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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 E(11-1)-2262 during fiscal year 1976. 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. 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 the response matrix method, Section 5 deals with collocation methods, section 6 is a discussion of nonlinear methods for finite element equations, and the last section deals with determination of equivalent contents.

2. METHODS FOR TIME DEPENDENT PROBLEMS

2.1 Finite Difference Methods

Much of the past work on this project has been concerned with solution of few-group, diffusion theory kinetics problems by finite difference methods^(1,2,3). The time-dependent spatially differenced equations can be written in the form

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

with $\underline{x}$ a column vector of the flux and precursor values at each spatial mesh point. The matrix A is a large, but relatively sparse, matrix. It has the property of being "stiff", that is the range of values of the eigenvalues of A span many decades.

Direct methods of solution of Eq. (1) may be severely limited by stability conditions for explicit methods, or severely limited by computing effort per step for implicit methods. We have been examining a variety of splitting methods for solving Eq. (1). The objective of the splitting methods is to generate stable methods of solution for which the computing effort for each step is small. In past work we have examined alternating direction implicit⁽³⁾, alternating direction explicit⁽²⁾, and "checkerboard"⁽⁴⁾ splittings. All of the methods are stable and require a small amount of computing time per step. Unfortunately the methods also

Fig. 1a ADI Discretization

Fig. 1b Modified ADI Discretization

suffer from a large temporal truncation error and hence require quite small time steps, particularly in comparison with implicit methods.

2.1.1 The Modified Alternating Direction Implicit Method

Recently some work has been reported by Werner⁽⁵⁾ on a splitting method that allowed the use of large time steps. This method is a modification of the ADI scheme. In Fig. 1a we show a simple mesh and the way in which an ADI method advances the solution. The points marked I are solved for simultaneously, while the points marked E are kept at their current value. In the usual ADI scheme the direction of the implicit solution is rotated each half-step.

The Werner scheme is shown in Fig. 1b. The solution is again obtained implicitly along an x-line. However the latest values of the solution at all points are used. (The figure assumes the x-lines are solved from bottom to top).

Mathematically the Werner scheme is simply a different splitting of the A matrix than the usual ADI scheme. The truncation error is of the same form and order but with different definitions of the splitting matrices. In order to illustrate this point we consider the following simple example of a two-dimensional, one-group, one-delayed group problem. The matrix A for a structure as shown in Eq. (2)

$$A = \left[\begin{array}{c|c} \text{diag} & \text{diag} \\ \hline \text{diag} & \text{diag} \end{array} \right] \quad (2)$$

A nonsymmetric ADI splitting would be defined as

$$\underline{x}^{n+1} - \underline{x}^n = \frac{\Delta t}{2} [A_1 \underline{x}^{n+1} + A_2 \underline{x}^n] \quad (3)$$

with

$$A_1 = \left[\begin{array}{c|c} \text{diag} & \text{diag} \\ \hline \text{diag} & \text{diag} \end{array} \right] \quad (4a)$$

and

$$A_2 = \left[\begin{array}{c|c} \text{diag} & \text{diag} \\ \hline \text{diag} & \text{diag} \end{array} \right] \quad (4b)$$

For the second-half step we have

$$\underline{x}^{n+2} - \underline{x}^{n+1} = \frac{\Delta t}{2} [A_3 \underline{x}^{n+2} + A_4 \underline{x}^{n+1}] \quad (5)$$

where

$$A_3 = \begin{bmatrix} \diagup & & & \\ & \diagup & & \\ & & \diagup & \\ & & & \diagup \end{bmatrix} \quad (6a)$$

$$A_4 = \begin{bmatrix} \diagdown & & & \\ & \diagdown & & \\ & & \diagdown & \\ & & & \diagdown \end{bmatrix} \quad (6b)$$

The Werner scheme would be written

$$\underline{x}^{n+1} - \underline{x}^n = \frac{\Delta t}{2} [A_1' \underline{x}^{n+1} + A_2' \underline{x}^n] \quad (7)$$

with

$$A_1' = \left[\begin{array}{c|c} \begin{array}{c} \diagup \\ \diagup \\ \diagup \\ \diagup \end{array} & \begin{array}{c} \diagdown \\ \diagdown \\ \diagdown \\ \diagdown \end{array} \\ \hline \begin{array}{c} \diagdown \\ \diagdown \\ \diagdown \\ \diagdown \end{array} & \begin{array}{c} \diagup \\ \diagup \\ \diagup \\ \diagup \end{array} \end{array} \right] \quad (8a)$$

and

$$A_2' = \left[\begin{array}{c|c} \begin{array}{c} \diagdown \\ \diagdown \\ \diagdown \\ \diagdown \end{array} & \begin{array}{c} \diagup \\ \diagup \\ \diagup \\ \diagup \end{array} \\ \hline \begin{array}{c} \diagup \\ \diagup \\ \diagup \\ \diagup \end{array} & \begin{array}{c} \diagdown \\ \diagdown \\ \diagdown \\ \diagdown \end{array} \end{array} \right] \quad (8b)$$

The second half-step would be

$$\underline{x}^{n+2} = \underline{x}^{n+1} = \frac{\Delta t}{2} \left[A_3' \underline{x}^{n+2} + A_4' \underline{x}^{n+1} \right] \quad (9)$$

with

$$A_3' = \left[\begin{array}{c|c} \begin{array}{c} \diagup \\ \diagup \\ \diagup \\ \diagup \end{array} & \begin{array}{c} \diagdown \\ \diagdown \\ \diagdown \\ \diagdown \end{array} \\ \hline \begin{array}{c} \diagdown \\ \diagdown \\ \diagdown \\ \diagdown \end{array} & \begin{array}{c} \diagup \\ \diagup \\ \diagup \\ \diagup \end{array} \end{array} \right] \quad (10a)$$

and

$$A_4 = \begin{bmatrix} & & & \\ & & & \\ & & & \\ & & & \end{bmatrix} \quad (10b)$$

The truncation error for the ADI method is

$$TE_{ADI} = h^2 [A - A_1 - A_3] A \quad (11a)$$

while for the Werner method the truncation error is

$$TE_W = h^2 [A - A_1^1 - A_3^1] A \quad (11b)$$

Thus, the truncation errors have the same order of convergence but may have different numerical coefficients due to the slightly modified definitions of A_1^1 and A_3^1 .

Much of the early work on this project has compared various AD methods and we find the nonsymmetric ADE method to be optimal in the sense of accuracy and computing time. We have tested the Werner method against the NSADE method for two problems. The first problem is a two-group problem we call test case 2. The data is given in Fig. 2, and Tables 1 and 2. Table 3 shows the calculated NSADE results for the thermal flux at the center of the perturbed zone of the assembly for different time step sizes. The present deviations are

Number of neutron groups - 2
Number of precursor groups - 1

Geometry:

$$\Delta x = 8.0\text{cm}$$

$$\Delta y = 8.0\text{cm}$$

Numbers indicate material compositions.

Fig. 2 Two Dimensional Test Case

Delayed Constants:

$$\lambda_1 = .08, \quad \beta_1 = .0075, \quad f_{11} = 1.0, \quad f_{21} = 0.0$$

	<u>GROUP 1</u>	<u>GROUP 2</u>
V	$.1 \times 10^8$	$.2 \times 10^6$
X	1.0	0.0

Material Properties:

Materials 1 and 2

	<u>GROUP 1</u>	<u>GROUP 2</u>
D	1.4	1.4
Σ_c	.0065	.05
ν	2.1877	2.1877
Σ_f	.0035	.1
$\Sigma_{g \rightarrow g+1}$	0.01	0.0

Material 3

	<u>GROUP 1</u>	<u>GROUP 2</u>
D	1.3	0.5
Σ_c	.0065	0.02
ν	2.1877	2.1877
Σ_f	.0015	.03
$\Sigma_{g \rightarrow g+1}$	.01	0.0

Table 1. Test Case 2 Data

Perturbation inducing transient:

Material 1

GROUP 2

Positive ramp: $\Delta \Sigma_c = \begin{cases} -.0035 (t/.2); & 0 \leq t \leq .2 \\ -.0035 & ; t \geq .2 \end{cases}$

