Report of the Panel on Future Directions in Computational Mathematics, Algorithms, and Scientific Software

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Werner C. Rheinboldt, Chairman

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CONTENTS

EXECUTIVE SUMMARY

The use of modern computers in scientific and engineering research and development over the last three decades has led to the inescapable conclusion that a third branch of scientific methodology has been created. It is now widely acknowledged that, along with the traditional experimental and theoretical methodologies, advanced work in all areas of science and technology has come to rely critically on the computational approach. Accordingly, for the advancement of the scientific and technological base of our nation, it is essential to maintain the U.S. leadership advantage in scientific computing.

In recent years, increasing concern has been voiced by various scientific and engineering groups and organizations about he competitive posture of the U.S. scientific computing enterprise. In particular, the Panel on Large Scale Computing in Science and Engineering [1], chaired by Professor P. Lax, identified the critical needs for supercomputers in science and engineering and recommended increased support for all related aspects of large-scale computing. During the past year several funding agencies have responded to some of the recommendations of this report and of the subsequent National Science Foundation (NSF) study [2]. These responses include the Fast Algorithm initiative of the Air Force Office of Scientific Research, the establishment of the Scientific Computing Program in the Office of the Director of Energy Research at the Department of Energy, and the formation of the NSF Office of Advanced Scientific Computing.

Both of the above mentioned reports noted the need for increased support of computational modelling and mathematics. In a detailed report, entitled "Computational Modelling and Mathematics Applied to the Physical Sciences" [3], the National Research Council (NRC) Committee on Applications of Mathematics forcefully detailed the integral and critical role of computational mathematics in the overall computational process.

The NRC report illustrated and explained the interdependence of the various stages of the computational modeling process. The committee observed that, at its best, computational mathematics involves the design and analysis of mathematical models and algorithms which are fully integrated with considerations about their implementation as scientific software in computational models. This is particularly important in the large scale scientific computing environment where new computer architectures are now being introduced. The NRC committee further recommended increased support for the entire computational mathematics enterprise.

In the fall of 1984 the Panel on Future Directions in Computational Mathematics, Algorithms, and Software was formed to review perceived needs and to identify possible courses of future action. The panel's deliberations were guided by the following realizations:

> Computational mathematics is a high-leverage element of our nation's scientific and technological effort. Its importance in scientific computing is increasing with the growing range and complexity of problems that have to be solved and with the demands of new generations of computers and new computer architectures.
>
> Modern research in computational mathematics increasingly depends on a multidisciplinary approach transcending the usual academic disciplines. Effective multidisciplinary teams typically consist of several scientists, engineers, and technicians who together cover the relevant scientific and engineering disciplines, applied mathematics, numerical analysis, statistics, probability theory, computer science and software engineering. Today, such research and engineering teams are found in the most advanced national and industrial laboratories, but are rarely located in universities.
>
> Although the field has developed vigorously during the past decades, there are serious reasons for concern about the future. There are presently substantial shortages of personnel on all levels and the existing educational opportunities are not producing the required personnel. At the same time, low funding levels and lack of stability in the support for facilities are hindering the research effort at academic institutions.

In order to overcome these problems and to provide for the needed strengthening of computational mathematics research in this country, the panel strongly recommends the following:

1. The appropriate federal agencies should strengthen their support for research in computational mathematics, methods, algorithms, and software for scientific computing.

2. The agencies should support the development of interdisciplinary research teams in computational mathematics and scientific computing.

3. Such support should permit the establishment and continued operation of a suitable research infrastructure for the teams, including computer hardware and software and the associated support personnel. Moreover, the support should be of sufficient duration to insure continuity and stability of the research effort in the academic environment.

4. The agencies should increase the support for graduate students and post-doctorals directly involved in the research of some interdisciplinary team in computational mathematics and scientific computing.

5. The agencies should increase the support for young researchers and cross-disciplinary visitors who can contribute to the research work of one of the interdisciplinary teams.

1. OVERVIEW

Scientific computation has become a vital component and even a basic mode for research and development in science and engineering. The impact of computers upon science and technology has already been extremely profound. A principal reason for this certainly is attributable to the fact that the computer has increased and will increase enormously the range of solvable problems. The rapid progress which we see today is a strong sign that this impact of computers may be expected to continue for some time to come.

A decade ago this nation was pre-eminent in all aspects of electronics, computers, and computational technology. This leadership position is being challenged from various sides. Some expressions of serious concern have already been presented in several reports. In particular, the report of the Lax panel [1] (see Appendix A) observed that "U.S. leadership in super-computing is crucial for the advancement of science and technology, and therefore, for economic and national security", but that "under current conditions there is little likelihood that the U.S. will lead in the development and application of this new generation of machines".

Computational mathematics plays a central and perhaps critical role in this connection. The computational solution of today's highly complex problems of engineering and science involves questions ranging from the design of suitable computer architectures and the study of algorithms to the modeling of physical, chemical, biological, and engineering processes by means of mathematical equations. These issues are tied together by mathematical theory, which seeks a full understanding of the nonlinear phenomena contained in the models, and by numerical mathematics which conceives, analyses, and tests the required computational methods. In a complementary and equally essential role, mathematics is the science of algebraic and logical manipulation which, in turn, represents the basis of such widely differing operations as the control of complex decisions through artificial intelligence, the design and encoding of large data sets, or the exact solution of scientific problems of an algebraic nature. The span of this wide range of activities forms the subject that has become known as computational mathematics.

Today's computer technology is dominated, on the one hand, by the introduction of micro-computers and their widespread acceptance, and, on the other hand, by the development of supercomputers with architectures that represent a major departure from traditional sequential machines. These supercomputers and other machines advancing the state of the art (e.g. in graphics or symbol manipulation), rather than the micros, are essential in areas of frontier science. In fact, it has been frequently observed that the most challenging problems always require more resources than can be provided by the fastest available computer. The reasons that these problems are under-computed is that each advance in computing-power or algorithm design opens up new possibilities for further research. Just as the increased resolution of the optical and electron microscope resulted in the discovery of whole new realms of science, so successive generations of computing hardware and software have led and will lead to fundamental advances in science and technology.

Here, more than ever, computational mathematics is of crucial importance. The effective utilization of supercomputers and, in particular, of the planned highly parallel architectures, is far from being understood. There is a critical need for developing new -- and re-examining old -- algorithms which will take full advantage of all the power of these computers. New advances in numerical mathematics, algorithm design, and computer languages, will be essential for learning to exploit the new facilities. It is expected that new research contributions of the community of computational mathematicians and computer scientists to these fundamental issues will be at least as important in the development of new generations of machines as the new hardware developments themselves.

