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**APPLIED MATHEMATICAL SCIENCES
RESEARCH AT ARGONNE**

October 1, 1978 - March 31, 1980

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ARGONNE NATIONAL LABORATORY, ARGONNE, ILLINOIS

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ARGONNE NATIONAL LABORATORY
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APPLIED MATHEMATICAL SCIENCES RESEARCH AT ARGONNE

October 1, 1978 - March 31, 1980

Applied Mathematics Division

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DISCLAIMER

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ABSTRACT

This report reviews the research activities of the Applied Mathematical Sciences Section for the period October 1, 1978, through March 31, 1980. The body of the report discusses various projects carried out in four major areas of research: applied analysis, computational mathematics, software engineering, and software clinics. Information on section staff, visitors, workshops, and seminars is found in the appendices.

APPLIED MATHEMATICAL SCIENCES RESEARCH AT ARGONNE

October 1, 1978 - March 31, 1980

Research in the Applied Mathematical Sciences Section at Argonne is carried out in both mathematics and computer science. The major goals are to reduce the cost of performing mathematical computations reliably and to exploit mathematical techniques to solve scientific problems. Our approach involves the formulation of new analytical and numerical methods, the design of computational algorithms, their implementation in computer programs, and their application in scientific and engineering problems. Activities range from studies of flow instabilities in reactor systems to automated program verification. Special attention is given to methods for creating collections of high-quality software--notably through work on algorithms, test programs, software evaluation techniques, and program transformation systems. Most of this work centers on numerical optimization, linear algebra, numerical integration, partial differential equations, and special functions. In addition, special efforts are made to facilitate the transmission of research results to DOE mission projects.

This report reviews the research activities in the Applied Mathematical Sciences Section for the period October 1, 1978 - March 31, 1980. During this period, significant progress was made in several areas:

1. A monograph was begun explaining the role of spectral methods in linear transport theory.
2. Substantial enhancements were made to the DISPL package for nonlinear systems of partial differential equations. The package has now been added to the National Energy Software Center.
3. The *Software Manual for the Elementary Functions* was completed and is scheduled for publication in April 1980. The collection of test programs from the manual is being used for benchmarking and certification of new software libraries.
4. The final version of MINPACK-1, comprising codes for the solution of nonlinear equations and nonlinear least squares problems, was sent to various sites for testing. Response to an earlier version of MINPACK-1 has been extremely favorable.
5. The LINPACK collection, together with a users' guide, was released to the public. The collection includes routines for solving linear systems and is designed to run without change on most computer systems. In its first nine months of distribution, over 200 computer centers have requested the package, and over 2000 copies of the guide have been sold.
6. An automated theorem-proving system, based on a flexible environmental approach, was distributed to several universities for practical applications, for example, in designing multivalued logic circuits.
7. Iterative techniques were successfully adapted from symmetric linear systems and applied to sparse, non-symmetric systems. Such techniques have proved valuable in solving problems in reactor analysis and design.
8. A collaborative project was organized with universities and with industrial and government research laboratories to produce an integrated collection of tools for numerically oriented Fortran programs.

These and other activities detailed below reflect the efforts of a permanent scientific staff of 19, many of whom work in more than one area of research. A complete list of section members, their publications, and their professional activities is provided at the back of this report. Also included is a list of faculty, students, and consultants who visited Argonne to conduct seminars, participate in workshops, or collaborate on special projects in mathematics and computer science.

I. APPLIED ANALYSIS

The essence of applied analysis research at Argonne is the application of analytical and numerical techniques to problems in the natural and engineering sciences. Broadly speaking, there are three aspects to this research: the mathematical modeling of observable phenomena, the analysis of the mathematical model, and the interpretation of the analytical results. Current interest centers upon the analysis of nonlinear evolution and boundary value problems.

A. Evolution Equations

Hans G. Kaper, Gary K. Leaf, and Bernard Matkowsky*

The multitude of nonlinear evolution phenomena in scientific and engineering applications makes nonlinear evolution equations a challenging area of study. In the applied analysis program, emphasis is placed on evolution equations that arise in fluid flow and gas dynamics problems and in reaction-diffusion systems. The long-term objective is to obtain qualitative and, possibly, quantitative information about a given physical system, through the design of reliable mathematical models and the development and application of efficient solution techniques.

1. Gas Dynamics

Hans G. Kaper and Gary K. Leaf

The ultimate goal of our research in gas dynamics is to give a mathematically satisfactory explanation of the relationship between the nonlinear Boltzmann equation of the kinetic theory of gases and the nonlinear Euler and Navier-Stokes equations of fluid dynamics. Heuristically, this relationship is established by the asymptotic expansion methods of Hilbert and Chapman-Enskog. Our recent efforts have focused on the Carleman model, which is a simplified version of the Boltzmann collision operator with a single collisional invariant. We prepared two articles for publication. In the first one, we reviewed the existing literature, corrected and improved some results of previous authors, and gave a unified presentation of two types of initial value problems: the pure initial value problem defined by the Carleman equation itself, and the initial value problem for the decay of solutions to the uniform steady state solution (the absolute Maxwellian for the Carleman model). In the second article, we presented a simple proof of a convergence result for nonlinear semigroups that could be applied to obtain the fluid dynamic limit of Carleman's equation. We were also able to identify explicitly the closed exponential generator of the limiting semigroup.

2. Bifurcation Theory

Hans G. Kaper, Gary K. Leaf, and Bernard Matkowsky*

We initiated a new research effort to investigate bifurcation and stability phenomena in reaction-diffusion systems. Such systems occur in chemical and biological environments. In particular, we considered catalytic systems (slabs, cylindrical shells, and spherical shells) reacting at their surfaces. Employing analytical as well as numerical methods, we exhibited all of the steady-state concentration profiles (symmetric and asymmetric, stable and unstable) as a function of the various parameters of the problem. We showed how parameter variations cause solution branches to shift, to split apart so that solutions are annihilated, and to recombine so that new branches appear. One manuscript has been accepted for publication in the open literature; another, by one of our summer students (B. Lucier), will appear as an ANL report. A second summer graduate student (D. Olagunju) applied bifurcation theory and asymptotic

* Northwestern University

analysis to a problem in the theory of combustion. He considered the stability of a uniformly propagating flame front subjected to infinitesimal perturbations, and described the bifurcation into periodic solutions that follows the onset of instability.

3. Linear Transport Theory

Hans G. Kaper

We started work on a research monograph entitled *Spectral Methods in Linear Transport Theory*. This project is carried out in collaboration with C. G. Lekkerkerker (University of Amsterdam, Netherlands) and J. Hejtmanek (University of Vienna, Austria). The monograph explains the characteristic spectral features of transport operators and their implications for the solution of many problems in neutron transport, radiative transfer, the kinetic theory of gases, and plasma physics.

Also in the area of linear transport theory, one of our summer visitors (R. Hangelbroek of the Virginia Polytechnic Institute) prepared an ANL report on finite slab and half space problems for the time-independent neutron transport equation in media with absorption and anisotropic scattering.

B. Differential Equations

Gary K. Leaf

This activity comprises three collaborative efforts with scientists in other Argonne divisions:

With T. C. Chawla from the Reactor Analysis and Safety Division, we are studying two-phase compressible flow in a channel. The research is important for the safety analysis of fast sodium-cooled reactors. For the single-phase portion of the flow, prior to boiling, we are implementing the method of characteristics; for the multiphase portion, during boiling, we have formulated an explicit procedure. This latter formulation has been tested successfully and awaits further work on the single-phase portion.