Table 2 Test Case 2 Data

Table 3 - Thermal Flux Results for the NSADE Method

<u>Time (secs)</u>	<u>h = 0.0005</u>	<u>h = 0.001</u>	<u>h = 0.005</u>	<u>h = 0.0125</u>
0.0	.3212	.3212	.3212	.3212
0.05	.3665	.3653 (-.33%)	.3315 (-9.5%)	.3364 (-11%)
0.10	.4318	.4325 (+.16%)	.3620 (-16%)	.3391 (-21%)
0.15	.5246	.5228 (-.34%)	.4296 (-18%)	.3594 (-31%)
0.20	.6652	.6647 (-0.8%)	.5494 (-17%)	.3903 (-41%)

Table 4 - Thermal Flux Results for the Werner Method

<u>Time (secs)</u>	<u>h = 0.0005</u>	<u>h = 0.001</u>	<u>h = 0.005</u>	<u>h = 0.0125</u>
0.0	.3212	.3212	.3212	.3212
0.05	.3688	.3537 (-3.5%)	.3290 (-10%)	.3252 (-11%)
0.10	.4308	.4428 (2.5%)	.3470 (-20%)	.3350 (-22%)
0.15	.5257	.5278 (.61%)	.3841 (-27%)	.3485 (-34%)
0.20	.6652	.6484 (-2.5%)	.4515 (-32%)	.3664 (-45%)

Critical Configuration 3

Number of neutron groups - 2

Number of precursor groups - 1

Geometry

$\Delta x = 10.0\text{cm}$

$\Delta y = 10.0\text{cm}$

Numbers indicate material compositions.

Fig. 3 Two Dimensional Test Problem

Delayed Constants:

$$\lambda_1 = .08, \quad \beta_1 = .0075, \quad f_{11} = 1.0, \quad f_{21} = 0.0$$

	<u>GROUP 1</u>	<u>GROUP 2</u>
V	$.1 \times 10^8$	$.2 \times 10^6$
X	1.0	0.0

Material Properties:Materials 1 and 2

	<u>GROUP 1</u>	<u>GROUP 2</u>
D	1.4	1.4
Σ_c	.0065	.05
ν	2.1877	2.1877
Σ_f	.0035	.1
$\Sigma_{g \rightarrow g+1}$	0.01	0.0

Material 3

	<u>GROUP 1</u>	<u>GROUP 2</u>
D	1.3	0.5
Σ_c	.0065	0.02
ν	2.1877	2.1877
Σ_f	.0015	.03
$\Sigma_{g \rightarrow g+1}$	.01	0.0

Table 5 Test Case Data

Material 5

$$\Sigma a_1(t) = \begin{cases} 1.040206 \times 10^{-2} & , 0 \leq t \leq 7.5 \\ 1.040206 \times 10^{-2} + 3.85 \times 10^{-4} \times \frac{1}{40}(t-7.5), & 7.5 \leq t \leq 47.5 \\ 1.078706 \times 10^{-2} & , t > 47.5 \end{cases}$$

$$\Sigma a_2(t) = \begin{cases} 3.76217 \times 10^{-2} & , 0 \leq t \leq 7.5 \\ 3.76217 \times 10^{-2} + 2.66 \times 10^{-3} \times \frac{1}{40}(t-7.5), & 7.5 \leq t \leq 47.5 \\ 9.032217 \times 10^{-2} & , t > 47.5 \end{cases}$$

Table 6 Test Case Data

calculated by assuming the value at $h = .0005$ seconds are "truth". The truncation error grows approximately linearly with Δt as expected. (Note that the truncation error expression, Eq. (11a), is for the error on one step, i.e. the local truncation error. The global error should be proportional to the local truncation error divided by h , or $O(h)$ in this case).

The same problem was run using the Werner method. The results are given in Table 4. It is apparent that the modified ADI method is not superior to the NSADE. Further the modified method required slightly longer computing time.

We ran various modifications of the methods including solutions of all group simultaneously. The general conclusion remained valid, that is the modified method is not better than the NSADE in regard to truncation error on running time.

The results reported by Werner⁽⁵⁾ included a problem with a slow ramp reactivity insertion for which large time step sizes were possible. We tested this identical problem using the NSADE method. The problem data is given in Fig. 3 and Tables 5 and 6. Results are given in Table 7 which show that the NSADE is again equivalent to the modified ADI (MADI) method. Further the running time of the NSADE is always less than the MADI method. We therefore conclude that the new method is not an improvement on past results.

2.1.2 Frequency Transformation

The temporal truncation error in various splitting methods has been shown to be improved by use of a change of variable which we call a frequency transformation. The original system of equations may be transformed by the change of variable

$$\underline{x} = e^{\underline{\Omega} t} \underline{z} \quad (12)$$

with $\underline{\Omega}$ a diagonal matrix to be determined. Inserting Eq. (12) into Eq. (1) yields

$$\frac{d\underline{z}}{dt} = e^{-\underline{\Omega} t} (\underline{A} - \underline{\Omega}) e^{\underline{\Omega} t} \underline{z} = \underline{A}(\underline{\Omega}) \underline{z} \quad (13)$$

If the behavior of $\underline{x}(t)$ is nearly exponential then we expect $\underline{z}(t)$ to be smooth in time. Thus, it is hoped a low-order temporal approximation may be satisfactory to calculate $\underline{z}(t+\Delta t)$ from $\underline{z}(t)$.

Past results have suggested that a unique value of the frequency for each mesh point should be computed. The most effective scheme found to date is based upon a pointwise calculation in the form

$$\underline{\Omega}_i = \frac{1}{h} \ln \frac{x_i(t)}{x_i(t-\Delta t)} \quad (14)$$

for point i . The value of $\underline{\Omega}_i$ computed as above, Eq. (14), is then used to find $x(t+\Delta t)$. Note that the frequency trans-

formation thus makes the solution at $t+\Delta t$ become a function of t and $t-\Delta t$. Thus the solution behaves as a second-order system. Indeed we do observe the feedback of the frequency solution onto the solution. In particular, for some problems we see underdamped behavior of the results for certain size time steps.

We have investigated a variety of alternative frequency solution methods to that given in Eq. (14). Among various methods we have tried are the following: define Ω from

$$\Omega \underline{x}_n = A \underline{x}_n \quad (15)$$

This could be called the "instantaneous frequency". Note however that small changes in any component of $\underline{x}$ can induce large changes in the corresponding component of Ω . Indeed, by experiment we have found the method to be unstable.

Another method is to use

$$e^{\Omega h} \underline{x}_n = e^{Ah} \underline{x}_n \quad (16)$$

but this requires knowing e^{Ah} which is, after all, the exact solution being sought. Nevertheless, various approximations to Eq. (16) can be used, such as

$$e^{\Omega h} \underline{x}_n \approx (I + hA) \underline{x}_n \quad (17a)$$

or

$$e^{\Omega h} \underline{x}_n \approx (I - h/2 A)^{-1} (I + h/2 A) \underline{x}_n \quad (17b)$$

Experiments with such methods led to stability problems.

Another scheme was tried involving a smoothing of the frequencies. A relation such as Eq. (17a) was used to calculate a value, say $\hat{\omega}_i$, and this was smoothed using the previous value of $\omega_i(t-\Delta t)$ in the form

$$\omega_i(t) = \frac{1}{2} [\hat{\omega}_i + \omega_i(t-\Delta t)]$$

Unfortunately, the smoothing did not prevent instabilities, but only delayed their occurrence.

A final modification was introduced based on an idea by Werner⁽⁶⁾ of using an average frequency for each group, but which is space independent. The group fluxes and precursor concentrations were averaged over the core and these values fit with an exponential as in Eq. (14). The approach was useful for problems with weak space dependence, i.e. space independent transients. However, for problems with a large spatial shift in the flux the method was worse than the usual NSADE method.

A completely independent variation of the original frequency transform method was examined to see if any improvement in the truncation error was possible. The original scheme, and the one used in the NSADE method, is written

$$\underline{x}(t+\Delta t) = B(\Omega, \Delta t) \underline{x}(t) \quad (18)$$

with

$$B(\Omega, \Delta t) = e^{\Omega h} [I - h(A_3 - \Omega)]^{-1} [I + hA_4] * \\ [I - h(A_1 - \Omega)]^{-1} [I + hA_2] e^{\Omega h} \quad (19)$$

where $h = \Delta t/2$.