These observations certainly support the conclusion that computational mathematics is a high-leverage element of our nation's scientific and technological effort. The field has developed vigorously during the past few decades. But the current vitality and level of achievement notwithstanding, there are reasons to be concerned about the future. There exists at present a considerable shortage of personnel on all levels in the area of computational mathematics. Moreover, the educational opportunities in the field are limited and do not produce the required people, especially the much needed young researchers. At the same time, the computational mathematics research effort in academic institutions is seriously hindered by low funding levels, lack of stability in the support for facilities and support personnel, and limited access to up-to-date computer equipment. These problems have already been noted by several previous reports. For instance, the NRC report [3] recommended the following:

1. Increased research support for computational modeling and applied mathematics.

2. Increased support for computing facilities dedicated to computational modeling and applied mathematics.

3. Increased support for education and manpower development in computational and applied mathematics.

In part, some of these problems reflect those of the mathematics community as a whole. In fact, as the David report [4] documents, "(s)ince the late 1960s, support for mathematical sciences research in the United States has declined substantially in constant dollars, and has come to be markedly out of balance with support for related scientific and technological efforts". Moreover, "(o)ver the historical period 1968-82 .. the annual number of U.S. citizens obtaining doctorates in the mathematical sciences from U.S. institutions has been cut in half, from over 1,000 to fewer than 500". "Overall demand for Ph.D.'s exceeds supply".

Computational mathematics has fared somewhat better with respect to federal research support than mathematics as a whole. But nevertheless this support lagged far behind the growth of the field. Moreover, with respect to manpower resources, the field clearly is in worse shape than most other parts of mathematics. The David report observes in this connection: "Particularly worrisome are the scarcity of senior personnel in this area and the extremely small number of young researchers and graduate students". "A major effort in this area is needed to attract, educate, and support graduate students, postdoctorals, and young researchers, and to provide the computational equipment essential for the proper conduct of this research". "Significant additional resources for the mathematics of computation may be needed in the years ahead".

In order to meet the immediate need for making supercomputers available to academic scientists and engineers, the National Science Foundation in April 1984 announced the formation of the Office of Advanced Scientific Computing. The office was formed to: (1) increase the access to advanced computing resources for the scientific and engineering research community, (2) promote cooperation and sharing of computational resources among all members of the community, and (3) develop an integrated research community with respect to computing resources. This is certainly a most important step toward overcoming some of the critical problems in scientific computing in the country.

But, in line with our earlier observations, any such program of expanded access to supercomputers can only be a first step. Its benefits to the country will remain severely limited unless there is the vigorous, accompanying program of academic research and education on computational mathematics, software, and algorithms necessary for the effective and efficient use of such large computer systems.

The panel does not find it sufficient to consider simply an increase in the funding level for support of the work of individual researchers in computational mathematics. The solution of today's computing research problems in science and technology requires an interdisciplinary approach involving contributions from various areas of science, engineering, applied and numerical mathematics, statistics, and computer science. Moreover, such work cannot proceed without appropriate computer hardware and software facilities and the associated support personnel. Indeed it will not be very effective unless there is a certain continuity and stability in this infra-structure which supports the research.

This calls for an increased emphasis on the support of teams which have a common intellectual focus but are sufficiently interdisciplinary to span a significant portion of the broad range from an application area through applied and numerical mathematics to scientific software and computer science. In order to assure the required stability and continuity of the research effort, such support has to have reasonably long duration. It also should include funds for the initial acquisition of the necessary hardware and software and for the subsequent operation and maintenance of these facilities. In this connection it is also important to foster more cooperation and coordination between researchers who often work on the same or similar problems. There is a great need for an extensive electronic network linking groups in mathematics, computer science, and related areas. Such a network would lead to greater standardization of software and less duplication of effort.

The proposed emphasis on group efforts does have the added benefit of optimal utilization of the limited number of active researchers in computational mathematics. Moreover, such groups provide an excellent training ground for graduate students and post-doctoral fellows. This would help in alleviating some of the manpower problems, although it would not remove the need for a more concerted program of strengthening the educational programs in the mathematical sciences in general and in computational mathematics in particular. A broad plan for educational support in mathematics has been presented in the David-report. In computational mathematics there appears to be some added urgency for increasing the level of support of graduate students and post-doctorals, and to study effective modes of undergraduate education which capture the experimental and laboratory components of the field.

On the basis of its findings the panel strongly recommends the following actions:

1. The appropriate federal agencies should strengthen their support for research in computational, methods, algorithms, and software for scientific computing.

2. The agencies should support the development of interdisciplinary research teams in computational mathematics and scientific computing.

3. Such support should permit the establishment and continued operation of a suitable research infrastructure for the teams, including computer hardware and software and the associated support personnel. Moreover, the support should be of sufficient duration to ensure continuity and stability of the research effort in the academic environment.

4. The agencies should increase the support for graduate students and post-doctorals directly involved in the research of some interdisciplinary team in computational mathematics and scientific computing.

4. The agencies should increase the support for young researchers and cross-disciplinary visitors who can contribute to the research work of one of the interdisciplinary teams.

2. RESEARCH OPPORTUNITIES

2.1 INTRODUCTION: In this section we discuss several research areas and directions in computational mathematics and examine how results in this field have a high leverage effect on broad areas of science and technology. The examples chosen are illustrative only and are not intended to be complete. Moreover, all the reports listed in Appendix A present such examples and there is certainly no need for duplication. Instead we endeavored to stress topics that were not covered very extensively in the cited reports.

In the last two decades many developments in numerical analysis have had a large impact on scientific computations. As examples we mention here only the fast Fourier transform, the evolution of the finite element methods, variable step/order ordinary differential equation solvers, adaptive mesh-refinements, spline approximations, spectral methods, fast matrix algorithms including, for instance, multigrid techniques, and effective optimization methods. But there are a host of problems waiting to be understood. Perhaps the greatest opportunity provided by the modern computational approach is that it has opened the wide realm of strongly nonlinear phenomena to systematic, relatively accurate, and efficient modeling, improving the chance that important phenomena can be isolated and analyzed. This represents one of the great challenges to numerical analysis today.

2.2 NONLINEAR ELLIPTIC EQUATIONS: The solution of coupled systems of nonlinear elliptic partial differential equations is important in many applications. These systems arise in steady state problems and as steady state subsystems or implicit solution steps within a dynamical problem. Many efficient discretization and solution methods have been developed over the past thirty years by computational mathematicians.

The solution of coupled nonlinear partial differential equations plays an especially important role in semiconductor simulation. It is now possible to analyze many different designs without building a prototype. The numerical problems encountered here, however, require computing equipment of the most modern type. Undoubtedly, more powerful computers will stimulate the use of more complex models, especially for three-dimensional problems.

The selection of suitable discretization procedures is influenced by various considerations. These include the goals of the analysis of the physical problem, known mathematical properties of that problem and of the solution algorithm, hardware considerations, such as parallelity, data management requirements and other computer science considerations, and, last but not least, restrictions on computation time and expense. For any choice of discretization there are questions about the accuracy and stability of the method, the efficient solvability of the resulting equations, the robustness of the method with respect to the input data, and, for nonlinear problems, the separation of legitimate approximate solutions from spurious approximate solutions, which do not correspond to any exact solution. Much important work on the various discretization methods remains to be done, especially when it comes to adaptive forms of these methods.

