Numerical Analysis - Final Report

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Report Number:
70-049
1. INTRODUCTION. This report summarizes the activities supported in full or part under contract N00014-67-A-0226-0011, Project NR 044-382 with the Office of Naval Research. The activities are broken into three major areas: The Special Year in Numerical Analysis, The Mathematical Software Symposium and Research.

2. SPECIAL YEAR IN NUMERICAL ANALYSIS. There were a number of activities associated with this special year. One of these, the Mathematical Software Symposium, is discussed in the next section.

   The Sets of Special Lectures. There were three sets of special lectures in numerical analysis. The idea was to invite several (four) leading experts in a special area to visit Purdue simultaneously and lecture on their current interests. The visits were for a 2-day period and allowed for close contact among the visitors as well as between the faculty at Purdue and the visitors. The lectures were publicized outside Purdue and a number of people from neighboring institutions attended.

   The lecturers and their topics are shown on the next page.
Special sets of lectures in numerical analysis given last year
as part of Purdue University's Special Year in Numerical Analysis.

**NONLINEAR EQUATIONS  NOVEMBER 10-11, 1969**

J.M. Ortega  A survey of convergence theorems for iterative
methods for nonlinear systems

A.S. Householder  Variations on a theme by Sebastiao e Silva

W.C. Rheinboldt  On M-functions and their application to nonlinear
Gauss-Seidel iterations and to network flows

J.F. Traub  Globally convergent polynomial iteration with a
posteriori error bounds

**QUADRATURE  DECEMBER 4-5, 1969**

A.H. Stroud  Integration formulas and orthogonal polynomials
of two variables

P.J. Davis  Double integrals, Schwarz functions and Hilbert
spaces

J.N. Lyness  Careful calculation of Fourier coefficients

R.E. Barnhill  Blending function cubatures

**SPLINES AND PROJECTION METHODS FOR OPERATOR EQUATIONS  MAY 18-19, 1970**

R.S. Varga  Improved error bounds for interpolatory spline
functions

G. Birkhoff  Practical generalizations for splines

M.H. Schultz  The computational complexity of the Rayleigh-Ritz-
Galerkin method

G. Strang  The finite element method and approximation theory
Other Activities. In addition to these short term visitors, there were
two longer term visitors. Miss Lois Mansfield spent the entire year at
Purdue as a postdoctoral fellow. Her interests are in the area of spline
functions and the estimation of linear functionals. She continued the
research started in her thesis and interacted considerably with Professor
Carl de Boor in this area. The second and third sets of lectures were
also especially relevant to her work. Mr. Sten Henriksson spent the
second semester at Purdue as a predoctoral instructor. His thesis
investigations (at Lund, Sweden) are extensions of some work of Professor
John Rice and they discussed these, and other, areas in some detail.

A number of advanced graduate students were involved in the activities
either as research assistants, participants in the numerical analysis
seminar or as attendees to the special lectures and the symposium. They
had an unusual opportunity to meet and hear a large number of the leading
workers in numerical analysis and related areas. The numerical analysis
seminar covered topics somewhat in conjunction with the visiting lecturers.
The topics and speakers are listed below.

A method of Powell's for nonlinear equations   - T. Aird (2 lectures)
An adaptive Romberg quadrature method        - C. de Boor
Constructive theory of Gaussian quadrature rules - W. Gautschi (2 lectures)
Optimal approximation and error bounds        - L. Mansfield
Minimization techniques and nonlinear approximiation - J. Rice (2 lectures)
Parallel processor methods for nonlinear equations - J. Rice
Optimization of non-convex problems            - A. Winston
2. **THE MATHEMATICAL SOFTWARE SYMPOSIUM**

**Organization.** An organizing committee was formed in the summer of 1969 by Professor John Rice. The other members were

- R.L. Ashenhurst University of Chicago
- C.L. Lawson Jet Propulsion Laboratory
- M.S. Lynn IBM - Houston Scientific Center
- J.F. Traub Bell Telephone Laboratories

This committee obtained sponsorship for the symposium from the Association for Computing Machinery and from the Special Interest Group in Numerical Mathematics. Ten leaders in the field were invited to speak at the symposium and they all accepted. They are indicated by an asterisk in the program given below. A call for papers was issued via journals and direct mailings and an additional 11 contributed papers were accepted for presentation. Publication of the proceedings were arranged with Academic Press in the ACM monographs series with Professor John Rice as editor.

He accepted the responsibility of preparing or obtaining several chapters of material in addition to the papers presented at the symposium.

**The Symposium.** The Mathematical Software symposium was held at Purdue University on April 1-3, 1970. The program of speakers is listed below.

**MATHEMATICAL SOFTWARE**

Program Schedule

**Wednesday, April 1**

- R.L. Ashenhurst, University of Chicago, Numeric Representation and Error Indications
- M. Goldstein and S. Hoffberg, New York University, The Estimation of Significance
- C.B. Dunham and H.C. Thacker, University of Western Ontario and Notre Dame University, Making Non-Standard Arithmetics Available
- J.F. Traub, Bell Telephone Laboratories, Status of the Bell Laboratories Numerical Mathematical Program Library Project
Wednesday, April 1 con't.
A.W. Dickinson, V.P. Herbert, A.C. Pauls and E.M. Rosen, Monsanto Company, The Development and Maintenance of a Technical Subprogram Library
A.C.R. Newbery, University of Kentucky, The Boeing Library and Handbook of Mathematical Routines
E.L. Battiste, IBM-Houston, Development of Mathematical Software for a Mass Audience - Problems and Attitudes
W.H. Payne, Washington State University, Continuous Distribution Sampling - Accuracy and Speed

