FINAL REPORT
for the project

NODAL METHODS:
AN INFORMATION-BASED ANALYSIS
Performance Period September 30, 1990 - September 30, 1992

1 Introduction

The basic objective of this project was succinctly described in the original proposal. "The purpose of the proposed project is to use the techniques of information-based complexity to analyze the degree of optimality of nodal methods (for both diffusion and transport theory), and to compare the capabilities and limitations of these methods to those of more classical methods (e.g., finite differences and finite elements)."

The detailed research plan for the project, as presented in this original proposal, comprised two basic tasks, that were further subdivided into a total of five subtasks, as follows:

Task I: Nodal Diffusion Methods

Subtask I.a: The initial effort will be directed toward studying ... optimality of nodal spatial approximations that use average node-surface partial current information. The focus in this subtask will be upon monoenergetic diffusion and methods that use rectangular nodes.

Subtask I.b: The effort of the preceding subtask will be extended to spatial approximations that use hexagonal nodes.

Subtask I.c: The results of the preceding subtasks will be extended in diverse directions, as project resources permit and results of the earlier subtasks suggest. Examples of possible directions of extension include higher-order methods, two-group problems and space-kinetic problems.

Task II: Nodal Transport Methods

Subtask II.a For monoenergetic neutron transport in two spatial dimensions it is proposed to study, from the viewpoint of the information-based theory ... spatial
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approximations that use average incident node-edge (or cell-edge) information. In particular this class of methods includes (but is not limited to) the constant surface-flux approximations that tended to be among the first developed for transport theory. It also includes some classical finite-difference/$S_N$ methods that are widely implemented in production codes, such as the (weighted) diamond-difference methods, and various versions of "step" methods.

Subtask II.b The effort indicated in the preceding task will be extended to encompass methods that use linear incident node-edge information. In particular this will encompass the linear nodal schemes of Badruzzaman$^8$, of Walters$^{16}$ and of Azmy,$^{3,4}$ along with linear characteristic methods.$^3$

It was originally$^8$ proposed "... that the majority of the effort during the first year of the proposed project will be directed toward study of coarse-mesh nodal methods for diffusion theory by means of the information-based complexity. The bulk of the effort during the second year will be directed toward similar analyses of nodal and finite-difference methods for transport theory, and a comparison of these." In point of fact the majority of the effort during the project was directed toward transport theory, and specifically toward subtask II.a, as described above. The decision to do this was based upon rather intriguing and promising results for one-dimensional transport that were discovered, partially during the time between submission of the original proposal$^8$ and the beginning of the project. These one-dimensional results are briefly summarized in Section 2 below. Similarly our results for transport in two spatial dimensions are briefly described in Section 3. Conclusions, including possible directions for future related research, are sketched in Section 4, and in Section 5 we report on miscellaneous administrative matters. Sections 6 and 7 consist of lists of, respectively, publications and conference papers resulting from this project.

2 One-Dimensional Transport

The technical results for one-dimensional transport were reported in detail in Refs. 11 and 12. A copy of Ref. 12, which is the more definitive of these works, is appended to this final report. Here we only briefly summarize the salient results.

Two classes of information regarding the underlying source density were considered, cell-average and point-evaluation information. Further, two popular transport algorithms, the step characteristic and diamond difference methods, were considered in the light of the information-based complexity theory. It was shown in particular that the diamond-difference method always has a smaller worst-case error than the step-characteristic method, when both use (the same) cell-average information. Further, optimal methods for these two types of information were obtained in the worst-case setting.

Although these optimal methods theoretically are the best possible, in the sense that they minimize the worst-case error, from the practical point of view they turned out to be
somewhat disappointing. For the optimal method under cell-average information, extensive computational experiments (not reported in the literature) showed that, although one could with sufficient effort find problems for which it was superior to the classical methods (i.e., step characteristics and diamond differences), for the vast majority of test problems used in emulating typical situations it was inferior to these classical methods, sometimes considerably so. The optimal method under point-evaluation information depends upon a priori choices of a bound for the source density and its derivative. This method was not tested computationally, because it was unclear how such bounds could be determined in practice. For later reference we note that the optimal methods in this case are nonlinear, and that because testing was not carried out it is unclear how sensitive is the optimal method to the precise value of these bounds.

3 Two-Dimensional Transport

The technical results for two-dimensional transport were reported in detail in Refs. 10, 13 and 19. A copy of Ref. 13 is appended to this final report. Here we only briefly summarize the salient results.