With N. Q. Lam from the Materials Science Division, we have completed a study of defect buildup in alloys under cyclically pulsed irradiation. A kinetic model developed earlier was extended to include techniques for preferential sputtering in alloys and provisions for both the approach-to-equilibrium and the final equilibrium state. This work was published in the open literature.

With W. T. Sha from the Components Technology Division, we have continued development of numerical techniques for solving transient two-phase fluid flow in three dimensions. In the present formulation, a boundary-value problem has to be solved at each time step for the pressure correction. The operator governing the pressure is more involved than the Laplacian; hence the numerical approximation leads to the problem of solving a sparse, large, non-symmetric linear system of equations at each time step. Because the operator has variable coefficients, methods such as FFT are not applicable, nor are direct methods appropriate because of storage limitations. We therefore surveyed iterative methods which could be applied to non-symmetric matrices, and we adapted from symmetric matrices a technique based on incomplete Cholesky factorization combined with conjugate gradients. Our efforts here satisfied the immediate needs of the Components Technology Division. Further work on this technique is being continued as a separate research activity under Computational Mathematics (see II.C below).

II. COMPUTATIONAL MATHEMATICS

Computational mathematics research at Argonne involves the design and analysis of numerical algorithms, the development of special techniques to measure algorithm reliability and efficiency, and the preparation of software based on broadly applicable computational methods. Our current efforts focus on five main areas: (1) investigation of unconstrained and constrained optimization algorithms, (2) design and dissemination of quadrature techniques, (3) work on linear algebra, (4) enhancement of the DISPL package for partial differential equations, and (5) development of new algorithms and software for elementary and special functions.

A. Optimization

Joseph M. Cook, Burton S. Garbow, Kenneth E. Hillstrom, Michael Minkoff, and Jorge J. More'

Optimization continues to play a major role in research activities at Argonne. One part of our studies is concerned with the development of new algorithms for general optimization problems. These algorithms can then be implemented in our MINPACK collection of high-quality optimization software. Another part of our studies focuses on specially structured optimization problems that arise in specific energy applications problems. We also carry out smaller programs of research in the evaluation of mathematical software and in systems modeling.

1. MINPACK

Jorge J. More', Kenneth E. Hillstrom, Burton S. Garbow, and Michael Minkoff

One of the major accomplishments during this period was the completion of the final version of MINPACK-1. This version contains new codes for the solution of nonlinear equations and nonlinear least squares problems, and includes an algorithm CHKDER for checking the consistency between function and gradient values. Future editions of MINPACK will address unconstrained minimization and unconstrained optimization problems.

As part of our research in constrained optimization, and in collaboration with R. Crane of the RCA David Sarnoff Research Center, we implemented an algorithm of J. Stoer and K. Schittkowski for solving linearly constrained linear least-squares problems, and revised the current implementation of M. Powell's recursive quadratic programming algorithm VMCON. The results from a numerical comparison of VMCON and an augmented Lagrangian algorithm were presented at the ORSA/TIMS meeting in Milwaukee. Research was also begun in collaboration with M. Lenard (Boston University) on alternative active set strategies for the linearly constrained linear least squares problem.

Research in unconstrained minimization led to a line search which guarantees (in the absence of round-off errors) global convergence of quasi-Newton methods for convex functions. Additional research was carried out in collaboration with D. Sorensen of the University of Kentucky on a Newton method that uses negative curvature and takes into account the structure (for example, banded) of the Hessian.

2. Optimization with Structure

Michael Minkoff

General mathematical programming methods are often inadequate for solving large-scale optimization problems that arise in energy systems analyses. We are therefore studying new approaches that explore the special structure of these problems. Our present work is carried out jointly with two other Argonne divisions.

A short-term project involves the study of constrained optimization to fit tritium reaction/absorption/release parameters. This work, pursued in collaboration with R. H. Land and V. A. Maroni of the Chemical Engineering Division, necessitates the fitting of experimental data with a model based on the solution to an ordinary differential equation (ODE) system. The mathematical problem thus involves minimizing a nonlinear least-squares function subject to ODE constraints. Further, the model provides bounds on the parameters. To deal with this specific structure, we used a constrained optimization technique in combination with an ODE solver. The final package provides parameter estimates that yield better results than previously available. The program has been submitted to the National Energy Software Center, and an ANL report is in preparation.

As a long-term project we are working with B. Toppel and R. Rudolph of the Applied Physics Division on optimization problems arising from the study of fuel cycle options for nuclear power-plant installations. A mathematical model for future energy demands and reactor technologies based on the ALPS system (Hanford Nuclear Laboratory) generates the basic optimization problem. This model is then interfaced with a linear programming (LP) package developed at Argonne to solve the optimization problem and report results in terms of the ALPS model. As a consequence of our interaction, the LP code has been substantially modified to ensure greater sensitivity and efficiency. A new model, AESOP (Argonne Energy Strategies Optimization Program), is now being developed which will necessitate further revision of the LP approach. We have therefore been considering decomposition and simplex techniques to improve the computational speed without reducing modeling accuracy.

3. Systems Modeling

Joseph M. Cook

Several years ago an executive systems modeling program was designed for use in optimized models of fusion power plants. In particular, strategies for constrained optimization problems were modified to interface with elements in MINPACK as part of a parameter optimization study of the theta-pinch reactor. More recently, recognizing the need for a generalization, we developed the General System Modeling Program (GSMP). In addition to overall model-organization and control, GSMP provides such features as parameter sweeps, sensitivity analysis, and user-tested error diagnostics. We are now working on the theoretical foundation for GSMP. Theory for the programming system is being founded on very recent work on program transformation methods, older general system theory on hierarchical decomposition, and categorical algebra as applied to abstract data types. Our objective is to establish a program capable of supervising concurrent processes. Such a program would enable a more natural and direct modeling of systems that are themselves composed of concurrent processes. Additionally, it would greatly reduce computation time on a multiprocessor. Preliminary work indicates that there are no fundamental conceptual barriers to this further development of GSMP.

B. Quadrature

James N. Lyness

The present thrust of our quadrature research comprises both the design of quadrature techniques and the dissemination of quadrature software.

Significant progress has been made in several areas of design. First, in collaboration with F. N. Fritsch (Lawrence Livermore Laboratory) and D. K. Kahaner (Los Alamos Scientific Laboratory), we completed work on two-dimensional quadrature using one-dimensional automatic quadrature routines. A report has been submitted for publication. Second, in collaboration with G. Monegato (the University of Turin, Italy), we completed a study of quadrature over a triangle with an integrand function having singularities at the vertices. Our results have been accepted for publication in the open literature. Third, in collaboration with E. de Donker (University of Leuven, Belgium), we are nearing

completion on a study of error functional expansions with an integrand function having coincident line and point singularities at the vertex of a square.

In the area of quadrature technique dissemination, we prepared a set of notes for a small part of the Quadrature Users' Guide. This is a problem-oriented manual, providing references on how to approach various quadrature problems.

C. Linear Algebra

James M. Boyle, Jack J. Dongarra, Gary K. Leaf, and Michael Minkoff

In the past few years we have been working on the design and testing of efficient, state-of-the-art algorithms that could be incorporated into a collection of high-quality Fortran routines for solving simultaneous systems of linear equations. The LINPACK package has now been completed and released for public distribution by the National Energy Software Center and International Mathematical and Statistical Libraries. Extensions to LINPACK are already under way, and new investigations in linear algebra have also been initiated.

1. LINPACK

Jack J. Dongarra and James M. Boyle

The LINPACK package has been very well received. In its first nine months of public distribution, over 200 computer centers have requested the package, and close to 2000 copies of the LINPACK Users' Guide have been sold. Most of the reports on LINPACK from users have been extremely favorable, and very little software maintenance has been necessary.

