes due to the decay of a unit, spatially flat source of delayed neutrons. All response matrices then refer to very fast processes. Thus the time integrals in Eq. (4) (rewritten adding extra terms to account for currents due to delayed neutrons) are determined by values of τ close to t . In addition we now assume that the response matrices appearing in these integrals depend on the instantaneous conditions of the material comprising the node. Thus we can update such matrices as the calculation proceeds.

We were led to this approach by examining the nature of response matrices computed (neglecting feedback effects) for homogeneous slabs by a one-group diffusion theory model, solutions being obtained by finite difference methods. Figure (4) shows some typical results for a 15 cm thick slab having properties characteristic of a LWR. It can be seen that, after an extremely fast, initial transient period, both R and T decay with the same, very fast ($\sim e^{-4000t}$) decay constant and then die away with a period characteristic of delayed neutrons. (The curve D(t) gives the rate at which the outgoing currents due to delayed neutrons emitted with a flat distribution at $t=0$, die away.) The advisability of separating prompt and delayed effects and the legitimacy of assuming constant nodal properties during the fast part of the decays is strongly supported by these curves.

An additional approximation that greatly eases the problem of finding the time dependent response matrices is also suggested by these curves. The fact that, after the very short transient period, the prompt decay period is the same for R, T and D(t) suggests that the neutrons involved in this decay belong to the fundamental ω -prompt mode, the solution of

$$D\nabla^2 \phi_\omega + [v\Sigma_f(1-\beta) - \Sigma_a - \frac{\omega}{v}] \phi_\omega = 0 \quad (5)$$

This in turn suggests that the prompt behavior of the response matrices can be expressed as a simple exponential decay. Thus we write, for example

$$R_i^+(t, \tau) = a_i^+ e^{\omega(t-\tau)} \quad (6)$$

Figure 4

where ω (a large negative number) is the eigenvalue of Eq. (5) written for node-i in a vacuum.

The coefficient a_i^+ can then be determined by imposing the rigorous relationship between static and time-dependent response matrices, namely that

$$R_{i\infty}^+ = \int_{-\infty}^t R_i^+(t, \tau) = -\frac{a_i^+}{\omega} \quad (7)$$

It appears then that a valid approximation (Eq. (6) and the analogous expressions for $T_i^+(t, \tau)$ and $D(t, \tau)$) for time dependent response matrices can be determined by finding the fundamental prompt decay period, ω , and static response matrices (such as $R_{i\infty}^+$) for the node with material properties characteristic of time t . We can thus determine time-dependent response matrices by solving only static problems.

The procedures outlined above have been successfully tested for several simple transients for reactors characterized by constant D 's and Σ 's. During the coming year we plan to extend this validation to a wider range of parameters that may be time-varying. The ultimate goal is to reduce the running time for space dependent transient reactor analysis by calculating time dependent partial currents on the surfaces of the nodes rather than time dependent fluxes throughout the nodes.

5.2 Connections Between Finite Element and Higher Order Nodal Methods

Finite element methods employing cubic Hermite interpolating polynomials as the element functions have been shown to yield accurate flux shapes and eigenvalues for large power reactors composed of large nuclearly homogenized nodes. Moreover such methods have a firm mathematical foundation, and, under certain conditions, precise statements about the dependence of rates of convergence on spatial mesh size can be made. Unfortunately efficient methods of solving the finite element equations have not yet been found so that even though the number of unknowns to be determined may be reduced by a factor of, say, 10, the running time may be reduced by only a factor of 2.

In contrast to this situation, certain higher order nodal methods ⁽¹⁴⁾ for analysing this type of reactor problem have been made very fast-running (essentially because the difference equations involved have the same form as conventional finite difference equations). However the theoretical foundation of these methods is not firm, and their accuracy must be established entirely empirically.

During the past year we have put some effort into bridging the gap between these two complementary approaches. The mathematical technique that makes such a connection possible is the method of collocation. This may be described as a weighted residual or variational method in which the weight functions, rather than being the expansion functions themselves (the Galerkin method), are Dirac delta functions. Thus the flux trial function is still expressed as a sum of finite element type expansion functions. However the combining coefficients are found by substituting that trial function

into the defining group diffusion equations and requiring the result to be valid at particular points rather than to be valid in an integral sense when multiplied by a weight function and integrated over the region where that weight function is non-zero. The advantage of this approach is that precise mathematical statements about the accuracy of the method can be made. In fact, with a proper choice of weight function and a given order of expansion polynomial its accuracy is equivalent to that of the finite element function. However the equations for the combining coefficients involve much less coupling and are closer to those of the nodal method than to conventional finite element equations. (We have not, however, been able to derive exactly the nodal equations of Reference (14) by this approach.) Currently we are examining the accuracy of this collocation approach when applied to the static group diffusion equations in one dimension. If results are encouraging, we intend to extend the scheme to two dimensions.

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