A more general representation might be

$$B(\Omega, \Delta t) = e^{\Omega \Delta t} \left\{ e^{-\Omega t_3} [I - h(A_3 - \Omega)]^{-1} e^{\Omega t_3 - \Omega t_4} * \right. \\ \left. [I + hA_4] e^{\Omega t_4} \right\} \left\{ e^{-\Omega t_1} [I - h(A_1 - \Omega)]^{-1} e^{\Omega t_1 - \Omega t_2} * \right. \\ \left. [I + hA_2] e^{\Omega t_2} \right\} \quad (20)$$

with

$$t_1, t_2 \in [0, h] \\ t_3, t_4 \in [h, 2h]$$

If we take $t_1 = t_2 = h = t_3 = t_4$ then we recover the original method. [This scheme was motivated by results of Hendricks⁽⁴⁾ in studying the use of the frequency transformation for the checkerboard method].

A very general study, including many choices of t_1, t_2, t_3, t_4 indicate that there is no noticeable difference in methods, at least for the ADE method. This result is in contrast to the results found by Hendricks for the checkerboard method, when stability was strongly dependent upon the

particular choices of t_1 , t_2 , t_3 and t_4 .

The conclusions reached from all of these experiments are detailed in a thesis reported as Reference 7. The general conclusions are that the NSADE remains the best overall splitting method, that the original frequency selection method and problem formulation are as good as any alternates, and finally that further improvements in kinetics methods will probably be found by other methods than splitting, or in entirely separate approaches such as the finite element method.

2.2 Finite Element Kinetics

Recent work in the study examining the application of finite element methods to reactor kinetics problems has considered additional analyses in Point Kinetics beyond those reported on in Reference 12, and analyses in two dimensions using one and two neutron groups.

2.2.1 Point Kinetics

Work in this area has examined two additional methods to the Hermite method described in References 8 and 12 that may be used with piecewise polynomial approximations to the neutron density and the precursor concentrations - a) a "Finite Element" approach and b) a Weighted Residual approach.

The point kinetics equations may be written in matrix form as:

$$\frac{d}{dt} \phi(t) = A(t) \phi(t)$$

(1)

where $\phi(t) = \text{col}\{n(t), C_1(t), \dots, C_I(t)\}$

$$A(t) = \begin{bmatrix} \frac{\rho(t) - \beta}{\Lambda} & \lambda_1 & \dots & \lambda_I \\ \beta_1/\Lambda & -\lambda_1 & & \\ \vdots & & \ddots & \\ \beta_I/\Lambda & & & -\lambda_I \end{bmatrix}$$

and I is the number of delayed neutron precursor groups.

Assume that a piecewise linear polynomial in time will be used to approximate the neutron density, $n(t)$, and the precursor concentrations, $c_i(t)$, i.e.

$$\phi(t) \approx \tilde{\phi}(t) = \tilde{\phi}_n^{0+}(t) + \tilde{\phi}_{n+1}^{0-}(t)$$

(2)

where

$$u_n^{0+}(t) = \begin{cases} (t_{n+1} - t)/\Delta t & t_n \leq t \leq t_{n+1} \\ 0 & \text{otherwise} \end{cases}$$

(3a)

$$u_{n+1}^{0-}(t) = \begin{cases} (t - t_n)/\Delta t & t_n \leq t \leq t_{n+1} \\ 0 & \text{otherwise} \end{cases}$$

(3b)

The "Finite Element" approach in time would proceed as follows:

1. Substitute the approximate solution given by equation (2) into the governing equation, (1).
2. Weight by $U_n^{0+}(t)$ and integrate from t_n to t_{n+1} .
3. Substitute the approximate solution for the time interval $[t_{n-1}, t_n]$ into the governing equation.
4. Weight by $U_n^{0-}(t)$ and integrate from t_{n-1} to t_n .
5. Combining the results, you obtain a relation of the form

$$B_{n+1} \overset{\uparrow}{\phi}_{n+1} = B_n \overset{\uparrow}{\phi}_n + B_{n-1} \overset{\uparrow}{\phi}_{n-1} \quad (4)$$

In the Weighted Residual approach⁽¹³⁾, you proceed as in steps (1) and (2) above, however, instead of weighting by $U_n^{0+}(t)$, you weight by $U_{n+1}^0(t)$. This yields a relation of the form

$$B_{n+1} \overset{\uparrow}{\phi}_{n+1} = B_n \overset{\uparrow}{\phi}_n \quad (5)$$

Equations (4) and (5) were used to solve for the results of a transient involving a positive ramp change ($\rho = \frac{\beta}{2} t$) in the reactivity of an initially critical thermal reactor. The precursor constants for this problem are given in Table 1, and $n(0) = 1.0$.

The results obtained for the neutron density at $T = 1$ sec. and $T = 2$ secs. are presented in Table 2. Also presented are the results obtained when the Hermite method is used with a

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 - POSITIVE RAMP
LINEAR PIECEWISE POLYNOMIALS
 $\rho = \frac{\beta}{2}t; \quad \Lambda = 5 \times 10^{-4} \text{ sec.}$

T(sec.)	Δt	Hermite	"Finite Element"	"Weighted Residual"	
1.0	0.5	1.9144001 (-1.83)*	2.0059683 (2.87)*	1.9646154 (.75)*	
	0.1	1.9482021 (-9.2x10 ⁻²)	2.0975429 (7.75)	1.9611691 (.57)	
	0.05	1.9495497 (-2.3x10 ⁻²)	2.0117334 (3.17)	1.9560554 (.31)	
	0.01	1.9499808 (-9.2x10 ⁻⁴)	1.9530412 (.16)	1.9512843 (.07)	
	0.005	1.9499942 (-2.3x10 ⁻⁴)	1.9507647 (.04)	1.9506461 (.03)	
	ORDER OF CONV.*	1.92	1.71	.95	
2.0	0.5	11.145270 (-.74)	9.9735595 (-11.18)	14.713169 (31.04)	
	0.1	11.243498 (.13)	11.900124 (5.98)	11.924599 (6.20)	
	0.05	11.232274 (3.5x10 ⁻²)	11.525365 (2.65)	11.564200 (2.99)	
	0.01	11.228529 (1.4x10 ⁻³)	11.243230 (.13)	11.293671 (.58)	
	0.005	11.228411 (3.5x10 ⁻⁴)	11.232114 (.03)	11.260909 (.29)	
	ORDER OF CONV.*	1.97	1.68	1.02	

*ORDER OF CONVERGENCE, AND % ERROR (GIVEN IN ()) ARE BASED ON:

$$n(1.0) = 1.9499987$$

$$n(2.0) = 11.228372$$

FROM CONVERGED CUBIC HERMITE SOLUTION FOR THIS PROBLEM.

linear approximation to the neutron density and the precursor concentrations. Percent errors, based on the converged solution are also given.

The results indicate that the Hermite method is a generally superior to both the "Finite Element" and the "Weighted Residual" approaches to treating the time dependence, both in terms of accuracy and order of convergence.

Use of a quadratic Lagrange approximation to the time dependent behavior of the neutron density and the precursor concentrations was also examined with the Hermite and Weighted Residual methods. The results obtained for the problem mentioned above when either of these methods is used with quadratic Lagrange elements were generally inferior, both in terms of accuracy and order of convergence, to those obtained with a simple linear approximation and the Hermite method.

2.2.2 Space Dependent Kinetics

The precursors integrated out form of the source free time dependent neutron diffusion equation is

$$\begin{aligned} \frac{1}{v(E)} \frac{\partial}{\partial t} \phi = & \left\{ \nabla \cdot D \nabla - \Sigma_f \right\} \phi + \int_E dE' \left\{ \Sigma_3(E' \rightarrow E) + \right. \\ & \left. (1-\beta) \Sigma(E) v \Sigma_f \right\} \phi + \\ & \sum_{i=1}^I \left\{ \lambda_i(E) \lambda_i C_{i0} e^{-\lambda_i t} + \lambda_i \beta_i \Sigma_i(E) \int_0^t e^{-\lambda_i(t-s)} \right. \\ & \left. * \int_E dE' v \Sigma_f \phi(E', s) ds \right\} \end{aligned} \quad (6)$$

with appropriate initial, boundary and continuity conditions.