We have begun work on extensions to LINPACK. In particular, we are developing sets of program transformations to construct a new, more efficient Fortran version of LINPACK. Building upon earlier work on transformations to replace BLA (Basic Linear Algebra) references by in-line code, we have implemented transformations for loop-unrolling and common-expression elimination. Work has also begun on transformations to convert from two-dimensional to one-dimensional arrays (including automatic linearization of subscript calculations); these transformations will be completed in a few months.

Somewhat longer-range efforts have also been initiated to construct alternate versions of LINPACK to handle matrices too large to fit into main memory (out-of-core techniques). Where possible, the new versions will be produced automatically from the standard version (or an abstraction of it). Otherwise, they will be constructed manually, adhering to LINPACK conventions for names, documentation, and parameters. The out-of-core methods will isolate any machine-dependent techniques for handling data transfers to and from secondary storage.

2. Eigenvalue and Eigenvector Refinements

Jack J. Dongarra

To date there has been no method available for improving the accuracy of an eigenvalue and eigenvector simultaneously once an eigensystem has been determined. We have therefore begun a new research effort to develop iterative techniques for improving the accuracy of a given eigenvalue and its associated eigenvector. The algorithm will use extended precision only at critical points. The method should require few iterations and should converge quickly if the original approximation is close to the true eigenvalue and eigenvector.

3. Non-Symmetric Linear Systems

Gary K. Leaf, Jack J. Dongarra, and Michael Minkoff

The increased demand for more detail in reactor analysis and design studies has focused attention on transient calculations of three-dimensional, two-phase fluid flow. A central feature of each calculation is the solution of large, sparse, non-symmetric linear systems arising at each time step. Because storage is limited, the solution must be iterative; and because the systems are solved repetitively, the solution must be fast. Continuing the work begun in applied analysis (see I.B above), we created two variants of an iterative technique involving conjugate gradients and incomplete Cholesky factorization. At present we are experimenting with various modifications of these algorithms in an effort to optimize the convergence rate. We will then compare and evaluate the algorithms in relation to other existing techniques.

D. Numerical Solutions of Partial Differential Equations

Gary K. Leaf and Michael Minkoff

This effort is concerned with the analysis of methods and software design for solving nonlinear systems of partial differential equations, including parabolic, mixed parabolic-elliptic, and some hyperbolic systems. We use the method of lines to reduce a system of PDE's to a system of ordinary differential equations. Reduction is achieved by means of a Galerkin procedure applied over an approximation subspace generated by a B-spline basis set. The resulting system of ODE's is solved with a variable order multistep stiff ODE package. This investigation led to the development of a software package DISPL1, which was extensively tested and used on a broad range of practical problems. The package allows one- and two-dimensional Cartesian, cylindrical, or spherical geometries; coefficient nonlinearities; fairly general nonlinear boundary conditions; material interfaces for problems in nonhomogeneous media; and steady-state, transient, and mixed-type problems. Software features include extensive dump/restart facilities; free-format input; and one-dimensional, contour, and three-dimensional graphics capability.

By the end of 1979, the primary, or "direct," version was in the National Energy Software Center. Another, or "geometric," version deals with general orthogonal geometries. It was enhanced to handle second-order cross-derivative terms; matrix valued diffusion coefficients; and highly nonlinear, periodic, and tangential boundary conditions.

We continued to interact with DISPL users. Three major studies are outlined below:

(1) with S. Das of the Materials Science Division, modeling of the melting and vaporization of oxide fuel pins. This activity involved creating a version of DISPL that was capable of handling multiphase heat-transfer problems.

(2) with R. Scattergood of the Materials Science Division, study of the migration of point defects in fuels.

(3) with G. E. Klinzing and G. D. Byrne of the Chemical and Petroleum Department, University of Pittsburgh, analysis of the effect of chemical reaction and the degree of contamination on mass transfer rates between discrete spherical particles and the dispersed phase. Results have been accepted for publication in the open literature.

In addition, we consulted on the installation and possible applications of the DISPL1 code with researchers at Yale University; the University of Pittsburgh; General Electric Re-entry and Environmental Systems Division; Chevron Research Laboratory; Sandia Laboratories, Livermore; and Lawrence Livermore Laboratory.

Other DISPL activities during this period included development of an interactive input generator and the capability of solving non-square systems of linear algebraic equations; the latter feature is useful for imposing constraints on the PDE system.

E. Approximation and Software Basics

W. J. Cody

In collaboration with W. Waite of the University of Colorado, we completed the *Software Manual for Elementary Functions*. The manual is intended as a guide to the implementation and testing of those subroutines for elementary functions ordinarily accompanying algebraic language compilers. It contains complete and detailed descriptions of algorithms, and a portable Fortran test program for each function discussed. The manual is scheduled for publication by Prentice-Hall in early spring.

In collaboration with D. Boss (a summer student), we also began work on a vector sine algorithm for the IBM 370. Preliminary results indicated that a significant savings in time was possible with a special subroutine which accepted a vector of arguments and returned a vector of results for each call. Additionally, we determined that a special subroutine which returned both the sine and cosine for a given argument operated at essentially the same speed as the standard system subroutine which returned only the sine.

Work has resumed on Bessel functions. We intend to develop new algorithms and software for those Bessel functions not included in FUNPACK. As a first step we are collecting readily available algorithms and software for Bessel functions of all kinds. We intend to survey this material for method and software performance, and to present the results of this survey at a special functions symposium at the University of Maryland in late 1980.

We have continued low-level participation in the IEEE Standards Subcommittee for Floating-point Arithmetic. Several papers were written in late 1979 in support of this activity.

III. SOFTWARE ENGINEERING

Software Engineering research at Argonne seeks ways to reduce the cost of producing highly reliable, easily usable computer software. Activities range from work on program transformation and verification to language-related studies on extensions to Fortran.

Having such a spectrum of activities makes it possible for Argonne scientists both to develop new software production tools and strategies and to test them in a working environment. For example, the TAMPR system was developed in the research on automated program transformations; it was subsequently used to produce LINPACK, to prepare input for the automated theorem prover and to study data and programming abstractions. In turn, these applications of TAMPR are generating input for the continuing research on program transformation methods.

One new activity is identified this year, Computer-Assisted Nuclear Power Plant Operations. We propose an interdisciplinary project--coordinated with industry, universities, and laboratories- to study ways of improving the efficiency and safety of nuclear power plants.

A. Program Development, Transformation, and Verification

James M. Boyle, Wayne R. Cowell, Kenneth W. Dritz, Brian T. Smith, and Lawrence T. Wos

These studies grew out of work on systematized collections of mathematical software. The ultimate goal is to reduce the cost of producing high-quality mathematical software--whether it be new software for inclusion in a package or an adaptation of existing software for a particular applications program. Emphasis is placed on creating reliable variants of software routines, assisting in their conversion to different computers, and analyzing program structure. Automated techniques for verifying the logical soundness of software are also under investigation.

1. Automated Program Transformation

James M. Boyle and Kenneth W. Dritz

Methods for specifying, implementing, and proving the correctness of program transformations are investigated. Particular attention is given to collections of transformations that are applicable to large classes of programs and that substantially modify them.

During the past eighteen months, we have made several enhancements to the existing TAMPR transformation system: We revised the interpreter to facilitate future proofs of correctness; we enhanced the formatter to permit quicker implementation of new global parameters; and we implemented two features to restrict the application of a transformation, thus reducing interference from other transformations.

A special formatting program was completed which produces "annotated structure-clarified Fortran," an executable version of Fortran with extensive comments describing its structure. It also appends to the Fortran program a "structure profile" to permit quick visualization of the overall program structure.