2.3 LINEAR AND NON-LINEAR EQUATIONS: The mentioned discretizations typically give rise to systems of linear equations. In particular, large sparse systems with tens or hundreds of thousands equations are relatively common, and the iterative solution of nonlinear problems usually involves such a linear system at each step. Much research has gone into the development of efficient methods for the solution of systems of linear equations. This includes direct solution techniques, such as the various forms of matrix decompositions, banded and frontal elimination techniques, nested dissection, and different approaches to sparse elimination, such as the minimal degree algorithm, etc. We also refer to iterative processes, such as the sucesive overrelaxation method, the alternating direction method, the conjugate gradient method, as well as the hybrid methods such as block and multi-grid methods. The study of efficient algorithms for solving large systems of linear equations remains a very active field of research. In particular, interest centers on fast methods for non-symmetric systems, the development of methods for computers with different architectures, especially parallel machines, and the development of methods which are effective for problems involving singularities. Moreover, partitioning of large problems has just begun to be studied and represents an area of considerable challenge.

There are various classes of solution algorithms which are of similar importance. These include, for example, methods for solving linear eigenvalue problems, and optimization methods for linear and nonlinear problems. For instance, large scale linear least squares problems come from a variety of sources. A particularly challenging set of such problems arises in geodetic computations. Here the data often are obtained from remote sensing devices and very large data sets are acquired. Fortunately, the nature of these problems leads to matrices which are highly structured and for which some of the modern iterative techniques are applicable. Other classes of such problems cannot be handled even with the most modern computing devices and in these cases new algorithms are required which take account of the fine structure of the matrices.

The optimal power flow (OPF) problem is an example of an important application whose solution has become practical only because of improved optimization methods. Broadly speaking, the goal is to optimize the distribution of electrical power over a network; the constraints are non-linear, and the number of variables in any realistic case is very large. The OPF problem occurs in many areas of power engineering and power engineers have been working on it for at least 20 years. The methods used in the 1960's -- when the computer solution of the OPF problem was first attempted -- were slow and unreliable. Because of inadequacies in the methods, it was widely considered that large OPF problems were essentially impossible to solve. For example, the objective function was believed to be almost "flat", with many local optima, simply because older methods usually failed to make any significant progress after the first few iterations. Within the last two years, however, sequential quadratic programming methods have been applied with great success to general OPF problems of a size previously considered intractable. In fact, very large OPF problems can now be solved routinely. This breakthrough received considerable attention in the power industry after the results were reported at a national power engineering conference in February 1984.

Despite such success stories, improved computational power is still necessary if certain problems are to be solved effectively. For example, stochastic linear programs have been the subject of intense study since World War II. The "natural" approach to such problems would be to explore the largest possible number of alternatives at each step of the solution process. However, the inherent complexity of this approach has meant that less satisfactory methods based on averaging had to be used instead. With the advent of new computer architectures involving substantial parallelism, it appears to be likely that, for the first time, stochastic problems can be treated in their "natural" most desirable way.

In the case of nonlinear equilibrium problems we usually encounter a number of parameters. Then the solution set forms a manifold in the combined state and parameter space, and for a deeper understanding of the system it is necessary to analyze the shape of this manifold. Here continuation methods are to be used. Moreover, questions about the stability of the solutions typically involve the determination of the location and character of the singular points of this solution set. Another important but as yet incompletely explored question concerns the comparison of the solution manifold of the original equations with the manifold defined by a discretized form of these equations.

The study of singular points on the mentioned solution manifolds constitutes an aspect of bifurcation theory -- the static case. The dynamic case is of equal importance in modern computational mathematics. In fact, it has been remarked that one of the most engaging problems in nonlinear dynamics is that of understanding how simple deterministic equations can yield apparently random solutions. Both static and dynamic bifurcation problems involve challenging mathematical and computational questions and represent active areas of research.

2.4 NONLINEAR HYPERBOLIC EQUATIONS: Nonlinear hyperbolic equations are equally important for a number of applications including, for instance, high speed gas dynamics. These problems are often characterized by the simultaneous presence in their solution of significantly different time and length scales. The solutions to these models will have regions of strongly localized behavior, such as shocks, steep fronts, or other near discontinuities. In recent years, a series of improved methods for these problems have been introduced by computational mathematicians, culminating in currently very refined agreement between computation and experiment for complex shock wave diffraction patterns. We refer here to upwind methods, flux limiters, higher order Godunov methods and methods based on solutions of Riemann problems. Areas of research important in coming years include the extension of such highly accurate solution techniques to more difficult problems, including those arising in reactive chemistry and combustion, and especially also to problems in three space dimensions.

2.5 ADAPTIVE MESH METHODS: In these problems, as well as in the earlier mentioned elliptic boundary value problems, adaptive mesh construction has come to be of critical importance. Such techniques allow extra computational effort to be concentrated in regions where the solutions are singular or nearly so. The design of efficient adaptive mesh refinement methods is an active research area. An important related research topic is the development and application of a posteriori error estimates. Such estimates can be used to assess the errors of the computed results and to form the basis of adaptive procedures. The requirement of designing error estimators with appropriate properties for realistic classes of problems, different solution methods, and suitable error norms certainly represents a demanding research task in computational mathematics.

Often local mesh refinement leads to nested levels of meshes which can be solved effectively on parallel computers as independent tasks. This makes this topic also very important for use in connection with modern computer architectures. For situations in which the localized behavior is known to be approximated well by very sharp fronts (e.g. shocks or flames), front tracking methods often have significant advantages. Such methods, as well as related vortex methods, insert analytic information concerning solution singularities into the numerical algorithm.

2.6 ILL-POSED PROBLEMS: The notion of a well-posed problem is due to Hadamard: a solution must exist, be unique, and depend continuously on the data. The term "data" can have a variety of meanings; in a differential equation it may include, for instance, the boundary or initial values, the forcing terms, or even the coefficients of the equation. Since data cannot be known or measured with arbitrary precision, it was thought for a long time that real physical phenomena had to be modeled by mathematically well-posed problems. This attitude has changed considerably in recent years, and it is now recognized that many important applied problems require the solution of less well-posed problems.

One important class of such applications falls, loosely speaking, under the heading of tomography. In a narrow sense, tomography is the problem of reconstructing the interior of an object by passing radiation through it and recording the resulting intensity over a range of directions. Tomography has also come to include applications where the source of radiation is inside the object or when radiation is reflected by features inside the object.

Probably the most widely known applications of tomography are in medicine. Computer assisted tomography (CAT scan) uses x-rays directed from a range of directions to recosntruct the density function in a thin slice of the body. Recent advances in medical tomography include nuclear magnetic resonance (NMR), where strong magnetic fields are used to make the hydrogen atoms resonate. By varying the fields and their direction the plane integrals of the density of hydrogen can be measured and an "approximate" two or three dimensional hydrogen density can be reconstructed. One advantage over the CAT scan is that the use of potentially harmful x-rays can be avoided.

