C00-2280-36

COMPUTATIONAL COMPLEXITY IN MULTIDIMENSIONAL
NEUTRON TRANSPORT THEORY CALCULATIONS

MASTER

Progress Report
for period September 1, 1976 - November 30, 1977

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Project Abstract

The objective of our research remain the same as outlined in the original proposal. They are in short as follows. Develop mathematically and computationally founded criteria for the design of highly efficient and reliable multidimensional neutron transport codes to solve a variety of neutron migration and radiation problems. Analyze existing and new methods for performance.

To achieve our goal we have subdivided the problem into three major steps:

Step 1: Automated error analysis over computational cells.

Step 2: Global error and stability analysis.

Step 3: Systems analysis and assessment of computational efficiency.

Each of these steps consists of three parts.

- a.) Rigorous analysis of the analytic behavior of the mathematical solution for any sub-problem.
- b.) Implementation of computer codes. Generation of representative benchmark problems for which the exact solutions are known.
- c.) Evaluation of test results and recommendations.

The exhibit on the next page summarizes the master plan of the research. The annual progress report, ERDA C00-2280-26, of last year described the work, which is still in progress, on pages 5 to 23 in a simplified manner.

QUANTITATIVE AND COMPUTERIZED ERROR ANALYSIS

A. CELL CALCULATIONS

CREATION OF EXACT
BENCHMARK PROBLEMS

NUMERICAL SOLUTION
BY APPROXIMATE METHODS

CALCULATION OF ERROR
CHOOSE APPROPRIATE NORM

QUANTITATIVE
ERROR
ANALYSIS

B. GLOBAL ANALYSIS

GLOBAL BACKWARD AND
FORWARD ERROR ANALYSIS

STABILITY ANALYSES OF
METHODS AND ALGORITHMS

CONVERGENCE ANALYSES

PROBABILISTIC
ERROR
ANALYSIS

C. COMPUTATIONAL COMPLEXITY

PERFORMANCE PREDICTION

CODE EVALUATION

DATA MANAGEMENT COST

COST
ANALYSIS

Scope of Investigations

Our aim is to develop a theory of error estimation for coarse network calculations in neutron migration problems and implement the results simultaneously in a computer code for use by engineers and scientists that need not be specialists in numerical analysis. At the same time, when gaps in the mathematical foundations are discovered, we make every effort to close them by working out an appropriate theory. As new analytical insight is gained, new numerical methods are developed and tested. We look at the problems from different points of view and then try to make a best judgement for implementation in a large scale computer code.

Significant Results Obtained by August 31, 1977

Synthetic Error Analysis: This theory was developed especially to predict the approximation error of irregular functions as they occur in solutions of partial differential and integral equations. The theory reduces all errors to a linear combination of elementary error functions which are obtained from the small class of functions $\{x^\alpha\}$, and $\{x^\alpha \ln^p x\}$ over the unit interval. This theory, for example replaces the classical convergence relation

$$(f - g)(r) = O(h^\nu)$$

by

$$(f - g)(r) = x^\mu h^\nu \{a_{n+1} h^{n+1} E_{n+1} + O(h^{n+k})\}$$

which explains why in certain practical calculations a lower order approximation can yield a better numerical result than a high order approximation, thus seemingly contradicting the classical asymptotic theory.

Another very important "negative" result is this. One may hope that by using a very fine network and very high precision in computing, the analytic behavior of a solution can be determined as a matter of routine performance by the computer, using approximation theory. The investigation shows that one cannot substitute accurate numerical methods for mathematical analysis to obtain the nature of a irregular solution. The converse however is true. A highly accurate numerical method can be used to verify the mathematical behavior of a solution, using the computer.

Statistical Aspects of Machine Rounding: The distribution of computer numbers is a fundamental concept to develop rules for rounding results of machine operations. All machine operations deal with magnitudes, and the allocation of signs is done by an auxiliary mechanism. Hence we came to the conclusion that the distribution of magnitudes is the important concept underlying the machine number distribution in floating point arithmetic. Using this new concept to construct rules for rounding, we introduced the logarithmic Gaussian distribution

$$f(x) = (2\pi ns^2)^{-\frac{1}{2}} x^{-(1 + (\ln x)/2ns^2)}$$

invoking the central limit theorem, and observing that for machine numbers of order 1, it approximates the reciprocal distribution $f(x) \sim x^{-1}$ which in turn has been shown to represent fairly well the observed number distribution.

We introduced also the sesqui-reciprocal distribution $f(x) \sim x^{-3/2}$ which also approximates the logarithmic Gaussian distribution for numbers of order 1 and has the additional property to provide bias free rounding. Obviously, the usual assumption of constant machine number distribution has, except for its simplicity, not much support, since it emphasizes large magnitudes contrary to observations. In addition, it is not bias free even in floating point arithmetic.

CRD Computer: We showed that a new computer arithmetic, the CRD-arithmetic enables the construction of a computer, that can multiply and divide any two machine numbers exactly within the constraints of a given word length. We recommend the construction of such a computer because of a number of additional attractive features.