We also demonstrated the use of transformation techniques to implement a tool for profiling the execution of a program with a given set of test data. The profile shows which program structures were not tested by the test data. Using program transformation techniques, we were able to implement this profiler with only one week of effort.

2. Abstract Formulation of Programs

James M. Boyle, Kenneth W. Dritz, and Brian T. Smith

This activity, begun in 1978, was motivated by the successful use of slightly abstract program formulations in LINPACK and by continuing studies of the transportability of numeric and non-numeric software. Its goals are (a) to investigate abstraction as a technique for producing reliable, highly adaptable software for basic computations and (b) to study the exploitation of adaptability for optimizing the software for use in particular applications programs and for use on different computers.

We have focused primarily on methods for abstractly describing rank-one processes in linear algebra. A description of matrices and matrix operations has been found which permits the storage reference patterns, as well as other properties of the programs, to be optimized. Transformations were studied for the very early and very late stages of converting abstract linear algebra algorithms to executable Fortran. These studies revealed a need for more information about strategies required for optimal implementation of an algorithm. Some of these strategies have now been designed and will be implemented as soon as we extend TAMPR to facilitate the manipulation of program properties.

We also briefly investigated abstract formulation of non-numeric programs, using the classic eight-queens problem as an example. Preliminary results have encouraged us to consider implementing transformations to convert a recursive pure-applicative specification of a program to an executable Fortran program employing iteration and assignment.

3. Automated Theorem Proving and Program Verification

Lawrence T. Wos and Brian T. Smith

In the past few years we have been developing an automated theorem proving program for proving program correctness. We have now completed a more flexible version of this program based on an environmental approach. The environmental version allows the user to choose values for the various input parameters and assignments for the various lists. The program has been released on a limited basis for such applications as designing a multivalued logic circuit.

Complementing the work on program verification, we developed a broadened unification module. By building some of the semantics of the given problem into the procedure to permit problem-dependent unification, we hope to improve the efficiency of automated program verification.

We also formulated and implemented a more sophisticated treatment of equality, that is, a generalization of the inference rule paramodulation. This new treatment, called hyperparamodulation, combines certain properties of paramodulation with others from hyper-resolution. Hyperparamodulation has already proved invaluable in algebraic investigations of Robbins algebra.

Finally, we have begun designing a new system for automated reasoning. Because of the dual concerns of portability and modifiability, the system will be written in a higher-level language. Included will be a multiprocessing capability, because the techniques and strategies used in an automatic deduction system are naturally suited to loosely coupled but separate tasks. The input language will permit present clause-oriented approaches, natural deduction, and lambda calculus.

4. Tools for Numerically Oriented Fortran Programs

Wayne R. Cowell and James M. Boyle

Software engineering research has resulted in a number of software tools that facilitate the development and testing of Fortran programs. During 1979, we

participated in an NSF-sponsored workshop which explored the feasibility of producing an integrated collection of these software tools. Eight groups agreed to collaborate on such a project (to be called Toolpack): Argonne, Bell Laboratories, International Mathematical and Statistical Libraries, Jet Propulsion Laboratory, Numerical Algorithms Group, Purdue University, University of California at Santa Barbara, and the University of Colorado. The background and goals of the project are summarized in AMD T.M. 341, *The Toolpack Prospectus*.

Argonne has played a lead role in defining the objectives and organization of the project, establishing a liaison with funding agencies, and identifying priorities for future work.

To date, some of the participating groups have made considerable progress in the construction of Toolpack components. Our own plans in this area are to prepare a transportable version of TAMPR beginning in late 1980.

B. Fortran Language Activities

Paul C. Messina and Brian T. Smith

Language research studies address the problem of ensuring that programming languages meet the diversified and changing needs of their users. Argonne is participating in two distinct projects, one involving revisions to the current Fortran standard, and the other involving design of a common programming language for use in the Department of Energy. Our special concern in both projects is the suitability of the language for numerical software development.

1. Fortran Standards Committee

Brian T. Smith

Since the 1977-1978 revision of Fortran, the X3J3 Fortran Standards Committee of the American National Standards Institute (ANSI) has been considering revisions to the current Fortran standard so that the language meets the changing needs of its users. To represent the interests of the numerical software community, Argonne and the SIGNUM organization (Special Interest Group for Numerical Software of the Association for Computing Machinery) have jointly supported a member of the X3J3 Fortran Standards Committee.

During 1979, a proposal to incorporate a general floating-point precision facility into the Fortran language was prepared and presented to the X3J3 committee. The general precision facility permits machine-independent specifications of precision in terms of a minimum precision specification and also permits a parameterized specification of the native floating data types. With the dual mechanism, portable Fortran programs will be more easily written for portable numerical algorithms, and non-portable programs will be easily parameterized in terms of a precision specification yielding transportable software.

Other proposals for the next revision were also evaluated, particularly with respect to their suitability for numerical software preparation. The goal is to have a draft of the next Fortran standard ready next year.

2. Language Working Group

Brian T. Smith and Paul C. Messina

In October 1976, the Office of Automated Data Processing Management of the Department of Energy established the Advanced Computing Committee (ACC) to study ways in which the large computing facilities at DOE sites could share computing expertise and resources. The ACC then formed the Language Working Group to recommend a common programming language so that software could be directly shared among the sites.

By the end of 1978, the Language Working Group (LWG) had formulated a language based upon extensions to the Fortran 77 language (ANSI X3.9). During the following year, Argonne had three participants in the LWG project who helped develop the functional specifications for the environmental inquiry feature, complex double-precision data type, and Level 3 specification, and assisted in the management and presentation of LWG reports. In addition, we provided about one-third of the effort involved in finishing a complete language design, integrated with Fortran 77.

Since October 1979, a representative from Argonne has been chairman of the Language Working Group. The functional specification and language design, recorded in a draft document, have been presented to DOE-supported groups. Based on comments about the draft, an amended report will be prepared and presented to the ACC.

C. Computer-Assisted Nuclear Power-Plant Operations

John R. Gabriel

Three Mile Island has focused attention on the need for increased computer assistance in nuclear power-plant operations. At issue is not simply what information-handling techniques can do to improve reactor safety, but how various groups from several disciplines can improve and ensure the human control of complex technical systems. Short-term solutions such as improved data logging are already being considered. There remain, however, important and very difficult problems, such as computer-assisted problem diagnosis, where the present state of the computing art is not known in the nuclear power community and the problems that arise in nuclear power plants are not known in the computer science community.

To understand better how to deal with these long-term problems, Argonne hosted a one-day workshop in January 1980. Representatives from universities, research laboratories, and industry gave presentations and participated in an afternoon round-table discussion. Several problems and potential solutions were outlined, but considerably more work is called for to determine where research is needed and how various groups can help.

We would like to explore these questions further, under formal endorsement from DOE. We have therefore proposed that DOE fund one year of effort each for appropriate outside consultants and for Argonne staff. The consultants would be chosen from a company that is well established in relevant computer science research activities. Argonne's role during this stage would be one of organization and coordination.

IV. SPECIAL PROJECTS

Among the special research projects supported by the Department of Energy are liaison activities intended to investigate ways of improving the flow of research results from the applied mathematical sciences into mission-oriented programs. The software clinics project addresses the specific problem of how to use software libraries and software tools effectively in developing computer applications.

Software Clinics

Wayne R. Cowell and Jesse Y. Wang*

A prototype clinic consortium was organized and began operation in late 1979. An overview of the project is presented in AMD T.M. 342, *Working Paper: Software Clinics in the Department of Energy*. Three sites--Argonne, Los Alamos Scientific Laboratory, and the NYU Courant Institute of Mathematical Sciences--are offering services in mathematical software consultation and in automatic structuring of Fortran programs.

