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Numerical Computation Breakthroughs and Future Challenges

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NUMERICAL COMPUTATION
BREAKTHROUGHS AND FUTURE CHALLENGES

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ABSTRACT

A list is given of significant accomplishments and breakthroughs in the past and of challenges for the future in the area of numerical computation. This list is compiled from the drafts of the panel on numerical computation of COSERS (Computer Science and Engineering Research Study). A selection of items from this list will be made to highlight in the final report. Suggestions for additions, deletions and improvements are solicited and will be greatly appreciated.

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The dates given below are approximate and/or averages of several pieces of work.

1. LINEAR ALGEBRA

   A. Valid error analysis for Gauss Elimination (1947)

   B. Backward Error Analysis Realization that Gauss Elimination is reasonable. (1952)

   C. SOR iteration (1954)

   D. QR transformation for eigenvalues. Orthogonal transformations in general. (1961)

   E. Error Analysis Developed (1962)

   F. Software - Forsythe & Moler (1967), Numerish Mathematik Handbook in Linear Algebra, EISPACK (1973)

   Future Challenges

   A. Techniques for sparse matrices of general and special types

   B. (?) Use of secondary storage for large matrices.

   C. (?) User-oriented software (may belong to Math software category)

2. OPTIMIZATION AND NONLINEAR EQUATIONS

   A. Recognition as a discipline for organized study (1947)

   B. Simplex method (1948)

   C. Dynamic Programming (1952)

   D. Continuation method for nonlinear equations (1952)

   E. Integer Programming techniques (branch-and-bound, integer-forms) (1958)

   F. Variable metric, update and quasi-Newton methods for unconstrained optimization and nonlinear equations (1964)

   G. Theoretical analysis of simplex method showing it could be very bad (1968)

   H. Numerically stable and compact algorithms (1973)

Future Challenges

A. Why is the simplex method so good in practice when theory says it can be so bad?

B. Techniques and aids for model construction

C. Understanding and taking advantages of various kinds of "structure" in optimization problems e.g. decomposability, staircase models, time-phased, hierarchical, sparseness

D. Better understanding and methods for integer programming problems

E. Understanding combination of problem and algorithm characteristics that give good results, creation of a methodology for evaluating algorithms and a set of reproducible experimental results that cover most types of applications

F. Better understanding of and better methods for the global convergence problem.

3. ORDINARY DIFFERENTIAL EQUATIONS

A. Discovery of stability criteria and stable methods (1954)

B. Variable step methods perfected (1959)

C. Methods for stiff problems (1970)

D. Reliable software and definitive comparisons and evaluation of methods for certain important problem areas. (1973)

Future Challenges

A. Methods that take advantage of special structures and properties of particular problems (e.g. sparseness, stiffness of various types)

B. Evaluation of the effectiveness of the many methods for boundary value and eigenvalue problems.

4. PARTIAL DIFFERENTIAL EQUATIONS

A. Stability analysis for initial value problems (1950)

B. Artificial viscosity (1948)

C. SOR iteration for elliptic problems (1954)

D. ADI methods (1956)

E. Finite element methods discovered (1958)

F. Tensor product and fast-Fourier-transform methods for separable equations (1964)

G. Systematic theoretical analysis of finite element methods (1970)

H. Large scale engineering oriented software packages (1970)

I. Nested dissection (1972)

J. Systematic exploration and use of higher order methods (1974)

Future Challenges

A. Analysis and application of parallel computation

B. Flexible methods with good accuracy for curved and complicated geometry, especially time varying surfaces and shocks.

C. Special methods for the sparse matrices arising from partial differential equations.

D. The effectiveness of finite element and other higher order methods for initial value problems.

E. Systematic evaluation and comparison of the many methods now available for use.

F. Extension of effective iterative methods to a wider class of problems (e.g. finite element methods for three dimensional problems)

G. Nonlinear elliptic problems

5. MATHEMATICAL SOFTWARE

A. Organized attempts made to collect and share useful programs (1960)

B. Creation of high quality and verified software for the elementary functions for some computers (1965)

C. Efforts to evaluate and enforce standards in published algorithms (1967)

D. Creation and dissemination of large packages of programs for particular applications areas (1967)

E. Recognition of mathematical software as a respectable subdiscipline with scientific content and methodologies (1970)

F. Systematic evaluation made for numerical quadrature and ordinary differential equations which identifies superior numerical methods and mathematical software (1972)

G. Systematized package for eigenvalue calculations and elementary functions developed by leading experts, exhaustively tested and evaluated and made available in a wide range of computing environments (1974)

H. Codification of the general principles for the creation and evaluation of software (1974)

Future Challenges

A. Creation and/or identification of quality software in various areas (statistics, linear algebra, partial differential equations, optimization)

B. User oriented interfaces with mathematical software, dissemination mechanisms

C. Codification of principles of software evaluation throughout the mathematical problem areas.

D. Portability standards and mechanisms, means of new software to build upon old software in a natural way

6. CURVES, SURFACES AND GRAPHICS

A. Orthogonal polynomial and related methods for least squares (1958)

B. Realization that classical (mostly linear) approximations theory methods cannot be adapted for successful use in a wide range of important applications (1962)

C. Use of splines and other piecewise polynomials (1962)

D. Use of B-spline basis for piecewise polynomials (1965)

E. Theoretical and algorithmic methods to compute nearly optimal locations of breakpoints for spline approximations (1968)

F. Moderately priced hardware for displaying graphics accurately and rapidly (1968)

G. Robust curve fitting methods that eliminate the effect of wild points (1970)

Future Challenges

A. Incorporation of piecewise polynomial methods for curves and surfaces into hardware and applications of graphics.

B. Efficient and reliable methods to generate smooth approximations to two and three dimensional surfaces of a general nature.

C. Approximation methods which greatly compactify the amount of data required to represent curves and surfaces.

7. OTHER AREAS OF NUMERICAL COMPUTATION

Mathematical Functions: Highly efficient and reliable algorithms for many functions (1965-75)

Future Challenges: Multivariate and complex valued functions; special computer architecture; incorporation into the hardware.

Quadrature: Adaptive quadrature (1966), Systematical evaluation of algorithms (1970), Principles of evaluation of algorithms (1974)

Future Challenges: Multidimensional quadrature

Monte Carlo and Random Numbers: Analysis of various pseudo-random number generators (1966)

Polynomial Roots: Recognition of the ill-conditioning of the problem (1960), Synthesis of a reliable and efficient algorithm for the roots of a general polynomial (1968)

Fast Fourier Transform: Discovery (1952)