If the standard few group approximation is made for the energy dependence, and if the spatial domain is discretized according to the Finite Element Method, the resulting equations may be written in matrix form:

$$V \frac{\partial}{\partial t} a(t) = \left\{ -L(t) + S + (1-\beta)F \right\} a(t) + \sum_{i=1}^I \left\{ \lambda_i C_{i0} e^{-\lambda_i t} + \lambda_i \beta_i \int_0^t e^{-\lambda_i(t-s)} F_d a(s) ds \right\} \quad (7)$$

Application of the Hermite method to (7) leads to a single step equation of the form:

$$B_{n+1} \hat{a}_{n+1} = B_n \hat{a}_n + \sum_{i=1}^I \left(e^{-\lambda_i t_n} - e^{-\lambda_i t_{n+1}} \right) d_{in} \quad (8)$$

(The details of going from equation (6) to equation (8) are contained in Reference 2).

A number of problems have been considered:

1. One neutron group, two dimensions

A homogeneous, square reactor 40cm x 40cm with group constants:

$$V = 2.2 \times 10^5 \text{ cm}^3/\text{sec.}$$

$$D = 0.4 \text{ cm}^2/\text{sec.}$$

$$\Sigma_T = 0.2 \text{ cm}^{-1}$$

$$v\Sigma_f = (0.218 \text{ cm}^{-1}) - \text{nominal value; a critical } v\Sigma_f$$

was found for each set of spatial basis functions and mesh sizes.

was subjected to a ramp change in reactivity given by

$$\Sigma_T(t) = \Sigma_{T_0} (1 - 0.01t)$$

Six delayed neutron groups were considered (Table 1).

The calculations were performed for $0 \leq t \leq 0.5\text{sec.}$

using both bi-linear and bi-cubic basis functions in

space, and the Hermite method with both linear and

cubic approximations in time. The cubic Hermite

equations were approximated by using second order

finite differences to replace the time derivatives at

t_n and t_{n+1} with appropriate linear combinations of

the unknowns at t_{n-1} , t_n and t_{n+1} . This resulted in a

"three level" formula for the "approximate" cubic Hermite

case rather than the "two-level" form represented by

equation (8). Time step sizes of $\Delta t = 0.1, 0.05, 0.01$

and 0.0005secs. were considered with spatial meshes

of $\Delta x = \Delta y = 10\text{cm}$ and 20cm for the bi-cubic spatial

basis functions, and $\Delta x = \Delta y = 10\text{cm}$ and 5cm for the

bi-linear spatial basis functions.

2. Two neutron groups, two dimensions

The heterogeneous, but symmetric reactor shown in

Figure 1 was subjected to three perturbations which

were induced by changing the group-2 capture cross-

section in the cross-hatched seed region in the fol-

lowing fashion:

(a) Positive step: $\Delta \Sigma_c = -.0035$

(b) Positive ramp: $\Delta \Sigma_c = -.0035 (t/.2) \quad 0 \leq t \leq .2$
 $= -.0035 \quad t > .2$

(c) Negative ramp: $\Sigma_c = t.03 (t/.02) \quad 0 \leq t \leq .02$
 $= t.03 \quad t > .02$

These problems used bi-linear basis functions in space and the Hermite method with linear piecewise polynomials to approximate the time behavior. Two spatial meshes were considered, as indicated in Figure 1, along with time steps of $t = 0.01, 0.005$ and 0.001 secs.

The solution procedure used for all the space dependent problems was Cholesky factorization along with forward elimination, back substitution to solve for the in-group fluxes, and a source iteration to perform the outer iterations required in the case of the two-group problems.

A number of preliminary observations may be made based on the results of these calculations.

1. One-Group

- (a) The linear Hermite method converges as approximately order $(\Delta t)^2$. Its stability is relatively insensitive to the spatial mesh size, and to whether bi-linear or bi-cubic polynomials are used in the spatial domain.
- (b) The "approximate" cubic Hermite method tends to oscillate, and appears to be affected by

both the spatial mesh size, and the order of the spatial approximation. Consequently, this approach has been discarded.

2. Two Group

- (a) Solutions for all the problems were stable for $\Delta t = .001$ secs. and for both spatial meshes.
- (b) The solutions for the negative ramp oscillated "slightly" for $\Delta t = .01$ and $.005$ secs with both spatial meshes.
- (c) The solution for the positive step oscillated with the "finer" spatial mesh for both $\Delta t = .01$ and $.005$ secs and with the "coarse" spatial mesh for $\Delta t = .01$.
- (d) Solutions for both the positive step and the positive ramp are quite accurate if the solution at $\Delta t = .001$ secs is taken as "exact", while the results for the negative ramp are generally very poor. (Table 3 presents the percent error in the thermal flux at the center of the reactor for a number of time points for all three perturbations).

TABLE 3
PERCENT ERROR IN THE THERMAL FLUX
AT THE CENTER OF THE REACTOR OF FIGURE 2

T	POSITIVE STEP	
	$\Delta t = 0.01$	$\Delta t = 0.005$
.01	- 1.98	0.94
.02	3.17	1.41
.03	0.12	0.94
.04	1.75	0.49
.05	- 0.64	0.24

T	POSITIVE RAMP	
	$\Delta t = 0.01$	$\Delta t = 0.005$
.05	0.0	-0.16
.10	0.0	0.0
.15	- 0.04	-0.04
.20	- 0.10	0.0
.25	- 2.21	-0.97

T	NEGATIVE RAMP	
	$\Delta t = 0.01$	$\Delta t = 0.005$
.01	10.84	-3.55
.02	-24.22	0.38
.03	31.06	7.51
.04	7.29	7.16

- (1) PERCENT ERRORS ARE BASED ON ASSUMPTION THAT $\Delta t = 0.001$ SOLUTIONS ARE "EXACT"
- (2) THE "FINE" SPATIAL MESH IN FIGURE 1 WAS USED.

Figure 1
Geometry and Constants
for 2-Group, 2-Dimensional Calculations

$$\lambda_1 = 0.8 \quad \beta_1 = .0075 \quad \chi_{d11} = 1.0 \quad \chi_{d21} = 0.0$$

$$V_1 = 1 \times 10^7 \text{ cm/sec} \quad V_2 = 2 \times 10^5 \text{ cm/sec} \quad \chi_1 = 1.0 \quad \chi_2 = 0.0$$

	D_1 (cm)	D_2 (cm)	Σ_{a1} (cm ⁻¹)	Σ_{a2} (cm ⁻¹)	Σ_{r1}
Seed	1.4	0.4	0.01	0.15	0.01
Blanket	1.3	0.5	0.008	0.05	0.01
	$\nu \Sigma_{fi}^*$ (cm ⁻¹)		$\nu \Sigma_{f2}^*$ (cm ⁻¹)		
Seed	7.6570265×10^{-3}		2.1877218×10^{-1}		
Blanket	3.2815828×10^{-3}		6.5631655×10^{-2}		

*These are nominal values. A critical $\nu \Sigma_{fg}$ was calculated for each spatial mesh prior to transient calculations.

3. FINITE ELEMENT METHODS

The finite element method has been used in structural mechanics for a number of years. Application of the method to neutron diffusion problems has been of considerable interest in recent years. The work on this project has concentrated on the use of Hermite polynomials for element functions. Kang⁽⁸⁾ showed how to couple the functions to satisfy current continuity conditions in one-dimensional problems. For two-dimensional problems he showed how to select a reasonably small set of functions to provide accurate solutions at singular points. The results of Kang's work, and that of Deppe⁽⁹⁾ and Kautz⁽¹⁰⁾ have led to the general conclusion that cubic elements provide an accurate spatial solution on a reasonably coarse mesh, i.e. mesh points at each corner of an assembly.

The results of the above work indicate that finite element solutions can achieve accuracies comparable to fine-mesh finite difference calculations with many fewer unknowns than finite difference methods. However, the finite element computing times are just as long as the finite difference computing times. This occurs because the finite difference matrices are more complicated than the finite difference matrices. There are more nonzero coupling coefficients in the finite element method.

The finite element results were obtained by a semi-

iterative scheme in which the fission source strength is estimated and then the group fluxes calculated by a direct inversion, using the Cholesky factorization scheme. We have undertaken a systematic study of the use of iterative methods for both the group fluxes and fission source⁽¹¹⁾. This is particularly important for three-dimensional problems where the number of unknowns per group will be too large to permit direct inversion.