Mathematical software consultation builds on existing consultant services but with a new emphasis on pooling of resources and information. Numerical computation has been a major thrust of DOE research and development programs. Expert capability exists but is somewhat dispersed, and there are serious communication gaps between mathematical software experts and mathematical software users. To facilitate information exchange, a clinician at each site writes up problems for circulation to mathematical software consultants, relays comments and questions back to the users, and circulates comments among the consultants. An electronic mail system is being used to broadcast abstracts of problems to clinicians and consultants at participating sites and to provide on-line files of abstracts of problems, feedback from consultants, and requests for formatting service.

Automatic program structuring involves the use of the TAMPR transformation system, developed at Argonne, to format Fortran source code. TAMPR is applied and the formatted program returned to the originator for use in DOE applications programs.

If the concept of software clinics proves successful, we intend to facilitate the establishment of clinics at all the national laboratories.

* Joint Appointment, User Services Section, Applied Mathematics Division

Appendix A

STAFF

J. M. Boyle, *Ph.D.*, Northwestern University, 1970
W. J. Cody, Jr., *M.A.*, University of Oklahoma, 1956, *D.Sc. (Hon.)*; Elmhurst College, 1977
J. M. Cook, *Ph.D.*, University of Chicago, 1951
W. R. Cowell, *Ph.D.*, University of Wisconsin, 1954
J. J. Dongarra, *M.S.*, Illinois Institute of Technology, 1973
K. W. Dritz, *M.S.*, Massachusetts Institute of Technology, 1967
J. R. Gabriel, *M.S.*, University of Otago, New Zealand, 1953
B. S. Garbow, *M.S.*, University of Chicago, 1952
D. V. Goetschel, • *M.S.*, Northern Illinois University, 1976
K. E. Hillstrom, *M.S.*, Northwestern University, 1957
H. G. Kaper, *Ph.D.*, Rijksuniversiteit, Groningen, 1965
G. K. Leaf, *Ph.D.*, University of Illinois, 1961
J. N. Lyness, *D. Phil.*, Oxford University, 1957
P. C. Messina, •• *Ph.D.*, University of Cincinnati, 1972
M. Minkoff, *Ph.D.*, University of Wisconsin, 1973
J. J. More', *Ph.D.*, University of Maryland, 1970
G. W. Pieper, *Ph.D.*, University of Illinois, 1969
B. T. Smith, *Ph.D.*, University of Toronto, 1969
J. Y. Wang, + *Ph.D.*, Washington State University, 1976
L. T. Wos, *Ph.D.*, University of Illinois, 1957

- Present address: Amerock Corporation, Rockford, Illinois
- Associate Division Director
- + Joint appointment, User Services Section,
Applied Mathematics Division

Appendix B

PROFESSIONAL ACTIVITIES

Members of the section participated in the following professional activities during the period October 1, 1978 - March 31, 1980.

J. M. Boyle	Chairman, DOE AMS Planning Group for Software Engineering Principal Investigator, Mathematical Software Research in U.S.-U.S.S.R. Science and Technology Joint Working Group in the Applications of Computers to Economics and Management
W. J. Cody	Associate Editor, Transactions on Mathematical Software Member, International Federation for Information Processing WG 2.5 for Mathematical Software Member, IEEE Standards Subcommittee for Floating-Point Arithmetic National Lecturer, ACM, 1979-1980
J. M. Cook	Consultant Systems Analyst, State of Illinois
W. R. Cowell	Council Chairman, Toolpack Project
K. W. Dritz	Member, SHARE PL/I Project
H. G. Kaper	Chairman, DOE AMS Planning Group for Applied Analysis Member, SIAM National Program Committee Visiting Professor, Northwestern University SIAM Visiting Lecture
J. N. Lyness	Associate Editor, Mathematics of Computation Associate Editor, SIAM Journal on Numerical Analysis Lecturer, Series of 25 Lectures on Numerical Analysis, Symposium for Post-Doctorate Students, organized by the Italian NSF, Perugia, Italy, July 16 - August 17, 1979
P. C. Messina	Chairman, DOE Advanced Computing Committee Language Working Group
J. J. More'	Associate Editor, SIAM Journal on Numerical Analysis Associate Editor, SIAM Journal on Scientific and Statistical Computing
G. W. Pieper	Instructor, Illinois Benedictine College
B. T. Smith	Member, DOE Advanced Computing Committee Language Working Group Member, International Federation for Information Processing WG 2.5 for Mathematical Software Member, X3J3 Fortran Standards Committee Member, Design Team for the LWG Fortran Language

Appendix C

PRESENTATIONS

The following list reflects articles published, reports distributed, and talks presented during the period October 1, 1978 - March 31, 1980

Publications

J. M. Boyle, *Extending Reliability: Transformational Tailoring of Abstract Mathematical Software*, SIGNUM Newsletter, 14, 57-62 (1979) (extended abstract)

J. M. Boyle, "Historical Development of the 'Software Applications' Project," *Summary of a Conference on the U.S.-U.S.S.R. Scientific Exchange Program in Computers and Management*, McKenney, Aufenkamp, and Austin, eds., Graduate School of Business Administration, Harvard University HBS 79-6

J. M. Boyle, "Possibilities for the Automatic Synthesis of Linear Algebra Programs by Program Transformation," *Numerical Analysis in Fortran*, Moscow State University, Moscow, U.S.S.R., 1979 (in Russian; to appear in English)

J. M. Boyle, "Program Adaptation and Program Transformation," *Proceedings of the Workshop on Software Adaption and Maintenance*, R. Ebert, J. Lueger, and L. Goeke, eds., North-Holland Publishing Co., New York, 1980

G. D. Byrne, *DISPL: A Software System for One and Two Spatially Dimensioned Convection-Diffusion-Kinetics Problems*, Proc. of the Third IMACS International Symposium on Computer Methods for Partial Differential Equations, Lehigh University, Pa., June 20-22, 1979 (invited paper)

W. J. Cody, "Discussion of 'Software for Numerical Computation,'" *Research Directions in Software Technology*, P. Wegner, ed., The MIT Press, Cambridge, Mass., 1979, pp. 793-794

W. J. Cody, *The Impact of the Proposed Standard on Numerical Software*, SIGNUM Newsletter, Special Issue on the Proposed IEEE Floating-Point Standard, October 1979, pp. 29-30

W. J. Cody, "Software Basics for Computational Mathematics," *Program Directions for Computational Mathematics*, R. Huddleston, ed., DOE, 1979, pp. 167-199

W. J. Cody, *Towards Sensible Floating-Point Arithmetic*, Proc. COMPCON 80, February 1980, pp. 488-490

W. R. Cowell, "Discussion of Session on Reliability and Warranty of Numerical Software," *Performance Evaluation of Numerical Software*, L. D. Fosdick, ed., North-Holland Publishing Co., 1979, pp. 169-171

J. J. Dongarra, *Some LINPACK Timings on the CRAY-1*, Proc. of the 1978 LASL Workshop on Vector and Parallel Processors, Los Alamos, New Mexico, September 20-23, 1978, pp. 58-75

J. J. Dongarra, J. R. Bunch, C. B. Moler, and G. W. Stewart, *LINPACK Users' Guide*, SIAM, 1979

J. J. Dongarra and A. R. Hinds, *Unrolling Loops in FORTRAN*, Software--Practice and Experience, 9, 219-225 (1979)

K. W. Dritz, *Portability of Numerical Software in PL/I: A Small Case Study*, Proc. of SHARE 52, 1, 596-623 (1979)

K. W. Dritz, Programmable Formatting of Program Text: Experiences Drawn from the TAMPR System, ACM SIGNUM Newsletter, 14, 71-72 (1979) (extended abstract)