Another important source of applications of tomography is non-destructive evaluation (NDE). There is considerable need in industry to evaluate the integrity and remaining reliable lifetime of components and structures, as, for example, nuclear reactor vessels, bridge girders, or turbine disks. Once again the component is subjected to penetrating radiation with the aim of deducing information about its internal state. Types of radiation used include ultrasound, x-rays, and neutrons. In other applications, electrical currents are induced in the material which produce fields that may allow the determination of existing cracks.

The search for oil depends heavily upon the analysis of seismic data. This is another example of the reconstruction of internal features of a body from monitored reflections of radiation or energy flows. Another example occurs in the study of confined plasmas in reverse-pinch machines that are being studied as a possible source of fusion energy. Radiation is reflected off the plasma in an attempt to determine the cross-sectional density function. In this example only a handful of data are available. In an even more compelling example, a suggested method of on-site monitoring of a limited test ban treaty depends upon the ability to resolve a problem of this type.

The idealized mathematical problem underlying all these problems is the reconstruction of a function f(x,y) of two variables from its integral along lines. This is an interesting example of a mathematical problem that was considered and solved long before its applicability was seen. In fact, this problem, as well as its three-dimensional version, was solved by J. Radon in 1917 and later rediscovered in various settings such as probability theory (recovering a probability distribution from its marginal distributions) and astronomy (determining the velocity distribution of stars from the distribution of radial velocities in various directions). Of course, much work was needed to adapt the Radon inversion formula to the incomplete information available in practice. The computational solution of ill-posed problems of the form arising in the general area of tomography is a very active research topic in computational mathematics. Recent years have brought much progress in this field, but much work remains to be done. Because of the overwhelming importance of the applications that lead to these problems, this area of research may be expected to yield many important dividends.

2.7 COMPUTATIONAL STATISTICS: As in mathematical physics and engineering, methodological breakthroughs in statistics tend to be a combination of many factors. For example, the major breakthrough in numerical spectrum analysis in the 1960's involved the theory of stationary stochastic processes, the fast Fourier transform, statistical sampling theory, and, behind all that, driving examples from geophysics. Statistical research is now poised for some major methodological advances through access to improved computing resources of various types.

An increase in computing power makes it feasible to approach problems that are intractable in closed form. This includes, for example, the establishment of properties of statistical procedures through Monte Carlo simulations (as, for instance, in Efron's bootstrap methods), and the solution of problems in Bayesian statistics through the direct computation of multi-dimensional integrals. On a more basic level, it now becomes possible to attack concrete statistical tasks through direct numerical optimization. We note here that a majority of statistical problems are naturally formulated in terms of optimality principles (such as the classical maximum likelihood estimates, optimal designs, robust alternatives to least squares, projection pursuit methods, etc.), but that they rarely have closed form, or even easily calculable solutions. Often, the function to be optimized is not available in closed form and must be found by integration and Monte Carlo simulation, or the optimization itself occurs inside a simulation loop. Frequently, not only the location of the optimum is needed, but also contour surfaces around the optimum (for confidence regions); this certainly compounds the computational problems. The research challenge here is to develop the methodology in a safe and efficient manner.

Large data sets represent a central problem for computational statistics. Here the computational work is typically storage bound rather than processor bound. The long range research challenge is to identify basic building blocks (both in hardware and software) that are suitable for massively parallel data base operations, and to build tools for analyzing large, highly structured, inhomogeneous data sets. Research opportunities in this area are wide open; in fact, none of the currently available data base management systems is designed to deal with the specific requirements of scientific/statistical data.

Statistical data analysis requires software and hardware suitable for interactive, often graphical, improvisation. The computing requirements here are similar to those in artificial intelligence work and include an integrated programming environment with instant, high resolution, easily improvisable, real-time graphics, and a mixture of symbolic and numerical manipulation capabilities. These requirements are beginning to be met by the single-user super-workstations now reaching the market (with a raw power exceeding that of a VAX-11/780). There are major challenges for the computational statistician; we need to develop better interactive languages for statistical data analysis, and we must design and implement effective methods that provide the required intelligent machine assistance to the analyst.

2.8 STOCHASTICS AND COMPUTATIONAL PROBABILITY: Stochastic processes and the need for probabilistic reasoning arise in the solution of numerous problems. These range from queuing and inventory studies to the fault tree analysis of safety design factors, and from economic and financial studies to the analysis of voting behavior. Modern applications of probability theory involve problems of very high dimension which present massive computational problems. The analysis of the related probabilistic models has called for new methodological approaches. Among recent advances are the product-form solution used in the analysis of networks of interacting queues, and the matrix-analytic methods of structured Markov chains. The product-form solution has stimulated extensive research on stochastic networks and is widely used in the design of interconnected computer systems. Structured Markov chains arise commonly in telecommunication engineering in the design of buffers and in the study of operating protocols. The computation of various measures of performance leads to the numerical solution of various types of nonlinear matrix-integrals and matrix-equations.

As noted earlier, most probability models lead to very high dimensional computational problems. Often already very simple descriptions require the study of a higher-dimensional stochastic process. For example, a typical econometric model of a country or group of countries may be characterized as a stochastic nonlinear system of hundreds or thousands of equations. They often involve some non-concavity in the system, and hence, already the computatational problems in analyzing the dynamic properties of the system are formidable. Moreover, the process of search for approximate optimal control strategies for policy authorities, especially when more than one active authority is involved, introduces game theoretical aspects. The resulting system will tax most of the available computing resources. As this example already indicates, progress in this area requires not only statistical methods of a nonclassical type, but also new approaches in nonlinear numerical analysis, and new techniques for data handling and computer graphics.

2.9 PATTERN RECOGNITION AND SYMBOLIC COMPUTATIONS: The area of pattern recognition, including image processing, acoustical processing and speech recognition, requires integrated mathematical techniques from several areas including signal processing, mathematical logic and linguistics, numerical mathematics, Fourier transforms, and algebra. The objective is a classification of sequences of images as they might arise in such widely differing applications as text reading or submarine detection. In the case of image reconstructions, random disturbances may blur or obliterate a transmitted image. One recently proposed method for the mathematical reconstruction of such images involves the use of stochastic dynamics based on Ising models. A dynamical evolution to an image with a lower Ising model energy filters out much of the noise while leaving the original image unchanged.