For the model two-dimensional problem considered the solution operator was taken as the flux along the top edge of an underlying rectangle, and the information regarding the underlying source that was assumed to be available was the cell-average value. An optimal algorithm was found, under this setup and in the worst-case sense. This algorithm was not explored computationally, but it seems clear that it very likely suffers from the same deficiencies as does the corresponding optimal algorithm for the one-dimensional case, as described in the preceding section.

In the context of this same model problem, three classical methods (the diamond-difference, step-characteristic and \((C, C)\) nodal methods) and one novel method (the corner-balance method\(^\dagger\)) were compared in the context of single-cell calculations, but with cells of variable sizes. The relative ranking of the three classical methods (in the sense of the worst-case error) was found to depend in a sensitive way upon both the cell size and the value of the angular variables, but there were some general trends. For sufficiently large cells (more than two mean free paths on a side) the step-characteristic was found to be best, and the nodal method worst, regardless of the value of the angular variable. (The latter of these conclusions provides a theoretical basis for earlier computational observations of Walters and O'Dell.\(^\dagger\)) As the cell size is decreased, the diamond-difference method begins to become superior to the step-characteristic method for smaller values of \(\eta\) (the direction cosine relative to the \(y\)-axis), and ultimately (i.e., for cell widths on the order of one-half mean free path) a pattern emerges in which the diamond-difference method is preferable for smaller values of \(\eta\), the nodal method for an intermediate range of values of \(\eta\), and the step-characteristic method remains best for larger values. When the corner-balance method enters the competition it is found to be the best of the four methods over a significant range.

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of values of the directional variable, but it is not uniformly so.

Altogether the results outlined in the preceding paragraph suggest the somewhat novel idea that one perhaps should consider the idea of implementations in which the underlying spatial approximation selected varies with the value of the angular variable. There would seem to be no practical difficulty with such implementation, so long as all spatial approximations employ the same information regarding the source, but it has not been tested computationally.

4 Conclusions and Recommendations

The results of this project confirm some results that had been previously noted computationally, and thereby suggest that the methodology of the information-based complexity theory has very considerable potential for the comparison of alternative spatial approximations in transport theory. They also suggest some novel ways of combining different methods. We recommend that additional computational experimentation and theoretical development be carried out to further explore this potential.

Having noted this positive aspect of the results, it should be noted that a disappointing aspect is the failure of the theoretically optimal methods that were identified to compete well in actual computational experiments. We believe this is due to the fact that the worst-case error criterion used in the studies described above gives undue weight to possible but highly unlikely types of source distributions. In theory this difficulty could be overcome by using a so-called\textsuperscript{15} average case error criterion, but this then raises the perplexing question of what measure should be used for the distribution of source densities. At the 1991 Dagstuhl Seminar on Algorithms and Complexity Continuous Problems Kon and others (p. 20 of Ref. 14 identified this as an important new research direction in the practical application of information-based complexity to numerical methods. (See the previous progress report for this project\textsuperscript{9} for a summary of other cogent matters related to this conference.)

Quite recent results have suggested an alternate view of this issue. Specifically, Walters and Waring\textsuperscript{18} noted that a nonlinear method previous shown by Mathews\textsuperscript{7} to have excellent accuracy can in fact be obtained as the exact method for the most probable source density, under the constraints imposed by the information known about the source. Here the “most probable source density” is to be interpreted as that source density that maximizes the associated entropy, where the “entropy” is interpreted in the classical sense of information theory as applied to statistical physics (e.g., Ref. 6). This suggests the idea that one adopt as a probability measure for the source densities those arising in this latter theory. Potentially even more importantly, it also suggests that there may be circumstances in which “nearly optimal” methods (in the average case sense) can be determined by tailoring methods to the most probable case. The importance of this stems from the fact that most probable values frequently are much easier to determine than the underlying distributions
per se,* so that such nearly optimal methods might be much more easily found than optimal methods.

5 Miscellaneous

DOE/ER-0249 "Application and Guide for the Special Research Grant Program 10 CFR Part 605" specifies a number of items that should be included in performance reports, beyond a description of the research carried out and its relationship to the established objectives, which are covered in the preceding section. This section is intended for discussion of such matters.

One such item was previously covered in the corresponding section of the performance report that was submitted at the end of the first year of the subject project.9 Here we wish only to mention further that his project provided the financial support for the Ph.D. research of Dr. Fan Yu. Reference 19 is his dissertation. Dr. Yu presently is employed as an analyst by Macromedia Corporation, in the Dallas, Texas area.

6 Publications


*This fact is responsible for much of the utility of information-theoretic techniques in classical statistical mechanics.

7 Conference Papers


REFERENCES


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