K. W. Dritz, "Removal of Data Structuring Abstractions from Linear Algebra Subroutines by Transformation and Optimization," *Numerical Analysis in Fortran*, Moscow State University, Moscow, U.S.S.R., 1979, pp. 131-150 (in Russian; to appear in English)

B. S. Garbow, *Algorithm 535. The QZ Algorithm to Solve the Generalized Eigenvalue Problem for Complex Matrices*, ACM Trans. on Math. Software, 4, 404-410 (1978)

R. J. Hangelbroek, "Derivation of Formulas Relevant to Neutron Transport in Media with Anisotropic Scattering," *Differential Equations and Applications*, W. Eckhaus and E. M. de Jager eds., North-Holland Publishing Co., 1978

G. A. Hively, *On a Class of Nonlinear Integral Equations Arising in Transport Theory*, SIAM J. Math. Anal., 9, 787-792 (1978)

H. G. Kaper, *Boundary Value Problems of Mixed Type Arising in the Kinetic Theory of Gases*, SIAM J. Math. Anal., 10, 161-178 (1979)

H. G. Kaper, *A Constructive Approach to the Solution of a Class of Boundary Value Problems of Mixed Type*, J. Math. Anal. & Appl., 63, 691-718 (1979)

H. G. Kaper, *Spectral Representation of an Unbounded Linear Transformation Arising in the Kinetic Theory of Gases*, SIAM J. Math. Anal., 10, 179-191 (1979)

H. G. Kaper and O. Diekmann, "On the Bounded Solutions of a Nonlinear Convolution Equation," *International Conference on Applied Nonlinear Analysis*, V. Lakshmikantham, ed., Academic Press, New York, 1979

H. G. Kaper and G. K. Leaf, *Improved Error Estimates for the Perturbed Galerkin Method Applied to a Class of Generalized Eigenvalue Problems*, Proc. Koninkl. Nederl. Akad. van Wetensch., Series A, 82, 307-316 (1979)

P. Keast and J. N. Lyness, *On the Structure of Fully Symmetric Multidimensional Quadrature*, SIAM J. of Num. Anal., 16, 11-29 (1979)

G. E. Klinzing, G. D. Byrne, G. K. Leaf, and M. Minkoff, *An Application of Spline-Galerkin Techniques to a Mass Transfer Problem*, Proc. of the Third IMACS International Symposium on Computer Methods for Partial Differential Equations, Lehigh University, Pa., June 20-22, 1979 (abstract)

N. Q. Lam, G. Leaf, and R. A. Johnson, *Defect Buildup and Solute Segregation in Alloys under Pulsed Irradiation*, J. of Nucl. Mat., 74, 277-289 (1978)

N. Q. Lam, G. K. Leaf, and H. Wiedersich, *Effects of Radiation-Induced Segregation and Preferential Sputtering Rate of Alloys*, J. Nucl. Mat., 85 & 86, 1085-1089 (1979)

G. K. Leaf, T. C. Chawla, and W. J. Minkowycz, *Numerical Methods for Hydraulic Transients*, Num. Heat Transfer, 2, 1-34 (1979)

J. N. Lyness, *The Affine Scale Invariance of Minimization Algorithms*, Math. Comp., 33, 265-287 (1979)

J. N. Lyness, *A Bench Mark Experiment for Minimization Algorithms*, Math. Comp., 33, 249-264 (1979)

J. N. Lyness, *Has Numerical Differentiation a Future?* Proc. of the Seventh Manitoba Conference on Numerical Mathematics and Computing, 1977, pp. 107-129

- J. N. Lyness, "Performance Profiles and Software Evaluation," *Performance Evaluation of Numerical Software*, L. D. Fosdick, ed., North-Holland Publishing Co., New York, 1979, pp. 51-58
- J. N. Lyness, *Quadrature over a Simplex: Part 1. A Representation for the Integrand Function*, SIAM J. of Num. Anal., **15**, 122-133 (1978)
- J. N. Lyness, *Quadrature over a Simplex: Part 2. A Representation for the Error Functional*, SIAM J. of Num. Anal., **15**, 870-887 (1978)
- J. N. Lyness and A. C. Genz, *On Simplex Trapezoidal Rule Families*, SIAM J. Num. Anal., **17**, 126-147 (1980)
- J. N. Lyness and P. Keast, *On p-Generator Fully Symmetric Quadrature Rules*, Num. Math., **30**, 51-62 (1978)
- J. N. Lyness and G. Monegato, *Quadrature Error Functional Expansions for the Simplex When the Integrand Function Has Singularities at Vertices*, Math. Comp., **34**, 213-225 (1980)
- M. Minkoff, "Nonlinear Constrained Optimization Methods," *Modeling and Simulation*, W. G. Vogt and M. H. Mickle, eds., Instrument Society of America, Vol. 10, Part 3, 1979, pp. 861-865
- G. Monegato and J. N. Lyness, *On the Numerical Evaluation of a Particular Singular Two-Dimensional Integral*, Math. Comp., **33**, 993-1002 (1979)
- J. J. More', "Implementation and Testing of Optimization Software," *Performance Evaluation of Numerical Software*, L. D. Fosdick, ed., North-Holland Publishing Co., New York, 1979, pp. 253-263
- J. J. More' and M. Y. Cosnard, *Numerical Solution of Nonlinear Equations*, ACM Trans. on Math. Soft., **5**, 64-85 (1979)
- J. J. More' and D. C. Sorensen, *On the Use of Directions of Negative Curvature in a Modified Newton Method*, Math. Prog., **16**, 1-20 (1979)
- J. J. More', R. Tapia, and M. Wright, "Optimization," *Program Directions for Computational Mathematics*, R. Huddleston, ed., DOE, 1979, pp. 129-166
- L. Nazareth, *A Relationship Between the BFGS and Conjugate Gradient Algorithms and Its Implications for New Algorithms*, SIAM J. Num. Anal., **16**, 794-800 (1979)
- L. Nazareth, *Some Recent Approaches to Solving Large Residual Nonlinear Least Squares Problems*, SIAM Review, **22**, 1-11 (1980)
- B. T. Smith, "Can Automated Theorem Provers Be Used to Evaluate Linear Algebra Software?" *Performance Evaluation of Numerical Software*, L. D. Fosdick, ed., North-Holland Publishing Co., New York, 1979, pp. 109-120
- B. T. Smith, "Portability and Adaptability--What are the Issues?" *Numerical Software -- Needs and Availability*, D. Jacobs, ed., Academic Press, 1978
- J. Y. Wang, *The Evaluation of Periodic Functions with Large Input Arguments*, ACM/SIGNUM, **13**, 7-9 (1978)
- J. Y. Wang, *On the Improvement of Some Mathematical Subroutines in the IBM S/360 FORTRAN IV Libraries*, Proc. of the IBM SHARE 54 Conference, Anaheim, Cal., March 3, 1980
- S. Winker, *Generation and Verification of Finite Models and Counterexamples Using an Automated Theorem Prover Answering Two Open Questions*, Proc. of the Fourth Workshop on Automated Deduction, Austin, Texas, Feb. 1-3, 1979, pp. 7-13