Thursday, April 2
C.W. de Boor, Purdue University, On Writing an Automatic Integration Algorithm
C.W. Gear, University of Illinois, Experience and Problems with Software for the Automatic Solution of Ordinary Differential Equations
P. Muller, Jet Propulsion Laboratory, A User's Experience with Sophisticated Least Squares Software in the Discovery of the Lunar Mascons
D.K. Kahaner, Los Alamos Scientific Laboratory, Comparison of Numerical Quadrature Formulas
O.G. Johnson and B.N. Parlett, IBM-Houston and University of California, Berkeley, Numerical Implementation of Variational Methods for Eigenvalue Problems
R.C. Bushnell, Ohio State University, User Modifiable Software

Friday, April 3
H. Kuki, University of Chicago, Mathematical Function Subprograms for Basic System Libraries - Objectives, Constraints and Trade-Off
L.R. Symes, Purdue University, Evaluation of NAPSS Expressions involving Polyalgorithms, Functions Recursion and Untyped Variables
Friday, April 3 con't.

J.E. Sammet, IBM Boston, Software for Non-Numerical Mathematics

W.J. Cody, Argonne National Laboratories, Software for the Elementary Functions

R. Bayer, Boeing Scientific Research Laboratories, Toward Computer Aided Production of Software for Mathematical Programming

C.L. Lawson, Jet Propulsion Laboratory, Applications of Singular Value Analysis

K.M. Brown and J.B. Dennis, Cornell University, A New Algorithm for Nonlinear Least Squares Curve Fitting

There was a banquet and reception for all the attendees on April 2. Several smaller, informal meetings were held by groups of those attending.

There were 155 registered attendees. The number was reduced slightly as some people (including the banquet speaker) were unable to reach Lafayette because of the air traffic controller's strike. Those registered came primarily from industry and universities (in about equal numbers) with a smaller number from government laboratories.

The Proceedings. Academic Press has the manuscript in production and publication is expected sometime in early Spring of 1971. The current estimates of the length and costs are 501 pages and $20.00, respectively. The table of contents is given (with the listing of the individual papers omitted). The chapters in the third part are papers (in the ordinary sense of the word) about specific mathematical software. They were not presented at the symposium.
MATHEMATICAL SOFTWARE
J.R. Rice, Editor

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Part 1 - Prologue

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I. Introduction
II. Chronological Record

Chapter two: THE DISTRIBUTION AND SOURCES OF MATHEMATICAL SOFTWARE - J. R. Rice
I. Introduction
II. Local Distribution Methods
III. Assessment of General Sources
IV. Summary

Chapter three: THE CHALLENGE FOR MATHEMATICAL SOFTWARE - J. R. Rice
I. Introduction
II. Algorithm Construction
III. Evaluation - Charting the Unknown
IV. Dissemination - Some Alternatives
V. Two Recommendations

Part 2 - Proceedings of the Symposium

Chapter four: DISCUSSION OF THE PAPERS - J. R. Rice

Chapter five: THE PAPERS

Part 3 - Selected Mathematical Software

Chapter six: SELF-CONTAINED POWER ROUTINES - N. W. Clark, W. J. Cody and H. Kuki
I. Introduction
II. A Fortran Program
III. An Assembler Language Program

Chapter seven: CADRE - AN ALGORITHM FOR NUMERICAL QUADRATURE - Carl de Boor
I. Introduction
II. Mathematical Analysis
III. Numerical Procedures
IV. Fortran Listing of CADRE
V. Testing and Examples
Chapter eight: SQUARS - AN ALGORITHM FOR LEAST SQUARES APPROXIMATION - J. R. Rice

I. Introduction
II. Mathematical Analysis
III. Numerical Procedures
IV. The Algorithm SQUARS
V. Example Program, Testing and Evaluation

Chapter nine: DESUB - INTEGRATION OF A FIRST ORDER SYSTEM OF ORDINARY DIFFERENTIAL EQUATIONS - P. Fox

I. Program Purpose and Use
II. Method
III. History
IV. Adaptation of the Program
V. Testing and Results
VI. Organization of the Program
VII. DESUB

3. RESEARCH. The research of two people were directly supported by this contract: Professor W. Gautschi (summer 1969) and Professor R. E. Lynch (summer, 1970). Professor Gautschi wrote the paper "On the construction of Gaussian quadrature rules from modified moments" which is now in the process of publication in Mathematics of Computation. The manuscript was distributed to ONR in October, 1969.

Professor R. E. Lynch is studying the estimation of solutions of differential equations with singular coefficients. Examples include Bessel's equation and the Poisson equation in cylindrical coordinates. The low order derivatives of solutions of such equations have singularities. He is investigating both the use of special finite difference schemes and of projection methods involving appropriately chosen basis functions. Specific applications to the Stephen problem is planned. Its solution is a mathematical model of the temperature field in a two-phase medium which is undergoing phase change at the interface. This occurs, for instance, in the melting of a solid. A manuscript has not been prepared yet, but a student, E. Pekarek, has completed a thesis under Professor Lynch's direction in this area.
Professor R. E. Lynch and John Rice have been collaborating on the development of an efficient, reliable algorithm for the numerical evaluations of the derivative of an arbitrary function. Such an algorithm will be a fundamental component of any automatic numerical analysis or mathematical software system. The work is an extension of previous work by Mr. J. J. Casaletto and Professor John Rice.

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Numerical Analysis

Final Report to Office of Naval Research (7/1/79 to 9/30/69)

John R. Rice

September 1, 1970

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None

CSD TR #49

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Office of Naval Research
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