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1. Multidimensional Finite Element Methods

We have completed an extensive study of the application of the Finite Element Method (FEM) to neutron diffusion problems in two and three dimensions. The study was designed to examine three distinct questions:

- (i) Comparison of direct and iterative methods for the solution of the FEM algebraic equations;
- (ii) Selection of element functions for three dimensional problems;
- (iii) Comparison of the FEM results with conventional finite difference (FD) methods.

With regard to the issue of solution methods for the FEM algebraic equations there is convincing evidence that, except for the most trivial of problems, iterative methods are superior to direct methods.

Table 1 shows some comparative results for a two-group, 3D, bare homogeneous reactor. The solution for each group in each plane, was found by direct inversion (Cholesky factorization) and by an SOR method. In some cases a Chebyshev extrapolation was used for the outer iterations. It is clear from the results that iterative methods are superior with regard to running time and I/O operations.

The question of element function selection is principally of concern in the third dimension. For 2D problems there is a body of evidence that suggests quadratic or cubic elements

Table (4.1.2) - Some overall results to compare SOR versus
Cholesky Factorization , plus extrapolation data.
(Code CHDZL)

Inner Tter. 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

are appropriate for realistic reactor problems. However, high-order elements in the third dimension can add considerable complexity to the calculation. For Hermite-type elements in 2D there are usually 36 non-zero coupling coefficients at each mesh point. If one uses linear elements in the axial dimension then there would be 3×36 nonzero coefficients. For cubic elements there would be 6×36 nonzero coefficients, thus doubling the number of coefficients.

Usually the solution for the flux is smooth in the axial direction and a coarse mesh can be used. Results comparing linear and cubic elements are given in Table 2, for the same problem as before. Our conclusion is that linear elements are satisfactory in that they are as accurate as cubic elements for the same number of unknowns. However linear elements, even with half the mesh spacing, will require fewer I/O operations.

The results comparing 3D FEM with FD methods are discouraging. The comparison was made on a benchmark problem for light-water reactors⁽¹⁾. Results are presented in Table 3 for some FEM results, denoted CHDZL, PDQ-7 results, and two nodal codes called QUABOX/CUBBOX and DANO. Detailed flux shape comparisons suggest that the PDQ-7 results are probably good to $\pm 20\%$ while the FEM results may be as much as $\pm 50\%$ in error.

It appears that for equal running time the usual FD methods are superior to 3D FEM methods. This conclusion may be sensitive to improvements in the iterative method used for the FEM, or to improved treatment of the coupling coefficients.

Table (4.1.5) - Overall results comparing
Linear versus Cubic Hermite
in the axial direction z

	Linear in z		Cubic in z
Iteration	SOR with Extrapolat.	SOR without Extrapolat.	SOR without Extrapolat.
No.Axial Planes	9	10	5
Unknowns/plane	32	32	64
k-eff	.9354648	.9354752	.9359021
Fast/Thermal flux ratio,000	3.364331	3.364348	3.364075
Dominance ratio	.6674681	-	-
k-eff conv. crit (10^{-4})	4.5125	4.4014	.1601
No.Outer Iters.	19	27	25
no.Inner Iters.	10	10	11
CPU-min.	.263	.735	.731
No.I/O Ops.	144	150	565

Table (4.5.1) - Overall Results for the 3D-LRA
Benchmark Problem

CODE	CHDZL				PDQ-7	QUABOX/ CUBBOX	DANO (1GRF)
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.

2. Non-Linear Methods for Solving Finite Element Equations

Although for a given degree of accuracy, the number of unknowns associated with finite element equations is far fewer than the number associated with finite difference equations, the coupling of unknowns is much greater for finite element equations. As a result the decrease in computation time associated with use of the finite element methods has been discouragingly slight.

One procedure which might improve this situation is to treat the more weakly coupled terms in the finite element equations in a non-linear fashion. For example, in two dimensions, the linear finite element equations are "nine-point", that is, the flux at point (i,j) is connected to those at $(i+1,j)$, $(i,j+1)$, and $(i+1,j+1)$. By replacing the $\phi_{i+1,j+1}^{(n)}$ at iteration (n) by $\alpha_{i+1,j+1}^{(n)} \phi_{i,j}^{(n)}$, where the

$$\alpha_{i+1,j+1}^{(n)} \equiv \frac{\phi_{i+1,j+1}^{(n-1)}}{\phi_{i,j}^{(n-1)}}$$

are flux ratios determined from the previous iteration, the nine-point formula is reduced to a five-point formula, and standard solution methods developed for finite difference equations can be applied. It is very difficult to prove anything about the convergence of this non-linear scheme. We have found empirically that it does converge for certain test cases. However the convergence is too slow to make the method attractive.

We are currently investigating alternative schemes for solving the finite element equations.

3. Collocation Methods

The investigation of collocation methods for obtaining approximate solutions to the group diffusion equations^(2,3) has been extended to the two dimensional, two-group model, and a summary report of the results has been issued⁽⁴⁾. The attractive feature of such schemes over finite element methods involving the same polynomial representation of the flux is that the coupling between unknown coefficients in the flux expansion is much less. Our empirical testing by comparison with the two-dimensional IAEA benchmark problem shows however that there are flux accuracy problems near the core-reflector interface. We do not intend to push further this particular use of collocation methods unless we can develop a method for overcoming these difficulties.

4. Time-Dependent Response Matrix Techniques

We have completed a study of the time dependent response matrix technique applied to the one-group diffusion theory model in one dimension⁽⁵⁾. Conclusions are that, for this model, the response method performs kinetics calculations with an accuracy comparable to that obtained from finite difference solutions and does so in a much shorter time and with a smaller storage requirement.

5. The Determination of Equivalent Homogenized Group-Parameters

The majority of 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 volume i is defined as:

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

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 $\int_{V_i} \phi_g(r) dV$, where $\phi_g(r)$ 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⁽⁶⁾. Recently, the response matrix technique has been used in determining "equivalent" parameters for two-dimensional, two-group diffusion problems⁽⁷⁾. It was found that for a symmetric, heterogeneous assembly, two-group equivalent diffusion parameters, constant over the entire assembly, could be calculated. When used in the full-core problem, these diffusion constants result in a more accurate prediction of the integrated reaction rates for each assembly than does the use of flux-weighted constants.

During the past report period we have been refining this response matrix technique for finding equivalent parameters. A method has been found by which the computational effort required to calculate the equivalent diffusion parameters can be substantially reduced. The next step will be an attempt to expand the method to non-symmetric assemblies.

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