The Corner Problem in Neutron Diffusion: The corner problem has been reduced to the problem of solving a system of boundary integral equations of lower dimension. While the problem is a classical one for convex bodies with certain types of exterior corners, the interior corner-and interface problems have so far not been treated rigorously in the literature. We observed that the current in radial direction is represented by a much smoother function than the flux, and thus better suited for numerical evaluation. The flux is then obtained from the current by an integral transform.

Compliance with Contract Requirements

To the best of the principal investigator's knowledge, all contract requirements have been fulfilled.

Time Effort

The principal investigator as well as his assistants have devoted more time on work for the contract than is required by the agreement. It is believed that the research results and the nine reports submitted to ERDA during the contract period provide amply evidence for this statement.

Summary of Work During September 1, 1976 to November 30, 1977

The major achievements have already been briefly mentioned above. Following are summaries of the work accomplished by August 31, 1977.

The Exact and Approximate Interior Corner Problem in Neutron Diffusion by Integral Transform Methods

The mathematical solution of the neutron diffusion equation exhibits singularities in its derivatives at material corners. We gave a mathematical treatment of the nature of these singularities and its impact on coarse network approximation methods in computational work. The mathematical behavior was deduced from Green's functions, based on a generalized theory for two space dimensions, and the resulting systems of integral equations, as well as from the Kontorovich-Lebedev Transform.

The effect on numerical calculations was demonstrated for finite difference and finite element methods for a two-region corner problem. It was shown that for coarse network calculations the addition of a single r^y element is in general not sufficient for flux calculations.

An Automated Approach to Quantitative Error Analysis

A method was described how a quantitative measure for the robustness of a given neutron transport theory code for coarse network calculations can be obtained. A code, that performs this task automatically and at only nominal cost, was described and implemented. This code generates also user oriented benchmark problems which exhibit the analytic behavior at interfaces.

ERDA Report	C00-2280-30	(163 pages)
ERDA Report	C00-2280-31	(6 pages)
ERDA Report	C00-2280-32	(27 pages)

Synthesis of Approximation Errors

A method was developed for the synthesis of the error in approximations in the large of regular and irregular functions. The synthesis uses a small class of dimensionless elementary error functions which are weighted by the coefficients of the expansion of the regular part of the function. The question was answered that a computer cannot determine the analytical nature of a solution by numerical methods. It was shown that continuous least squares approximations of irregular functions can be replaced by discrete least squares approximations and how to select the discrete points. Using the elementary error functions, it was shown how the classical convergence criterions can be markedly improved.

ERDA Report C00-2280-34 (152 pages)

Statistical Aspects of Machine Rounding

Rounding is used on computers because exact results of machining operations are in general not machine numbers. The nature of the rounding depends on statistical presuppositions which were examined. Specifically rounding to the midpoint of a rounding interval of real numbers implies that the distribution of numbers in the interval is such that the mean of the distribution is the midpoint. This is true for the uniform distribution, but not for other possible distributions such as the Gaussian, the logarithmic Gaussian, and the reciprocal distribution, which have justification on theoretical and empirical grounds and which were studied. For these more realistic distributions, conventional rounding introduces bias, or systematic errors. Systematic error is introduced in floating point representations in any case because of the presence of transitional intervals which are due to the hybrid nature of floating point arithmetic. Besides examining rounding in the conventional number representations on computers under different distributions, geometric rounding was also treated in a new computer number system in which rounding occurs only in addition and subtraction. The biases for the different distributions were ordered. The problem of removing the bias under the reciprocal distribution of numbers is solved, both theoretically and practically.

Basics of the CRD-Computer

A new kind of computer arithmetic (CRD-arithmetic) was investigated that has some very attractive features:

The stored result of multiplication or division of two machine numbers is exact; i.e., no rounding error is introduced.

The radix of the system is not an essential ingredient.

In the course of computing, the precision may be changed gradually to meet the accuracy requirements of intermediate calculations and thus permits dynamic precision.

The representational efficiency is 100%.

The mathematical foundations were studied for implementing a Constant Relative Difference (CRD) computer, including input and output conversions.

The existence of a CRD-computer will have a profound impact on numerical analysis, since algorithms emphasizing multiplications, divisions, and exponentiations will be the preferred ones, and the error analysis will be simplified.

It was also shown that the representational efficiency of an ordinary binary computer can be improved from 50% to 100%, and at the same time its precision increased.

1972 - 1973

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30. Bareiss, E. H. and Paul Michel, "Synthesis of Approximation Errors," Northwestern University ERDA Report COO-2280-33 (July 1977) 152 pp.
31. Grau, A. A. and E. H. Bareiss, "Statistical Aspects of Machine Rounding," Northwestern University ERDA Report COO-2280-34 (August 1977) 29 pp.
32. Bareiss, E. H. and A. A. Grau, "Basics for the CRD Computer," Northwestern University ERDA Report COO-2280-35 (August 1977) 60 pp.
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