Numerical and non-numerical computing are often regarded as two different areas which use their own software, interfaces, and algorithms even when sharing the same hardware environments. An important form of non-numerical computation involves the use of symbolic manipulation systems for carrying out algebraic operations on a computer. These systems perform indefinite integration, factor polynomials, simplify complex expressions, and operate on matrices. They have been applied very successfully in several situations, for instance in the computation of orbits of space objects, and in the calculation of Feynman integrals in physics. In each of these cases the required algebraic computations were so extensive that only computers could perform them sufficiently rapidly and accurately. The development of computer algebra systems required the invention of numerous new algorithms and the adaptation of various old ones. Some of the most notable ones are those for indefinite integration and polynomial factorization. Further work is needed on algorithms that are more efficient than presently known ones and on algorithms than can deal with new classes of problems. There is also need for new computer-algebra systems that are more portable than present ones, run on smaller machines, and can be interfaced more easily with other programs. Moreover, there is a strong need for studying more closely the coupling of automatic reasoning algorithms with mathematical modeling and data base techniques to produce effective control processes for complex systems and for effective modeling of complex systems involving human and mechanical components.

2.10 COMPUTATIONAL METHODS IN PURE MATHEMATICS: Some of the most interesting applications of symbolic mathematics are in mathematics itself. Areas of both pure and applied mathematics, including coding theory, cryptography, probability theory, analysis, combinatorics, and number theory, have all gained from the availability of symbolic manipulation tools. These tools have been used to prove a number of results directly. Their main application, however, has been to obtain insight into behavior of various mathematical objects, which then led to conventional proofs. This rather new, direct impact of computation upon pure mathematics is not limited to symbolic manipulation and will no doubt expand considerably in coming years. In doing so it may lead to the development of computational tools, methods, and concepts of broad applicability. For instance, the four color problem was reduced to a check of a very large but finite number of specific cases. This final step, too tedious for humans, was performed on a computer. Computers have been used in exploratory studies of the iterates of mappings which in turn led to new insight into the nature of chaos and turbulence. They also played a role in the classification of all finite simple groups. Finite groups certainly play a very important role in the study of many topics in applied mathematics and science, such as discrete computational structures, enumeration of combinatorial designs, the definition of stereo-isomers in organic chemistry, the cataloguing of crystallographic structures, etc.

The recent invention by Lovasz of a fast algorithm for finding good bases for lattices has had a striking impact on several fields. The problem of finding the shortest nonzero vector in a high-dimensional lattice is considered to be very hard, but has been of great interest because many other problems in diverse areas can be reduced to it. The Lovasz algorithm does not in general find the shortest nonzero vector, but it does rapidly find a relatively short one, and in many situations that is sufficient. The algorithms has been applied, for example, to the determination of integer solutions of linear programs and to the factorization of polynomials. But perhaps its most important application is to cryptography. Among public key secrecy ssystems (that is, those that do not require the two communicating users to exchange secret keys beforehand) there was a large class for which the presumed security relied on the difficulty of solving the knapsack problem. Essentially all of these knapsack-based secrecy systems have been shown to be breakable by application of the lattice-basis reduction algorithm. As a result the only public key cryptosystems that still appear credible are those for which security depends on the difficulty of factoring large integers or computing logarithms in finite fields.

2.11 QUALITY SOFTWARE: Quality software is an indispensible tool in many modern science and engineering projects. The continuing developments in micro-electronics will decrease the cost of computing and increase the speed and memory available. But these hardware improvements will allow present codes to be pushed only a limited amount beyond their current capabilities. Additional capabilities must come from better mathematical models and more efficient numerical methods. Because computer architectures will certainly change, there is a need to re-examine traditional methods and to develop new methods that use the inherent structure of the new machines. But, at the same time, it will be important to avoid locking the software into a particular architecture. Software flexibility, modularity, reliability, efficiency, restricted data flow and documentation are here fundamental requirements. There is certainly a need for the development of high quality mathematical libraries to support large-scale scientific computing. This will require close cooperative work between applications programmers, numerical analysts, and the scientific computing research community.

2.12 PARALLEL COMPUTING: Despite the fact that electronic components are becoming faster, the limits of raw machine speed are now clearly visible. Further gains will eventually have to be made by the use of novel architectures and algorithms, and, in particular, by some form of parallelism. Many of the new designs now under consideration represent a sharp break from previous computer architectures and introduce issues of scheduling, coordination, and communication which previously did not arise. Thus it will be necessary to rethink and reconstruct the vast number of familiar numerical methods from the point of view of these new issues. It appears that in many cases software, not hardware, will pose the most difficult problems and will account for the most impressive advances.

As an illustration we discuss here some issues relating to parallel computing. Recent progress toward solving large problems, such as full body air flow simulations, has concentrated on the use of local mesh refinements and adaptive methods. Data structure design is evolving toward the production use of networks of overlapping grids some of which are coarse and stationary while others are fine grids which may be moving to track a front. For the solution of elliptic problems the algorithms that show the greatest promise are multilevel methods such as hybrids of multigrid methods and methods that are well suited to substructured grids, such as the conjugate gradient method. From the point of view of software design there are two important features of these techniques. First, the algorithm and data structure are dynamic. Second, while the global grid structure is very non-uniform, the local structure is based on deformations of uniform grids. These two facts have a large impact on the problems of programming the next generation of computers. In particular, we face three fundamental research problems:

(1) Numerical algorithms: We must understand the dynamic structure and formulate the mathematical model in terms of high level parallel operations. For example, the computation may be viewed and expressed as a system of higher order tasks which encapsulate the large scale dynamic/adaptive structure of the algorithm. Each higher order operator can be composed of lower order parallel operations on uniform fine structures such as subgrids of a large network. The point is that no matter how the algorithm is formulated, we will need to employ much more parallelism than we currently do in order to utilize the power of a massively parallel machine.

(2) Algorithm analysis: A more accurate model of parallel algorithms is needed to describe the expected performance of the new software. In particular, parallel algorithm analysis must capture the cost of communication, process synchronization, and initiation. An ideal model would be machine independent but have parameters that are easily set to a specific architecture. Such a model also could be of great value in the design of new architectures.

(3) The mapping problem: Given a parallel architecture and a parallel specification of an algorithm, find an optimal mapping from one to the other. This problem takes on special significance in the case of massively parallel non-shared memory systems. In this case, the machine can be viewed as a graph where processors are nodes and the communication network describes the edges between the nodes. The algoithm is a graph of communicating processes (or data flow graph) which, in the case of adaptive methods, has a dynamic structure.

Clearly, as this brief sketch already shows, research in this important area of computational mathematics will require well integrated team efforts between algorithm designers, numerical analysts, and researchers in the applications areas.

3. NEW MODES OF RESEARCH

Traditionally, individual researchers working alone or in pairs have characterized the style of much of the work in the mathematical sciences. This situation is different in computational mathematics where increasingly a multidisciplinary team approach is required. There are several compelling reasons for this.

First and foremost, as noted already several times in the previous section, problems in modern scientific computing transcend the boundaries of a single discipline. In general, the computational approach has made science more interdisciplinary than ever before. There is a unity among the various steps of the overall modeling process from the formulation of a scientific or engineering problem to the construction of appropriate mathematical models, the design of suitable numerical methods, their computational implementation, and, last but not least, the validation and interpretation of the computed results. For most of today's complex scientific or technological computing problems a team approach is required involving scientists, engineers, applied and numerical mathematicians, statisticians, and computer scientists.

