FINAL REPORT on CONTRACT E(11-1)-3021

Contract E(11-1)-3021 represents a continuation of Contract AT(30-1)-3971, and it seems appropriate to review briefly in this Final Report the work done under both contracts.

The stated purpose of Contract AT(30-1)-3971 was twofold: (i) to develop efficient and accurate variational methods for solving the multi-group diffusion equations and related elliptic systems, using piecewise polynomial approximating functions (e.g., bivariate cubic splines), and (ii) to appraise the extent to which such improved variational methods could advantageously replace the difference methods currently used to solve such equations (and systems).

Much of the work was done in collaboration with George Fix. Our work during the years 1968 through 1970 led us to conclude that such variational finite element methods are "more efficient for getting very accurate solutions... in certain typical [reactor] geometries" (underlines added). However, to achieve this high accuracy at moderate cost, one must use special "singular elements" that we had invented (see [3], [4]), adding considerably to the programming complexity.

Moreover such high accuracy is of little practical value. Therefore, in the second phase of our work, we investigated the overall practicality of the higher-order finite element approximations that we had developed. Thus, to make our approach more widely applicable, we supplemented the rectangular elements that were the main object of our earlier study by triangular elements. Although most of our analysis of triangular elements was carried out in other contexts, one innovative idea conceived while working on Contract E(11-1)-3021 was announced in [5]. Another "spinoff" from the research performed under this contract consisted in material published in the last three chapters of [8].

Our conclusions concerning higher-order finite element methods were reported orally at various meetings sponsored by the ANS and AEC, and at some length in writing in a widely distributed report [6]. Various relevant new technical results were published separately in [7]†. Our main conclusion

†Various extensions of the results of [7] are currently being worked on by Drs. Louis Hageman and I. Abu-Shumays at the Bettis Atomic Laboratory.

was that a great deal of high-level developmental work would be required before finite element methods could advantageously replace the standard 5-point difference approximation now used in multigroup diffusion codes.

At the same time, we tried to evaluate the practicality of the great variety of direct and iterative algorithms that have been proposed during the past 25 years for solving large systems of linear algebraic equations having sparse coefficient-matrices. Our aim was to see whether one could advantageously replace the SOR methods used in the PDQ codes for determining flux distributions that were developed at the Bettis Atomic Power Laboratories during the late 1950's, by newer methods.

Our conclusions concerning this question were also reported in [6]. Slightly paraphrased, our main conclusions concerning both questions can be summarized as follows:

I. Considerably more development work would be required to make higher-order methods useful for solving complex reactor problems.

II. Iterative methods (among which SOR has the great advantage for "production codes" of requiring the least "fine tuning") seem preferable for criticality problems involving very large numbers (say 2000 or more) unknowns.

III. However, for relatively simple reactor configurations which have smoothly varying physical properties, highly accurate solutions can usually be obtained most accurately by higher-order methods.

The preceding conclusions refer to the "state of the art" as of 1972. They could be made obsolete by new sparse matrix algorithms (see below), new finite elements, or by improved parallel processing (including "pipelining") and core storage capacity (including "virtual memory").

Since 1972, when George Fix left Harvard for a tenure position at the University of Maryland, I have continued to monitor developments, assisted by Surender Gulati. We have considered other possible improvements in the standard 5-point difference approximation used in neutron diffusion codes. This is

$$(1) \quad A_{i,j}u_{i,j} = b_{i'-1,j}u_{i-1,j} + b_{i',j}u_{i+1,j} + c_{i,j'-1}u_{i,j-1} + c_{i,j'}u_{i,j+1} + s_{i,j'}$$

plus an error term. In (1), $i' = i+1/2$, $j' = j+1/2$, and the coefficientmatrix is a diagonally dominant, 2-cyclic, positive definite symmetric matrix. Formula (1) is given in another notation in Varga's classic Matrix Iterative Analysis, Prentice-Hall, 1962, p. 186; a formula for the error term in terms of u_{xxxx} and u_{yyyy} is given there on p. 190.