Reports

- J. M. Cook, *User's Guide for GSMP, A General System Modeling Program*, ANL/MHD-79-11
- J. J. Dongarra, *LINPACK Working Note No. 3: Fortran BLAS Timing*, ANL 80-24
- R. J. Hangelbroek, *On the Derivation of Some Formulas in Linear Transport Theory for Media with Anisotropic Scattering*, Katholieke Universiteit Nijmegen Report 7720, April 1978
- H. G. Kaper and G. K. Leaf, *Ergodic Theorems for Nonlinear Contraction Semigroups in a Hilbert Space*, ANL 79-50
- H. G. Kaper and G. K. Leaf, *Nonlinear Ergodic Theorems for Abel Means*, ANL 79-49
- G. K. Leaf, M. Minkoff, G. D. Byrne, T. Bleakney, and J. Saltzman, *DISPL: A Software Package for One and Two Spatially Dimensioned Kinetics-Diffusion Problems*, ANL 77-12 (Rev. 1)
- O. L. Mangasarian, *Iterative Solution of Linear Programs*, ANL 79-75
- S. Reich, *On the Equivalence Between Resolvent Consistency and Convergence for Nonlinear Quasi-Contractive Algorithms*, ANL 79-53
- S. Reich, *Nonlinear Ergodic Theory in Banach Space*, ANL 79-69
- M. Rose, *Numerical Methods for a Porous Medium Equation*, ANL 78-80
- L. Rudinski with G. W. Pieper, *Evaluating Computer Program Performance on the CRAY-1*, ANL 79-9
- L. Rudinski with G. W. Pieper, *Production Runs on the CRAY-1*, ANL 79-68

Technical Memoranda

- W. J. Cody, *Draft - Software Basics for Computational Mathematics*, T.M. 328
- L. Cornwell, P. Hutchison, M. Minkoff, and H. Schultz, *Test Problems for Constrained Nonlinear Mathematical Programming Algorithms*, T.M. 320 (Rev. 1)
- W. R. Cowell and W. C. Miller, *The Toolpack Prospectus*, T.M. 341
- W. R. Cowell, *Working Paper: Software Clinics in the Department of Energy*, T.M. 342
- J. J. Dongarra and A. R. Hinds, *LINPACK Working Note No. 12 - Unrolling Loops in Fortran*, T.M. 327
- J. J. Dongarra and C. B. Moler, *LINPACK Working Note No. 13 - Implementation Guide for LINPACK*, T.M. 330
- D. V. Goetschel and J. K. Kalita, *Two Experiments Involving the Implementation and Use of Nonlinear Optimization Software on a Minicomputer System*, T.M. 331
- J. N. Lyness, *Performance Profiles and Software Evaluation*, T.M. 343
- L. Nazareth, *A Relationship Between the BFGS and Conjugate Gradient Algorithm*, T.M. 282
- R. C. Raffanetti, *A Comparative Study of the Fortran Development Environment Provided by the VAX/UNIX Operating Systems*, T.M. 346

Oral Presentations

- J. M. Boyle, "Abstract Formulation of Algorithms in Linear Algebra," Seminar, SRCC, Moscow State University, Moscow, U.S.S.R., November 21, 1978
- J. M. Boyle, "Introduction to the TAMPR Program Transformation System," Seminar, Technical University of Munich, Munich, FRG, December 19, 1978
- J. M. Boyle, "Software Adaptability and Program Transformation," NSF Workshop, Software Engineering, A National Issue, RPI and GE R&D Center, Albany, Schenectady, and Troy, New York, May 30-June 1, 1979
- J. M. Boyle, "The TAMPR Program Transformation System," Seminar, Computing Center of the Academy of Sciences, Novosibirsk (Akademgorodok), U.S.S.R., November 16, 1978
- J. M. Boyle, "Towards Automatic Synthesis of Linear Algebra Programs," Conference on the Production and Assessment of Numerical Software, Liverpool, England, April 9-11, 1979
- W. J. Cody, "Computation and Testing of Elementary Functions," Wisconsin Section MAA Workshop on Mathematics, Computers, and Calculators, Ripon, Wis., November 10, 1979
- J. J. Dongarra, "LINPACK: An Example of Mathematical Software," Seminar, Stanford University, March 30, 1979
- J. J. Dongarra, "LINPACK and LINPACK Timings," NASIG Meeting, Lawrence Livermore Laboratory, April 2, 1979
- J. J. Dongarra, "LINPACK," A.E.R.E., Harwell, October 11, 1979
- J. J. Dongarra, "Mathematical Software for Linear Systems," Reading University, October 19, 1979
- J. J. Dongarra, "LINPACK, A High Quality Software Package for Linear Algebra," Eidgenossische Technische Hochschule, Zurich, October 25, 1979
- J. J. Dongarra, "LINPACK: An Example of Mathematical Software," Seminar, Northern Illinois University, November 1979
- K. W. Dritz, "The TAMPR System Formatter," Seminar, Computing Center, Siberian Division of the Soviet Academy of Science, Novosibirsk, November 16, 1978
- H. G. Kaper, "Boundary Value Problems of Mixed Type in the Kinetic Theory of Gases," Kent State University, Kent, Ohio, October 1978
- H. G. Kaper, "Initial-Value Problems for the Carleman Equation," Department of Mathematics, Indiana University, Bloomington, Indiana, December 1978
- H. G. Kaper, "Recent Results in Nonlinear Transport Theory," Sixth Conference on Transport Theory, Tucson, Arizona, April 1979
- H. G. Kaper, "Asymmetric Steady-States in Catalytic Reactors," SIAM Fall Meeting, Denver, Col., November 1979
- G. K. Leaf and M. Minkoff, "Some Comments on PDE/ODE Software Interfaces," Panel Discussion on Numerical Methods of Linear Software, SIGNUM Numerical Ordinary Differential Equations Meeting, Champaign, Ill., April 3-5, 1978
- G. K. Leaf and M. Minkoff, "DISPL1: A Software Package for Solving One and Two Spatially Dimensioned Kinetics-Diffusion Problems," Sandia Laboratories, Livermore, February 1980

J. N. Lyness. "The Role of Adaptive Quadrature Routines in Large Scale Calculations," SIAM Fall Conference, Denver, Col., November 14, 1979

J. N. Lyness. "When Not to Use an Automatic Quadrature Routine," RCA Laboratories, Princeton, New Jersey, December 5, 1979

J. N. Lyness. "When Not to Use an Automatic Quadrature Routine," NBS, Washington, D.C., February 1, 1980

P. C. Messina. "Beyond Fortran 77," SHARE 54, Anaheim, Ca., March 3, 1980

M. Minkoff. "Testing of Augmented Lagrangian and Constrained Variable Metric Methods," ORSA 1979 Fall National Meeting, Milwaukee, October 15-19, 1979

J. J. More'. "Nonlinear Least Squares Calculations," Imperial Chemical Industries, England, November 2, 1978

J. J. More'. "Directions of Negative Curvature and Modified Newton Methods," National Physical Laboratory, England, January 10, 1979

J. J. More'. "Directions of Negative Curvature and Modified Newton Methods," Cambridge University, England, January 22, 1979

J. J. More'. "Directions of Negative Curvature and Modified Newton Methods," Manchester University, England, February 7, 1979

J. J. More'. "Numerical Solution of Systems of Nonlinear Equations," Reading University, England, February 27, 1979

J. J. More'. "Directions of Negative Curvature and Modified Newton Methods," Atomic Energy Research Establishment, England, March 1, 1979

J. J. More'. "Numerical Solution of Systems of Nonlinear Equations," Imperial College, England, March 14, 1979

J. J. More'. "Directions of Negative Curvature and Modified Newton Methods," Umea University, Sweden, April 23, 1979

J. J. More'. "Numerical Solution of Systems of Nonlinear Equations," Lulea University, Sweden, April 25, 1979

J. J. More'. "Implementation and Testing of Optimization Software," Linköping University, Sweden, April 27, 1979

J. J. More'. "Numerical Solution of Systems of Nonlinear Equations," University of Kent at Canterbury, England, June 8, 1979