A number of comparison calculations are shown in Table 1 where the Cholesky method is compared with the SOR method. The procedure was to use the Cholesky method in each axial plane, or an inner iteration using SOR. After a new solution was found at each plane one outer iteration was complete. In some instances a Chebyshev extrapolation was used for the outer iteration. Such cases are marked "yes" in the Table. A "no" means no outer acceleration.

It is clear from the results that an SOR scheme without acceleration is equivalent to the Cholesky scheme for the smallest number of unknowns. As the number of unknowns increases the superiority of the SOR method becomes very obvious. Furthermore, it is relatively easy to use the Chebyshev acceleration for the SOR method and to further improve the rate of convergence. We found it very difficult to apply the extrapolation to the Cholesky method in a stable

Table 1 - Some overall results to compare SOR versus
Cholesky Factorization , plus extrapolation data.
(Code CHDZL)

Inner Iter. Extrapolation	Cholesky no	SOR no	SOR yes	Cholesky no	SOR yes	Cholesky no	SOR yes
No.AxialPlanes	9	9	9	17	17	9	9
No.Unks/Plane	32	32	32	32	32	128	128
k-eff	.9354708	.9354852	.9354708	.9358649	.9358824	(.9380816)	.9354815
Fast/Thermal Flux ratio,000	3.364282	3.364205	3.364225	3.364168	3.363442	-	3.364139
Dominance Ratio	-	-	.6716115	-	.6489813	-	.7315012
(10^4)k-eff Convergence	4.2945	4.4484	4.2945	.2374	.0504	-	4.3341
No. inner iterations	-	12	9	-	9	-	10
No. outer iterations	25	25	18	39	24	9	17
CPU-min	.272	.339	.226	.909	.619	3.981	1.434
No. I/O Operations	133	123	123	133	126	116	123

manner. Thus the comparisons are always with extrapolation for SOR but not for the Cholesky scheme. The results clearly indicate that iterative method for the finite element method are to be preferred.

The selection of element functions for the axial direction was investigated along with the study of iterative versus direct methods. Cubic elements have been shown to be approximately optimal in two-dimensional problems in that they provide reasonable accuracy for the computing cost. The use of linear elements requires more computing time than cubic elements for the same accuracy. Elements of higher order than cubics are not justified since the material heterogeneities will not permit a mesh coarser than the assembly size itself, and elements of higher-order then use more unknowns than cubics.

It is not clear that a similar argument would hold in the axial direction since material properties are usually rather slowly changing in the axial direction. Comparisons were made using linear and cubic axial elements for several problems, including a bare homogeneous core, a 3-region reflected reactor, and a reactor with continuously varying material composition.

Table 2 shows a comparison of data for the three-region, two-group problem. The results suggest that linear elements on a coarse mesh appear almost as satisfactory as cubic

Table 2 - Overall results for the 3-Regions
Problem using Linear and Cubic
Hermite in z through CHDZL and CHDZC

	Linear expansion in z - CHDZL			Cubic in z CHDZC
Iteration	SOR without Extrapolat.	SOR without Extrapolat.	Cholesky without Extrapolat.	SOR without Extrapolat.
No. Axial planes	11	19	19	11
Unknowns/plane	32	32	32	64
k-eff	.9510739	.9511698	.9511908	.9512900
Fast/Thermal flux ratio, 000	3.358271	3.359533	3.359598	3.357919
No. Outer Iters.	40	51	51	40
No. Inner Iters.*	7.16	6.5	-	9.2
CPU-min.	.820	1.327	1.752	2.578

*- Average no. per outer iteration

elements on the same mesh. Further, the computing time for the linear elements is much less than for the cubic elements.

Table 3 shows comparative data for the thermal flux distribution. The cubic element distribution is more accurate than the linear results, for either mesh spacing. This is particularly true at the core-reflector interface. However, the overall results suggest that linear elements are satisfactory.

The principle motive for investigating the finite element method is to see if it provides an economic means of generating accurate solutions for three-dimensional diffusion theory problems. The earlier work led to the conclusions that iterative methods should be used to solve the algebraic equations, and that linear elements were satisfactory for use in the axial direction.

A complex, three-dimensional benchmark problem was used to provide an exacting comparison between the finite difference and finite element method. The problem was developed at Munich⁽¹⁴⁾ and is referred to as the LRA benchmark problem. The core layout and mesh configuration is shown in Figs. 1 and 2. The compositions are given in Reference 14 and will not be repeated here.

The finite element results used cubic elements in each radial plane, and linear elements in the axial direction.

Table 3 - Normalized Thermal Flux for the
Three-Regions Problem as
obtained through CHDZL and CHDZC
(10^{-2})

Z	Analytic	Linear in z			Cubic z 11-SOR
		11-SOR	19-SOR	19-CHLSKY	
0	1.05427	1.0637	1.05669	1.05667	1.0559
5	1.04300	-	1.04334	1.04333	-
10	1.00944	1.0190	1.00783	1.00782	1.0143
15	.954301	-	.95104	.95103	-
20	.878766	.88573	.87423	.87423	.88600
25	.784447	-	.77913	.77914	-
30	.673367	.68412	.66720	.66722	.68176
35	.548101	-	.54551	.54553	-
40	.419833	.39028	.37613	.37615	.43137
41	.401272	-	-	-	-
42	.393387	-	-	-	-
42.5	.396830	-	-	-	-
43	.408277	-	-	-	-
44	.471289	-	-	-	-
45	.635557	.51716	.50852	.50854	.61019

The LRA Benchmark Core layout

Fig. 1 - Mesh arrangements for the 3D-
LRA Benchmark Problem

Fig. 2 - Blocks and Planes specifications for the 3D-LRA Benchmark Problem.

Eigenvalue comparisons are given for a number of finite element calculations, and comparisons with PDQ-7 finite difference results in Table 4. (Some nodal results for other codes used in developing the LRA problem are included.)

The thermal flux in the core midplane is shown in Fig.3 for a diagonal line from the core center. The discrepancy is very large, ~ 25% between the results. It is unclear which code is closer to the exact answer, as a detailed calculation would be prohibitively expensive. In order to estimate the quality of the two solutions a time-mesh, two-dimensional PDQ-7 calculation was performed for the central plane with an assumed axial buckling. The comparison suggested that the PDQ-7 3-D flux shape was more accurate than the CHDZL results. By extrapolating from calculated 2D results, and small 3D calculations we can estimate computing costs and accuracy comparison for PDQ-7 and CHDZL. Table (5.1) shows actual 3D cost comparisons and Table (5.2) shows estimated costs to achieve acceptable accuracy. Note that the finite element running times were longer but total costs due to smaller amounts of I/O. However the results are sensitive to the type of charging scheme used at a computing center. More detailed results and comparisons are given in Reference 11.

The conclusions drawn from this study are the following:

Table 4 - Overall Results for the 3D-LRA
Benchmark Problem

CODE	CHDZL				PDQ-7	QUABOX/ CUBBOX	DANO (1GRP)
Mesh	7x7	8x8	8x8	8x8	33x33	19x19	18x18
No. Axial Planes	10	10	11	11	17	16	18
Core Fraction	1/4	1/4	1/4	1/8*	1/8	1	1
Unknowns/ Plane-Group	154	208	208	208	1089	361	312
k-eff	.994756	.995636	.995014	.996050	.997307	.99530	.99935
ϵ_{λ}^+ , 10^{-4}	.37	1.4	1.6	.78	.295	-	-
ϵ_{ϕ}^+ , 10^{-3}	2.7	3.7	3.2	3.2	.95	-	-
Outer Itrs.	30	30	30	40	29	-	-
Inner Itrs.	4.1	4.38	4.15	11.18	-	-	-
Relax Fac. 1	1.3594	1.1956	1.1967	1.2347	-	-	-
Relax Fac. 2	1.2913	1.2934	1.2940	1.3701	-	-	-
I/O-Operats.	208	236	4783	6292	30491	-	-
CPU-min.	8.244	14.842	13.416	22.218	18.154	-	-
ϵ_{SOR}^+ , 10^{-3}	5	5	5	1	-	-	-

* Axial Symmetry - Z-mesh space = 1/2 of 1/4 core case.

+ Convergence Criteria.