Unlike theoretical mathematics, computational mathematics, by its very own nature, has a strong experimental component. As a result, research work proceeds in part in a laboratory mode similar to that in the experimental sciences. The laboratory equipment required for modern scientific computing ranges from local workstations, micro- and mini-computers, to mainframe machines of various sizes and super-computers. This hardware is complemented by appropriate software systems and libraries. Moreover, the multidisciplinary nature of the work requires a new level of interchange between researchers in widely different fields. For this the communications capabilities of modern computer networks form an ideal mechanism to link scientists from widely differing fields and to allow them to share ideas and information. As in the traditional laboratory sciences, support personnel is required to ensure efficient usage of all facilities and to avoid any unnecessary waste of research time. Under current funding practices projects involving support staff are certainly not very common in mathematics.

Clearly, the investment costs, as well as the longer duration of typical computational projects -- especially when extensive software development is involved -- necessitate a certain continuity and stability of the entire research infra-structure and hence calls for a sharing of the facilities among several researchers. Once again research teams are best suited to sustain such an operation.

As has been noted before, computational mathematics currently faces a critical manpower problem. Any national effort to strengthen the field has to take special account of this fact and has to include steps toward making optimal use of existing manpower resources. In the opinion of the panel, the most advantageous approach will be to ensure the establishment of a sufficient number of viable research teams in computational mathematics. Such groups are not only most appropriate for research in the field, but they ensure that the most effective use is made of the scarce talents of established researchers, and they provide a means of bringing additional young researchers as quickly as possible into the mainstream of the work.

Generally, the emphasis should be on a concentration of effort. In other words, teams should have a common intellectual focus yet be interdisciplinary, spanning a significant portion -- and ideally all -- of the broad range from an application area through applied mathematics and numerical analysis to mathematical software and computer science. This concentration of effort on a common research interest will allow the group to take a problem all the way from the application to working software. This commonality and range of research interest is considerably more important than a particular administrative structure, such as a center or institute. Of course, for vitality of such an organizational unit it may be desirable to ensure a certain stability in a particular academic setting, but it should not be the sole driving force.

In order to be viable, it appears that a group should consist of at least three faculty level researchers, one post-doctoral fellow, five to eight Ph.D. level graduate students and one full-time support person. In most cases it will be highly desirable to include additional junior faculty level researchers in such teams. The support person would do both systems and applications programming for the group, and generally ensure smooth operation of the local computing facilities. While some groups might survive without such a person, they would do so only at the expense of researchers performing these tasks which is a waste of valuable and scarce talent.

As noted before, each group will require some local computing facilities, but access to supercomputers can be provided by suitable high-speed networks. The quality of the computing facilities has a decisive effect on the overall research effort. It is highly desirable that the group has at least high-performance personal workstations, to support the research work of the individual members, to provide for efficient access to appropriate large computing facilities, and to allow for very-high bandwidth communication, such as needed in graphical post-processing. If the group has to operate more substantial computing facilities, then there should be at least two support people. But in all this, it is important to note that the requirements described here are minimal rather than average. Some further discussion of possible laboratory facilities is presented in Appendix B below.

In order to assure the required stability and continuity of the research effort, funding should be provided on a multi-year basis, say, on the order of five years. Moreover, it is necessary to support both the initial purchase and the subsequent annual maintenance of the hardware and software. The overall funding for such a group need not be in the form of one large institutional grant, but may well be in the form of several grants and contracts from from different funding sources. In some cases, it may also be appropriate to establish cooperation with industrial research groups and to secure some support from non-governmental sources.

This multidisciplinary team work in a laboratory setting represents a significant departure from the traditional style of research in mathematics. It is also a departure from the standard funding mode of the federal agencies supporting computational mathematics. It will take special efforts on the part of these agencies and the mathematical community to accept the changing situation and to help in the development of this new mode of research in computational mathematics. In line with this, it is of considerable importance that the proposed new funding effort for the establishment of such research teams is meant to complement rather than replace the traditional project support for individual researchers in the field. The proposed team approach is intended to focus on different categories of scientific computing than are feasible for individual researchers and to strengthen the productivity and effectiveness of the researchers involved in such interdisciplinary projects.

4. EDUCATIONAL NEEDS

The Lax report [1] (see Appendix A) recommended a long-term National Program on Large-Scale Computing which included as one of its goals the "(t)raining of personnel in scientific and engineering computing", and in [3] this was re-iterated in the form of a recommendation for "(i)ncreased support for education and manpower development in computational and applied mathematics".

Basically, the educational needs addressed here are part of a much broader problem concerning all of mathematical education in the country. Throughout the past two years several pieces of legislation were introduced in the Congress in response to the report of the National Commission on Excellence in Education entitled "A Nation at Risk". Then, in August 1984 the President signed into law the "Emergency Mathematics and Science Education and Jobs Act".

The David report [4] addressed some of the educational problems in mathematics on the post-secondary level. Its fundamental observation was that "(t)he field is not renewing itself".

There is little question that there are formidable problems with our undergraduate and graduate educational programs in all areas of mathematics; that is, in pure mathematics, computational and applied mathematics, statistics, operations research, etc. The quickly broadening need for computational modeling in all areas of science, engineering, and business has produced an increasing demand for more college-level mathematical education. This is evident by the 33% increase of enrollments in the mathematical sciences at four year institutions during the period 1975-80. But during the same period the number of faculty members increased only by 8%. At the same time, mathematics is failing to secure its share of qualified young people. When compared with 1970, the number of undergraduate degrees in the mathematical sciences has decreased by 40%, and the number of Ph.D.degrees has been dropping monotonically since 1970. Moreover, the percentage of foreign recipients of the Ph.D. in mathematics has now increased to about 40% of the total. As the David report observes a "gap has been created between demand for faculty and supply of new Ph.D's. It may well widen as retirements increase in the 1990's".

The reasons for the difficulties in the mathematical sciences are complex. A strongly contributing factor is certainly to be found in the drastic decreases in federal funding for mathematics during the past fifteen years as documented in [4]. Another factor is the earlier noted and widely discussed range of problems with mathematics education at the elementary and high school level. At the same time, the typical undergraduate mathematics curricula are largely inflexible and have not responded well to the challenges introduced by the fact that today much of the student-interest centers in areas of applied mathematics, computational modeling and scientific computing. As a result, talented young people often turn away disappointedly from the field.

The problems are even worse in computational mathematics. The rapid growth of the field has largely outstripped the available educational opportunities. There is a profound lack of senior faculty members in the field and a paucity of graduate students and young researchers. At the same time, there has been a growing demand for computational mathematicians in industry. In fact, during the last few years nearly one-third of the new Ph.D.'s in the mathematical sciences have taken positions in industry. At the same time students often terminate their studies early to accept high paying positions in the computing industry. Similarly, the best young faculty members in computational mathematics are frequently lured away to industry not only by the attraction of higher salaries but also by the much better computing environments.