J. J. More'. "On the Design of Optimization Software," International Conference on Nonlinear Optimization and Applications," L'Aquila, Italy, June 18-20, 1979

J. J. More'. "Directions of Negative Curvature and Modified Newton Methods," Heidelberg University, Germany, June 22, 1979

J. J. More'. "Numerical Solution of Systems of Nonlinear Equations and Nonlinear Least Squares Problems," Massachusetts Institute of Technology, Boston, Mass., October 3, 1979

J. J. More'. "Implementation and Testing of Optimization Software," ORSA 1979 Fall National Meeting, Milwaukee, October 15-19, 1979

J. J. More'. "Numerical Solution of Systems of Nonlinear Equations and Nonlinear Least Squares Problems," Rice University, Houston, Texas, October 29, 1979

J. J. More', "Numerical Solution of Systems of Nonlinear Equations and Nonlinear Least Squares Problems." Yale University, New Haven, Conn., March 27, 1980

B. T. Smith, "A Comparison of Two Recent Approaches to Machine Parameterization for Mathematical Software," ACM/SIGNUM Conference on the Programming Environment for Development of Numerical Software, Pasadena, Ca., October 18-20, 1978

J. Y. Wang, "The Numerical Computation of Inverse Eigenvalue Problems." NASIG 79 Meeting, Lawrence Livermore Laboratory, May 1, 1979

Appendix D

VISITORS PROGRAM

The Visitors Program encourages interactions with the applied mathematical sciences research community. Following is a list of students and visiting scientists who came to Argonne for special work in mathematics and computer science during the period October 1, 1978, through March 31, 1980.

Faculty and Staff Appointments

Eugene Barston	University of Illinois, Chicago Circle
Thomas Coleman	University of Waterloo, Canada
Roger L. Crane	RCA David Sarnoff Research Center
Elise H. De Doncker	Katholieke University, Leuven, Belgium
Richard Goodman	University of Miami
Rutger J. Hangelbroek	Virginia Polytechnic Institute
Johann Hejzmanek	Universitaet Wien, Vienna, Austria
Larry Henschen	Northwestern University
C. Gerrit Lekkerkerker	Universiteit van Amsterdam
Melanie Lenard	Boston University
Olvi Mangasarian	University of Wisconsin
Giovanni Monegato	University of Torino, Italy
Philip Rabinowitz	Weizmann Institute of Science, Israel
Steven Winker	University of Illinois, Chicago Circle

Graduate Student Appointments

Dale Boss	Purdue University
Gregory Halac	Johns Hopkins University
John Kalita	Western Illinois University
Barbara Kerns	Massachusetts Institute of Technology
Bradley Lucier	University of Chicago
David Olagunju	Northwestern University
Robert Veroff	Northwestern University
Withold Wojciechowski	Illinois Institute of Technology

Undergraduate Student Appointments

Patricia Managan	Bayer University
Gerold Perham	St. Joseph's University
Andrea Sha	University of Illinois
Daphne Smith	Spelman College
Mary Sullivan	Clarke College
Karen Wiekert	Oregon State University

Appendix E

CONSULTANTS

Garrett Birkoff
James Bunch
George Byrne
Larry Cornwell
William Davidon
John Dennis
Olvi Mangasarian
Bernard J. Matkowsky
Cleve Moler
Larry Nazareth
J. Ben Rosen
Hilbert Schultz
Danny Sorensen
Gilbert Stewart
William Waite
David Young

Harvard University
University of California, San Diego
University of Pittsburgh
Western Illinois University
Haverford College
Rice University
University of Wisconsin, Madison
Northwestern University
University of New Mexico
Self
University of Minnesota
University of Wisconsin, Oshkosh
University of Kentucky
University of Maryland
University of Colorado
University of Texas, Austin

Appendix F

MEETINGS AND WORKSHOPS

1. Applied Analysis Workshop - December 6-7, 1978

Fifteen mathematicians from DOE laboratories participated in a two-day workshop to discuss DOE research in applied analysis. The workshop, hosted by Argonne National Laboratory, focused on the preparation of a planning document detailing a research program in applied analysis.

2. ANL-LBL Workshop on Tools for Software Development - May 10, 1979

A one-day workshop was held at Argonne to discuss the current status and plans of Lawrence Berkeley Laboratory's Advanced Systems Group and Argonne's role in the proposed Toolpack project. Potential areas for collaboration between the two projects were also considered.

3. Chicago Area Applied Mathematics Consortium - May 14-15, 1979

Distinguished mathematician Harold Grad (Courant Institute of Mathematical Sciences, New York University) presented two lectures on kinetic theory and plasma physics. The consortium is sponsored jointly by Argonne National Laboratory, the University of Chicago, the University of Illinois at Chicago Circle, and Northwestern University.

4. Toolpack Council - June 14-15, 1979

The first meeting of the Toolpack Council was held at Argonne to deal with basic questions about project organization and funding. The council chairman, Wayne R. Cowell, was responsible for preparing the agenda and coordinating the discussion.

5. SIMS Research Applications Conference on Energy Conversion and Fluid Mechanics - June 25-29, 1979

Mathematicians and computer scientists met at Alta, Utah, to discuss mathematical problems in energy conversion. The meeting was partially funded by Argonne National Laboratory.

6. ELLPACK Workshop - July 27-28, 1979

Numerical analysts and computer scientists from several universities and DOE laboratories met at Argonne to review the progress of the ELLPACK project. This project is a cooperative effort led by Purdue University to provide a research and educational tool for evaluating and developing software to solve elliptic partial differential equations. Included in the program were reports on the advantages and disadvantages of ELLPACK and a discussion of future efforts.

7. ACC/LWG Meeting - September 17-20, 1979

The DOE Advanced Computing Committee Language Working Group held its thirteenth meeting in Chicago. Fourteen representatives from national research laboratories discussed the continuing work on ACC Fortran and the future role of the Language Working Group.

8. Computer-Assisted Nuclear Power-Plant Operation - January 18, 1980

Representatives from industry, universities, and laboratories attended a one-day seminar at Argonne to hear scheduled presentations on the interplay between human factors and nuclear power-plant operation. Round-table discussions followed in the afternoon.

Appendix G

SEMINARS

During the period October 1, 1978 - March 31, 1980, the Applied Mathematical Sciences Section sponsored numerous seminars in mathematics and computer science. These are listed below.

Douglas Arnold

University of Chicago

Superconvergence of Finite Element Methods

January 9, 1979

Shih-Ping Han

University of Illinois

Quasi-Newton Methods for Solving Minimax Problems

January 12, 1979

Jose' Vega

Northwestern University

Singular Perturbation Techniques and Langmuir-Hinshelwood Type Kinetics

January 25, 1979

Russell Caflisch

Courant Institute of Mathematical Sciences

The Fluid Dynamic Limit of a Model Boltzmann Equation

February 1, 1979

T. Mahar

The Technological Institute, Northwestern University

Oscillations in Systems of Nonlinear Difference Equations

March 1, 1979

Michael Overton

Stanford University

The Projected Lagrangian Algorithms for Solving the Nonlinear Minimax Problems

March 6, 1979

Walter Gautschi

Purdue University

Constructive Aspects of Gaussian and Related Quadrature Rules

March 8, 1979

Sudarshan K. Loyalka

University of Missouri

Kinetic Theory of Cross-Effects in Rarefied Gases

March 15, 1979

Thomas Coleman

University of Waterloo

An Exact Penalty Function Approach to the Nonlinear Programming Problem

March 22, 1979

Bernd Kiekebusch-Muller

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