Table (5.1) - Computing Costs and No. of Unknowns for the 3D-LRA Benchmark Problem as evaluated through PDQ-7 and CHDZL.

CODE	PDQ-7	CHDZL
Mesh	33x33x16	8x8x11
No. of unknowns(2Grp)	34848	4576
No. Outer Iters.	30	40
CPU-min	18.154	22.218
Running Time, min.	33.470	25.994
I/O Ops.	30965	15740
Cost, \$	425.35	321.53

Table (5.2) - Estimated Costs, Accuracy, and escalated No. of Unknowns for the 3D-LRA Benchmark Problem.

CODE	PDQ-7	CHDZL
Mesh	78x78x51	11x11x37
NO.of Unknowns(2Grps)	620568	31672
No. Outer Iters.	100	300
Scaling Factor	59.36	51.91
Estimated CPU-Hour	17.96	19.22
Estimated Cost , \$	25,248.57	16,690.61
Estimated Error , %	2	5

1. Iterative methods should be used for solving the FEM algebraic equations. No detailed study of iterative methods was performed beyond the standard SOR method.
2. The FEM can provide solutions of equal accuracy to finite difference solutions for roughly the same computing costs, but with fewer unknowns.
3. Unless the FEM algebraic system can be simplified, or fast methods of solutions developed, there is little motive to change from finite difference to finite element physics codes for static calculations.
4. Since the FEM results use fewer unknowns than finite difference methods it may be attractive to consider FEM's for kinetics calculations, even if the initial static solution determination is not cheaper than finite difference.

4. THE RESPONSE MATRIX TECHNIQUE FOR TIME DEPENDENT PROBLEMS

During the past year we have developed a method for analyzing reactor transient problems by response matrix techniques and have applied it to slab geometry problems using a one-group diffusion theory model. The results are reported in detail in Reference (14).

For the one-group model, if we partition the slab 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

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

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 (+) direction 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 equations similar to (1) for all nodes the $J_i^+(t)$'s can be determined, and by finding auxiliary response matrices specifying the power level in node (i) at time t due to unit current entering its faces at time τ , the power histories of all the nodes can then be determined.

We reported in the 1975 annual Progress Report⁽¹²⁾ that the problem of representing the reflection and transmission matrices in Eq. (1) is greatly simplified if delayed neutrons are treated separately and assumed to be distributed uniformly throughout the node and if prompt parts of the response matrices are assumed to depend on the instantaneous reactor conditions.

We also reported in Reference (12) that a simple exponential representation of the time dependent matrices was possible. It seemed adequate to fit matrices such as $R_i^+(t, \tau)$ by

$$R_i^+(t, \tau) = a_i^+ e^{\omega(t-\tau)} \quad (2)$$

where a and a_i^+ are found by matching to the zeroth moment (equal to the static response matrix for the node) and to the prompt asymptotic decay constant of the exact result. (Both

of these quantities may be found by solving static problems.)

Further study however indicated that the contribution to the asymptotic delayed precursor population of the very fast decaying transient nodes is lost by this matching process.

Instead we found it much more accurate to approximate the

$R_i^+(t-\tau)$ and $T_i^+(t-\tau)$ by expressions such as

$$R_i^+(t-\tau) = A S(t-\tau) + a e^{\omega(t-\tau)} \quad (3)$$

where the constant A is now available to account for contributions to the delayed precursor population from modal components of the transient caused by the initial burst of incoming current. We again set ω equal to the time constant of the prompt die-away mode and find A and a by matching the exact zeroth and first moments. Thus we require that

$$R_0 \equiv \int_t^\infty R_i^+(t-\tau) d\tau \Big|_{\text{exact}} = A + a/\omega \quad (4)$$

$$R_1 \equiv \int_t^\infty (\tau-t) R_i^+(t-\tau) d\tau \Big|_{\text{exact}} = a/\omega^2 \quad (5)$$

As mentioned before, R_0 is the static response function. The first moment can be found as the derivative of the Laplace transform of R_i^+ .

$$R_1 = \frac{d}{ds} R_i^+(s) \Big|_{s=0} \quad (6)$$

For a heterogeneous cell $\frac{d}{ds}R_i^+(s)$ can be found numerically by finding $R_i^+(s)$ for, say, three values of s , fitting the result to a quadratic function of the transform variable, s , and taking the derivative as $s \rightarrow 0$.

If the material properties of the node vary in time, it is sufficient to represent the response matrices in the form Eq. (3) but with ω changing in time with the material properties. It is when such feedback effects are present that dealing with prompt and delayed neutrons separately becomes essential if the equations are to remain tractable. With the spatial distribution of delayed precursors assumed flat, an expression of the form (3) can be used to give output partial currents from a unit source of delayed neutrons having that flat distribution. The parameters in the expression will depend on the material properties of the node at the time that the delayed neutrons are emitted. Thus in all the response expressions such as Eq. (3), the ω 's are large in magnitude.

In order to test the validity of the approximations made, several typical problems were solved using computer codes RESKINPAR and RESKINCAL, the former to calculate the parameters of individual slabs and the latter to perform the reactor calculation.

One test problem for a heterogeneous assembly dealt with four slabs as shown in Figure (1). The two central slabs are

heterogeneous, but have symmetry with respect to their center lines. The compositions of the different homogeneous regions are presented in Table (1).

Fig. 1
Heterogeneous Slab Reactor

TABLE 1. DATA FOR HETEROGENEOUS SLAB PROBLEM

SLAB	REGION	L(cm)	D(cm)	$\Sigma_f(\text{cm}^{-1})$	$\Sigma_a(\text{cm}^{-1})$
1	1	15.0	0.15	0.0	0.01
2	2	7.0	0.30	0.02	0.04
	3	1.0	0.15	0.0	0.015
	4	7.0	0.30	0.02	0.04
3	5	7.0	0.30	0.02	0.04
	6	1.0	0.15	0.0	0.015 $\rightarrow$ 0.05 linear $0 \rightarrow 10^{-2}$ sec
	7	7.0	0.30	0.02	0.04
4	8	15.0	0.15	0.0	0.01

Slabs 1 and 4 have the same material composition, simulating a "water reflector". Slabs 2 and 3 are heterogeneous. Each contains two "fueled regions" separated by a "water slot".

The transient studied was a linear increase in Σ_a in the water slot region 6, in slab 3, representing the insertion of a control rod into a fuel assembly.

Since the relation between the response parameters and Σ_a is not linear, parameters of slab 3 had to be calculated for five values of Σ_a over the total range of variation (0.014 to 0.5cm^{-1}). RESKINCAL interpolates other values linearly at each time step.

For the other three (unchanged) slabs, only one set of parameters is necessary. Slabs 1 and 4 have identical parameters and slab 2 has the same set of parameters as the initial condition of slab 3. Thus, only six sets of parameters had to be calculated, and only three were used at any given time. These sets of parameters are presented in Table 2.

A great advantage of the response method is that heterogeneous cells are represented by the same number of parameters no matter how complex their internal structure. The main advantage, however, is the reduced number of unknowns in the kinetics calculation. In this case only eight partial cur-

TABLE 2. PARAMETERS OF SLABS FOR HETEROGENEOUS SLAB PROBLEM

	SLABS 1 & 4	SLAB 3					
		$\Sigma_{a6}=0.025^*$	$\Sigma_{a6}=0.1$	$\Sigma_{a6}=0.2$	$\Sigma_{a6}=0.3$	$\Sigma_{a6}=0.4$	$\Sigma_{a6}=0.5$
ω	3214.62	2218.56	3812.43	5035.62	5836.81	6389.56	6789.54
A	0.74751	0.71674	0.65164	0.60211	0.56922	0.54773	0.53358
a/ω	0.10791	0.24141	0.26305	0.29678	0.32229	0.33941	0.35062
B	-0.00786	-0.05310	-0.03831	-0.02779	-0.02093	-0.01599	-0.01274
b/ω	0.01348	0.12958	0.07224	0.04690	0.03353	0.02500	0.01952
D	0.06261	0.05836	0.04908	0.03986	0.03398	0.03157	0.02895
d/ω	0.16898	0.46785	0.32708	0.28290	0.26456	0.25309	0.24669
F	0.0	0.00170	0.00140	0.00114	0.00097	0.00089	0.00080
f/ω	0.0	0.01088	0.00779	0.00685	0.00647	0.00624	0.00611
G	0.0	0.00046	0.00023	0.00014	0.00007	0.00007	0.00006
g/ω	0.0	0.03068	0.01866	0.01454	0.01271	0.01160	0.01094

* Also slab 2, constant properties

rents are necessary in the costly time dependent problem.