Significant additional manpower resources for computational mathematics will be needed in the years ahead. In fact, the David report presents the following estimate: "Expectations are that a few hundred supercomputers for acedmic, industrial, or governmental use will be put in place over the next decade. Each machine will require approximately 10 scientists with sophisticated knowledge of applied mathematics related to computation. Demand for such new scientists may run 500-800 per year. Even though numbers of these scientists will come from computer science, the physical sciences, or engineering, the demand for new Ph.D. mathematical scientists in computing could easily reach 100 per year in the future. Federal support of a subfield of this size could not be absorbed within the resources we have recommended". The projections of the report appear to be rather conservative. In fact, recent studies by the Institute for Constructive Capitalism of the University of Texas at Austin indicate that by 1990 the projected number of supercomputer installations will be most likely around 200 per year and that worldwide supercomputer sales may exceed 1,500 per year by 1993.

These brief remarks already indicate that there is no easy response to the recommendations in [1] and [3] that there be an increase in the education and manpower development in computational and applied mathematics. The

David report recommended a broad "National Graduate and Postdoctoral Education Plan in the Mathematical Sciences". There is no need to repeat here the details. But we note particulary the strong emphasis on additional support for graduate students, post-doctorals, and young investigators.

The special situation of computational mathematics requires added attention to these recommendations. In the field there exists a very urgent need for increased support of graduate students to help in inducing more of them to continue their studies up to the Ph.D. degree. However, care needs to be taken that such students are not assigned to standard teaching duties but should participate as much as possible in the work of multidisciplinary research teams in computational mathematics.

In contrast to chemistry, physics, and biology, there exists very little funding for post-doctoral positions in mathematics. In part this corresponds to the sociological fact that post-doctoral studies are not a traditional requirement in the core areas of mathematics. In computational mathematics, however, there are growing indications that this situation is changing. Typically a new Ph.D. has had time to become somewhat familiar only with one particular application area. As in the other experimental sciences, there is a need for a subsequent deeper involvement in some other application and problem area. Without such additional post-doctoral experience the young Ph.D.'s research is likely to remain severely restricted. At the same time, the proposed research teams represent an ideal training mechanism for such post-doctoral fellows. We recommend strongly that the National Science Foundation increase its support for post-doctoral positions in computational mathematics.

In view of the severe shortage of computational mathematics faculty, it appears to be desirable to consider retraining qualified persons from other areas of mathematics or other fields. In part, this process can be aided by means of longer visits of such people at places where there are established computational mathematics teams. Some consideration should be given to providing appropriate support for such visits, for example, in the form of competitive grants to the potential visitors.

There appears to be a need for a closer study of suitable modes of undergraduate education in computational mathematics. In analogy with the experimental sciences, courses certainly require a meaningful laboratory component. This raises questions about suitable hardware and software, and even more critically about well designed textual material. The funding agencies, and, in particular, the National Science Foundation may be able to stimulate some developments in this area by means of some well targeted support. For instance, this may be in the form of some support for interdisciplinary study groups to prepare material for novel courses in computational mathematics, or of challenge grants to design new and innovative programs. But this also raises the question of funding of appropriate computational facilities for educational purposes.

5. FUNDING CONSIDERATIONS

In paraphrasing the Bardon-Curtis report [2] (see Appendix A) the Committee believes strongly that the general role of the Federal funding agencies supporting scientific computing should be to maintain strong programs that are designed to provide:

support of basic and applied research in universities in computational mathematics and advanced computer concepts including software, algorithms, architecture, subsystems, and components;

support of basic and applied research in problems that require computing across all areas of science and engineering;

training of mathematicians, scientists, and engineers in the concepts, design, and use of computing systems;

assured access for researchers and graduate students to computing facilities.

During the past year several funding agencies responded to some of the recommendations of the Lax report [1] and the Bardon-Curtis report [2]. We mention here only the Fast Algorithm initiative at the Air Force Office of Scientific Research, the establishment of the Scientific Computing Program in the Office of the Director of Energy Research at the Department of Energy, and the formation of the Office of Advanced Scientific Computing at the National Science Foundation.

The Air Force initiative is based on the earlier noted observation that new advances in numerical analysis, and algorithm design are required to exploit the new computer architectures that are now being introduced. In line with this, a moderate number of team-research efforts for the development of "fast algorithms" for large scientific problems are being funded.

The aims of the Scientific Computing Program at DOE agree closely with many of the ideas and recommendations described in Section 3. The program consists of the Applied Mathematical Sciences Resarch Program and the Energy Research Advanced Computation Project. The Applied Mathematical Sciences Program has initiated several major interdisciplinary projects at universities and laboratories through its initiative in the development of Advanced

Computing Concepts and the Energy Research Advanced Computation Project in providing access to supercomputers at the NMFECC and the Supercomputer Computation Research Institute at Florida State University via the nationwide MFE network.

The formation of the Office of Advanced Scientific Computing (OASC) by the National Science Foundation represents an important step toward providing much needed supercomputer service for a broader community involved in academic research and science education. The OASC Supercomputing Centers Program is supporting access to advanced scientific computing resources and advanced prototype computers, as well as projects in the area of software productivity and computational mathematics for supercomputers. In addition the OASC Networking Program will facilitate the establishment of a national network and support of local access to that network.

In connection with the OASC support for software productivity and computational mathematics it should be noted that the emphasis is here not on basic research but on projects that enhance the effectiveness of scientists and engineers in their use of supercomputers. But as pointed out in Section 1 above, there is a fundamental need for establishing a companion program of support for research and education in computational mathematics itself. Evidently this is not part of the current program of OASC, although there may well be reasons to consider modifications of that program.

As summarized in Section 1 our fundamental recommendation is to expand and strengthen the programs of the various funding agencies in support of research and education in the computational mathematical sciences and scientific computing. In line with the discussions in the previous sections, such expanded programs should have at least the following components:

1. New funding programs specifically focused on the establishment of a number of viable research teams in computational mathematics and scientific computing and on ensuring the continuity of their work for several years.

2. Support programs for establishing and maintaining an appropriate research infra-structure for such research teams consisting of suitable computer hardware and software and the associated support personnel.

3. A concentrated effort for overcoming some of the manpower shortages in computational mathematics. This should include, in particular, support for graduate students, post-doctoral fellows, and young researchers.

In order to give some indication of the required funds, the following table presents an estimate of the yearly cost of a team of five researchers: (All figures are in thousands of dollars)

SALARIES		
5	investigators at an average of $45 two months summer support each	$50
	two months released time per academic year each	50
2	full time support persons	60
1	post-doctoral fellow	25
		185
FRINGE BENEFITS (at 25%)		46
GRADUATE STUDENTS		
8	students at $12 each for stipend and tuition benefits	96
ASSOCIATED RESEARCH COSTS		
	secretarial costs, printing and reproduction, travel, etc (5 times $7)	35
		$362
INDIRECT COSTS (50% of direct costs)		181
TOTAL PER YEAR		$543

There are currently about 15-20 small more or less informal research groups in computational mathematics and scientific computing around the country. Clearly they would constitute natural nuclei for the proposed research teams. This would suggest that funds are needed for the establishment and continued support of about 3-4 such teams each year for a period of five years.