Specifically, we have studied replacing the concentrated source term $s_{i,j}$ in (1) by a distributed source

$$S_{i,j} = w_{i,j}s_{i,j} + w_{i'-1,j}s_{i+1,j} + w_{i,j'-1}s_{i,j-1} + w_{i,j'}s_{i,j+1}$$

The use of distributed sources was suggested by our paper [7], which showed that properly distributed sources give systematically at least an order of magnitude‡ more accuracy in the 3-point one-dimensional analog of (1). Although no such systematic error reduction is possible for (1), except in the case of the Poisson equation by using a 9-point formula. We had reasons for hoping that the average error might be reduced.

Statistical error analysis. The relevant considerations involved a new concept: that of the statistical optimization of algorithms. In the summer of 1973, we began developing this concept in collaboration with Prof. Bona of the University of Chicago. We also tested our ideas in the special case of the Poisson equation $-\nabla^2 u = s$ in a square S, with $u = 0$ on δS. Although we wrote several drafts of a paper on the subject, and made extensive tests on the error distributions associated with various assumed random distributions of s, we must report with regret that: (i) we obtained no dramatic improvements, and (ii) we were not satisfied with our exposition of what we had found out.†

‡ Here "order" of magnitude" means order of infinitesimal, not a factor of 10. Although the result is well-known in other contexts (Størmer-Numerov method, it is overlooked in most discussions of the multigroup diffusion equations.

† We have included with this Final Report copies of the following partial MSS. in draft form:
[M1] G. Birkhoff, "Solution of the Poisson DE in a square," (dated 8-30-73).
[M2] G. Birkhoff and J. Bona, "Statistically optimal 5-point discretizations, (dated 9-3-73)
[M3] Letters from S. Gulati to J. Bona dated 10-25-73 and 11-29-73.
[M4] G. Gulati, "Optimal 5-point discretizations," (MS. dated 7-31-75).

Accordingly, during the present year, we tested source problems somewhat more typical of reactor criticality calculations. Again, although we reduced the error in most cases by a factor of about two by using properly distributed sources, this required "fine tuning" for which we found no good *a priori* prescription.

We plan to write up our ideas for publication during the coming year, and still hope that further careful study of the evidence will turn up a systematic replacement for (1) which will substantially reduce the average error by redistributing the source term. However, do not feel justified in asking for further support for this work.

Two-way dissection. My monitoring of new developments which might lead to improved techniques for solving reactor problems has not been confined to the ideas reported on above. For example, I have considered the desirability of replacing relaxation methods with the "nested dissection method" invented by Alan George. After considerable reflection‡ I have concluded that a modification of this method which I plan to call 'two-way dissection' seems to hold the most promise. Having only reached this conclusion during the present summer, it also remains to work it out in detail.

I hope that this Final Report is adequate, and that the work under Contracts AT(30-1)-3971 and E(11-1)-3021 will prove to have been a good investment of research funds.

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‡ For dissection techniques, see [9].

REFERENCES

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[2] G.J. Fix and G. Strang, "Fourier analysis of the finite element method...," Studies in Applied Math. 48 (1969), 265-73.

[3] Garrett Birkhoff, "Angular singularities of elliptic problems", J. Approx. Theory 6 (1972), 215-30.

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[6] Garrett Birkhoff and George Fix, "Higher-Order Finite Element Methods," 34 page report distributed to many contractors and AEC Distribution Center at Oak Ridge.

[7] Garrett Birkhoff, and Surender Gulati, "Optimal few-point formulas for linear source problems", SIAM J. Numer. Analysis 11 (1974), 700-728.

The following references cover work referred to in this Final Report, but not supported by the AEC-ERDA.

[8] Gilbert Strang and G.J. Fix, An Analysis of the Finite Element Method, Prentice-Hall, 1973.

[9] Garrett Birkhoff and J. Alan George, "Elimination by Nested Dissection," pp. 221-270 in Complexity of Sequential and Parallel Numerical Algorithms, (J.E. Traub, ed.), Academic Press, 1973.