The resulting fluxes at the interfaces between slabs are shown in Fig. 2. Similar calculations using the finite difference code GAKIN II⁽¹⁵⁾ (also shown in Fig. 2) require the use of as many as 60 mesh points, thus requiring 60 dependent variables in the time dependent calculation.

Fig. 3 shows the flux as a function of position at $t = 0$ and $t = 0.1$ sec. Also shown is the flux obtained using response kinetics calculation dividing the reactor into eight homogeneous slabs. The differences in the values of the flux, compared with GAKIN II results is due to the assumption of uniform delayed-neutron precursor distribution, here not a good assumption because of the small size of the reactor and consequent large flux curvature.

It is clear from Fig. 3 that GAKIN II results provide much more detail about the neutron population. But, since important quantities like the average flux, average power or flux at peak points can be obtained from the response kinetics solutions when and where needed, one concludes that Response Matrix Techniques save effort expended by finite-difference methods to determine results of little importance.

We conclude that the response method developed performs kinetics calculations with an accuracy comparable to that obtained from finite difference solutions. It does so in a much shorter time and with a small storage requirement.

Fig. 2. HETEROGENEOUS PROBLEM: FLUX. VS. TIME

Fig. 3. HETEROGENEOUS PROBLEM: FLUX. VS. POSITION

5. COLLOCATION 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 or even less.

In contrast to this situation, certain higher order nodal methods⁽¹⁶⁾ for analyzing 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 completed an effort that bridges 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 function 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. Moreover, 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 tested the method for static problems in both one and two dimensions using both Lagrange and Hermite interpolating polynomials to approximate the flux within nodes and deriving the approximate flux equations using variational principles made stationary by both the P-1 and diffusion theory approximations to the transport equation. Detailed results are reported in Reference⁽¹⁷⁾.

Expanding the fluxes within a node in cubic Hermite polynomials and requiring that this form fit the diffusion equation in a weighted integral sense seems to yield the most efficient procedure. The weight functions, rather than being Hermite polynomials as in the finite element method⁽⁸⁾, are Dirac delta functions. Thus the approximate polynomial expressions for the group fluxes throughout a given node are required to obey the group diffusion equations at certain particular mesh points (collocation points) within the nodes. In one dimension there are optimal locations for these collocation points. Thus with cubic polynomials and a mesh interval extending from x_i to x_{i+1} ($h_i \equiv x_{i+1} - x_i$) there are two optimal locations t_{ik} ; $k = 1, 2$ for collocation. They are given by

$$t_{ik} = (x_i + x_{i+1} + \rho_k h_i) / 2 \quad ; \quad k = 1, 2 \quad (7)$$

where

$$\rho_1 = 1/\sqrt{3} \quad ; \quad \rho_2 = -1/\sqrt{3}$$

This collocation procedure has been applied to a one-dimensional two energy group reactor physics problem⁽⁶⁾ in which the solution interval is $[0, L]$ with $L = 60\text{cm}$. The material properties within the region, $[0, 20]\text{cm}$, are like those in the water reflector of a light water reactor. The region $[20\text{cm}, 60\text{cm}]$, has material properties like those in a light water reactor core. Zero flux boundary conditions are imposed at

$x = 0$ and zero current conditions are imposed at $x = 60\text{cm}$.

Figure 4 is a graphic description of the problem and a graph of the thermal flux computed using fine mesh FD equations⁽⁸⁾.

Table 3 shows computed values for the eigenvalue, the thermal (energy group 2) flux at $x = 40\text{cm}$, $\phi_2(40)$, and integrated flux, $\int_0^L \phi_2(x) dx$, when $|\rho|$ is taken equal to $\frac{1}{\sqrt{3}}$.

The results are excellent. Errors are acceptable for $h = 20\text{cm}$, and convergence rates appear to be approaching the theoretical value of 4. For comparison, finite element (cubic Hermite polynomials) results with $h = 20\text{cm}$ are $\lambda = 1.02145$, $\phi_2(40) = .81027$, and $\int_0^L \phi_2(x) dx = 37.970$ ⁽⁶⁾.

5.1 Effect of Collocation Point Location

In order to assess the effect of collocation point location on solution accuracy and convergence, the example problem was solved with various values of ρ in Eq. (7). Figure 5 shows graphs of the errors in the approximate eigenvalue, λ , and approximate flux at $x = 40\text{cm}$, $\phi_2(40)$, for $h = 20\text{cm}$ versus ρ . Examination reveals that, as theoretically predicted, accuracy and convergence are best when the collocation points are located near the Gaussian points. Near these points the dependence of solution accuracy on ρ seems to be mild.

In order to test further the capabilities of the collocation method, the IAEA two-dimensional two-group benchmark problem (see reference 18) was solved. Figure 6 is a graphic

Figure 4
Description of the One-dimensional Two-group Problem.

Computed values			
h (cm)	λ	$\phi_2(40)$	$\int_0^L \phi_2(x) dx$
20	1.02022	.80060	37.816
10	1.02023	.78761	38.217
5	1.02080	.79054	38.428
2.5	1.02090	.79126	38.472
Reference	1.02091	.79133	38.478

Flux normalization: $\phi_2(60) = 1.0$

Table 3

Results for One-dimensional Two-group Problem,

$$|\rho| = 1/\sqrt{3} \approx .57735.$$

Figure 5
Effect of Collocation Point Placement on Solution Accuracy.

Numbers in the upper right hand corner of each assembly refer to the material composition. ✓

Axial buckling = $.8 \times 10^{-4}$ for all regions and energy groups.

Figure 6

Description of Two-dimensional IAEA Benchmark Problem.

description of the problem. Materials 1 and 2 are characteristic of fuel assemblies in a light water reactor, the group parameters for material 3 are similar to those for a light water reactor fuel assembly with a control rod present, and material 4 is characteristic of a water reflector. Figure 7 shows the errors in the approximate assembly average powers obtained using 20cm mesh spacing throughout the region of solution. The reference solution is a finite difference calculation in which 1cm mesh spacing was used throughout⁽¹⁸⁾.

The results are disappointing; 18 percent error is unacceptable. However, we note that the errors are largest in those nodes close to the fuel-reflector interface. This interface has required special treatment when finite element methods have been used⁽¹⁹⁾.

As a test of this hypothesis, a second solution for the two-dimensional IAEA problem was obtained, this time using 6.666cm mesh spacing for $x > 110\text{cm}$ and $y > 110\text{cm}$ (20cm mesh was used for $x < 110\text{cm}$ and $y < 110\text{cm}$, as before). In this case, most nodes contiguous to the fuel-reflector interface are treated with a refined mesh. The exceptions are the nodes (refer to Figure 6) $I = 6, J = 6$; $I = 7, J = 5$; and $I = 8, J = 3$. In these nodes the mesh has not been refined in the x and/or y direction.

The results are shown in Figure (8). They support the hypothesis that more effective treatment of interfaces where

Error (%) in approximate average assembly power
for IAEA problem; 20cm mesh.

Figure 7

Results for Two-dimensional IAEA Benchmark Problem,
Coarse Mesh.

Error (%) in approximate average assembly power
for IAEA problem, 6.666cm mesh for $x > 110\text{cm}$
or $y > 110\text{cm}$.

Figure 8

Results for Two-dimensional IAEA Benchmark Problem,
Locally Refined Mesh.

large material discontinuities exist should improve the accuracy of the collocation approximations.

Even with the smaller mesh spacing near the reflector interface, the results for the collocation method are somewhat inferior to those obtained by the standard finite element method (for which the maximum error in the average assembly power was found to be ~ 7% with 20cm mesh spacing used throughout the region of solution⁽¹⁰⁾). The collocation points for the calculations leading to Figures (7) and (8) were determined by applying Eq. (7) for each direction separately. However, in two dimensions, there is no longer any mathematical reason to expect that the choice will be optimal. Evidently it is not, since the standard finite element method based on the same polynomial flux expansions, yeilds more accurate results (although at the cost of solving more complicated equations for the polynomial expansion coefficients). Since in three dimensions the efficiency of the standard finite element method seems inferior to that of the finite difference method, and since the same collocation equations (although cheaper to solve) yield less accurate results, we do not plan at present to investigate the collocation method further.

6. NON-LINEAR METHODS FOR SOLVING FINITE ELEMENT EQUATIONS

The unknowns of the finite element equations are much more extensively coupled to one another than those of the finite difference equations. For example use of the simple linear element function leads to a coupling of 9 points in two dimensions and 27 in three dimensions (compared to 5 and 7 points for finite difference equations). The increased computation time per unknown for finite element equations is certainly partly due to this increased coupling.

During the past year we have looked at non-linear methods for decreasing the degree of coupling among the unknowns. For example, in the two-dimensional linear finite element case, the flux ϕ_{ij} at point (i,j) is coupled to eight other fluxes, (those at $(i \pm 1, j)$, $(i, j \pm 1)$, $(i \pm 1, j \mp 1)$ and $(i \mp 1, j \pm 1)$). Thus the matrix to be inverted at any given step, n , of the iteration process is nine-stripe. If, however, the fluxes $\phi_{i+1,j+1}^{(n)}$, $\phi_{i+1,j-1}^{(n)}$, $\phi_{i-1,j-1}^{(n)}$ and $\phi_{i-1,j+1}^{(n)}$ at iteration n are replaced by (for example) $[\phi_{i+1,j+1}^{(n-1)} / \phi_{ij}^{(n-1)}] \phi_{ij}^{(n)}$, $[\phi_{i+1,j-1}^{(n-1)} / \phi_{ij}^{(n-1)}] \phi_{ij}^{(n)}$, etc. (where superscript $(n-1)$ refers to a previous iteration) the matrix becomes 5-stripe, and the standard methods applied to finite difference equations can be used to invert it.

We have investigated non-linear methods of this type as well as those that apportion the corner-point fluxes at iteration- n

partly (or wholely) to the side-face fluxes ($\phi_{i+1,j}^{(n)}$, $\phi_{i,j+1}^{(n)}$, etc.).

Results have been generally discouraging. The iterations needed to invert the 5-stripe matrix that results (the coefficients of which have to be up-dated as the calculations proceed) either diverge or converge very slowly. We were unable to find a systematic, problem-independent way to improve the efficiency with which the original nine-joint equations can be solved.

7. THE DETERMINATION OF EQUIVALENT HOMOGENIZED GROUP-PARAMETERS

Most of the practical numerical methods for solving the group diffusion equations for large reactor geometries such as finite difference, nodal, and finite element methods are prohibitively expensive unless large regions of the reactor can be homogenized by determining "equivalent" homogeneous diffusion theory parameters. The most common method of finding such parameters is to flux-weight the spatially dependent cross sections and diffusion coefficients over the region to be homogenized by estimating the flux shape in that region *a priori*.

For example, the spatially constant cross section for reaction α , energy group g , and volumes i is defined as:

$$\Sigma_{\alpha g}^i = \frac{\int_{V_i} \Sigma_{\alpha g}(r) \phi_g(r) dV}{\int_{V_i} \phi_g(r) dV} \quad (8)$$

Two mathematical inconsistencies exist in such a flux-weighting procedure. First, even if $\phi_g(r)$ can be accurately predicted *a priori*, $\int_{V_i} \phi_g(r) dV$ is unlikely to equal $\int_{V_i} \bar{\phi}_g(r) dV$, where $\bar{\phi}_g(r)$ is the flux shape found using the equivalent constants in the reactor problem. Unless these two integrals are equal for all volumes i , the integrated reaction rates will not be preserved. Second, flux-weighting the spatially dependent diffusion coefficient (or even its inverse, as in the most common procedure) is theoretically unsound and has little physical significance for large heterogeneous zones.

A particular scheme for finding "equivalent" diffusion theory parameters for slab geometry by matching fluxes and currents on the boundaries of the slab has been examined and found to be highly successful for symmetric slabs⁽²⁰⁾. Recently, the response matrix technique has been used in determining "equivalent" parameters for two-dimensional, two-group diffusion problems. It was found that for a symmetric, heterogeneous assembly, two-group equivalent diffusion parameters, constant over the entire assembly, could be calculated. When used to represent the subassemblies making up a full-core, these diffusion constants result in a prediction of the integrated reaction rates for each assembly that is more accurate than that obtained when flux-weighted constants are used.

In the new method⁽²¹⁾ the equivalent constants are found essentially by matching the response matrices of the heterogeneous subassembly to those of the equivalent homogenized subassembly.

Suppose for example that the heterogeneous subassembly has a square cross section, has 90° rotational symmetry about its axis and contains a cross shaped control rod.

If, for simplicity, we consider a one-group diffusion theory model, a spatially flat partial current of neutrons entering one face of the square will give rise to a flux $\phi(\underline{r})$ throughout the heterogeneous assembly and to reflected, sideways-transmitted and through-transmitted partial currents

R, S and T. Application of Eq. (8) will then give a first order approximation to $\bar{D}^{(1)}$, $\bar{\Sigma}_a^{(1)}$ and $\bar{\nu}\bar{\Sigma}_f^{(1)}$, the one-group homogenized parameters.

If then, with the subassembly represented by these homogenized parameters, a flat input partial current is again imposed on one face, a flux $\bar{\phi}^{(1)}(\underline{r})$ will be obtained for the homogenized assembly, and the improved homogenized parameters

$$\bar{\Sigma}_\alpha = \frac{\int_{V_i} \Sigma_\alpha(\underline{r}) \bar{\phi}^{(1)}(\underline{r}) dV}{\int_{V_i} \bar{\phi}^{(1)}(\underline{r}) dV} \quad (9)$$

Now a new value $\bar{D}^{(2)}$, the homogenized diffusion coefficient, can be found by requiring that the largest of the partial output currents, $\bar{R}$, for the homogenized subassembly, calculated using $\bar{D}^{(2)}$, $\bar{\nu}\bar{\Sigma}_f^{(2)}$ and $\bar{\Sigma}_a^{(2)}$ match the corresponding output current, R, of the heterogeneous subassembly.

The flux $\bar{\phi}^{(2)}(\underline{r})$ associated with the improved set of parameters is then used in the denominator of (9), and values $\bar{\Sigma}_a^{(3)}$ and $\bar{\Sigma}_f^{(3)}$ result. A search for the values $\bar{D}^{(3)}$ that again causes $\bar{R}$ to match R can be made and the whole procedure continued to convergence. The homogenized parameters $\bar{\Sigma}_a$, $\bar{\nu}\bar{\Sigma}_f$ and $\bar{D}$ that eventually result, if used in the homogeneous assembly will yield exactly the same values of the $\int_{V_i} \Sigma_\alpha(\underline{r}) \phi(\underline{r})$; $\alpha = a, f$ and R as those obtained when the heterogeneous parameters are employed.

As stated earlier, homogenizing parameters obtained in this

way provide improved predictions of power distribution when used for a reactor made up of homogenized subassemblies. However a rather clumsy, double iteration procedure is required to obtain the parameters. Accordingly we have been searching for a more efficient method for carrying out the required calculations.

Results to date are encouraging. We have found an improved scheme for determining the converged denominator of Eq. (9). It is based on the fact that the flux throughout the homogenized subassembly is smooth in shape and can be well approximated by bicubic Hermite polynomials. These can be specified in terms of the fluxes and currents along the edges of the square, and these in turn can be found from the input and output partial currents ($\phi = 2(J^+ + J^-)$; $J = (J^+ - J^-)$). But, since we are matching response matrices, we want the partial currents for the homogenized subassembly to equal those of the heterogeneous subassembly, and these are known from the initial calculation that yields $\phi(\underline{r})$. Thus the response matrices of the heterogeneous subassembly yield directly an excellent approximation to the flux integral $\int_{V_i} \phi(\underline{r}) dv$ for the homogenized subassembly. (There is a slight dependence on $\bar{D}$, but even use of $\bar{D}^{(1)}$ yields a value for $\int_{V_i} \phi(\underline{r}) dv$ only a few tenths of a percent in error.)

We now feel that the computational expense of determining the improved homogenized group parameters is comparable to that required to find conventional flux weighted numbers. Further testing of the basic method, however, remains to be carried out.

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