As noted in the earlier sections, this support need not be in the form of one grant. In particular, funding for the work of the senior investigators might already exist in the form of project grants. However, the currently available support for post-doctoral fellows, support personnel, and additional graduate students is certainly inadequate and needs to be expanded. Moreover, most importantly, some mechanism has to be found to ensure some stability and continuity in the support of such a team over a period of several years. For this the current, relatively short term project grants, are not well suited. A long-range approach can substantially increase the productivity, and efficiency of computational mathematics research in this country.

The above figures do not include computer costs. Here funds are needed for the acquisition of computer hardware and software, the continued operation and maintenance of these facilities, and access to national networks and super-computers.

The existing support program for computer equipment appears to be in need of considerable expansion if it is to meet the requirements of the proposed strengthening of computational mathematics research and the formation of the indicated research teams. Some cost-data for these laboratory facilities are given in Appendix B. As summarized there the minimal equipment cost for the above research team is of the order of $250,000 to 300,000.

The cost of operating and maintaining computing equipment is an increasingly difficult problem for most colleges and universities. In fact, frequently, institutions find it easier to acquire some computing equipment through one-time funds, gifts, or bequests, than to operate and maintain it. Such costs have been estimated at about 15-20% of equipment costs per year. Since these computing facilities are an essential part of the computational mathematics research, there is a need to establish some support for these ongoing costs as part of the normal funding of this work.

The mentioned third component of support for computational facilities, namely, the access to a national network and suitable supercomputers is a part of the already established program of the NSF Office of Advanced Scientific Computing. But as noted earlier there is an equal need for a broadly based network which links groups in mathematics, computer science, and related areas, and which provides the much needed closer cooperation and coordination between researchers who often work on the same or similar problems.

As discussed in Section 4 above, there is no easy solution to the required strengthening of the educational situation in mathematics, in general, and in computational and applied mathematics, in particular. The proposed establishment of a number of research teams in computational mathematics will certainly have a positive effect in this regard, at least on the graduate and post-doctoral level. As noted earlier, these teams can also provide the opportunity for faculty level visitors interested in switching to computational mathematics. All funding agencies should give strong consideration to an expansion of their support for graduate research assistants, post-doctoral fellows, young investigators, and faculty level visitors in the general area of the computational mathematical sciences. In addition, through support of studies by professional societies and special groups, there exist possibilities for mobilizing the mathematical sciences research community to address the critical problems of mathematical education in this computer age.

APPENDIX A
LIST OF RELATED REPORTS

[1] REPORT OF THE PANEL ON LARGE-SCALE COMPUTING IN SCIENCE AND ENGINEERING, Sponsored by DOD and NSF in cooperation with DOE and NASA, P.D.Lax, Chairman, National Science Foundation, Dec. 26, 1982

[2] A NATIONAL COMPUTING ENVIRONMENT FOR ACADEMIC RESEARCH, NSF Working Group on Computers for Research, K.K.Curtis, Chairman, Report prepared under the direction of M.Bardon, National Science Foundation, July 1983

[3] COMPUTATIONAL MODELING AND MATHEMATICS APPLIED TO THE PHYSICAL SCIENCES, National Academy of Sciences/National Research Council, Committee on the Applications of Mathematics, W.C.Rheinboldt, Chairman, National Academy Press, 1984

[4] RENEWING U.S.MATHEMATICS, CRITICAL RESOURCE FOR THE FUTURE, National Academy of Sciences/ National Research Council, Ad. Hoc Committee on Resources for the Mathematical Sciences, E.E. David, Chairman, National Academy Press, 1984

APPENDIX B
LABORATORY FACILITIES FOR SCIENTIFIC COMPUTING

The Committee discussed various workstation network configurations which would be suitable for scientific computing teams. On the basis of this discussion, one of the committee members, D. Gannon, compiled the following summary.

A basic laboratory suitable for three senior researchers and five graduate research assistants should consist of a network file server and gateway to a long haul network to supercomputers, two high performance workstations and four low end workstations. These pieces of equipment should have the following minimal characteristics:

1. The network (X.25) gateway and file server should have at least 500 MBytes disk storage and tape backup. The cost range for such a file server ranges between $50,000 and $100,000 or more.

2. The two high end workstations should have at least 4 MBytes memory each, and should include color grahpics (approx. 1024 by 1024 and 8 to 24 bit planes) as well as hardware floating point accelarators. The cost range is about $40,000 to $80,000 each, but may easily be much higher than that.

3. The four low end workstations should have at least 3 MBytes of memory each and a bit mapped black and white display. They need not incorporate floating point hardware. The cost range is about $15,000 to $20,000 for each station, but once again can go also much higher.

4. The software requirements will vary considerably, but FORTRAN and C compilers, UNIX, and network support are most likely needed. For some networks the cost of such software may be as high as $25,000 while in other cases only $1,000 to $3,000 may be required.

The performance of the currently available systems of this type varies as much as the cost. In fact some of the lower priced systems may need to be connected to a suitable super-mini computer to form an acceptable configuration. The cost of the above laboratory -- after customary university discounts -- is at least of the order of $250,000 to $300,000, but may easily be double that amount. The yearly maintenance for this equipment is roughly 15-20% of the purchase price per year.

A general overview of the computing facilities needed in support of a small research team in scientific computing was prepared by the Computing Center of the University of Michigan. In the remainder of this appendix we present a verbatim copy of this thoughtful specification:

Computing facilities to support a small group of researchers in scientific computation should consist of a collection of workstations of varying and/or specialized capabilities joined in a LAN with one or more especialized servers and network gateways. The workstation capabilities and specialized servers must be selected to meet the general requirements delineated below as well as any special requirements needed by the researchers for whom the system is designed. Facilities custoized for specific research areas should be anticipated. For example, workstations providing unique computing capabilities and servers for specialized hardware devices (high-quality printing, hardcopy graphics, or photographic output) should be anticipated.

The workstations can be characterized in terms of five quantitative requirements: megapixel displays, megabytes of RAM, MIPS of computing power, megabytes of storage, and megabit transmission rates within the LAN. These five criteria provide the outline of a "5M" workstation and will be assigned different emphasis depending on the specific research activities under consideration. For example, a (1,4,2,1,1) configuration might be used for computationally intensive activities, while a (8,4,1,4,1) might be more appropriate for graphic intensive applications.

Although written in terms of hardware characteristics, the 5M criteria should be viewed in the context of the LAN. Thus, for example, reduced function workstations need not have these hardware characteristics in isolation from the LAN provided that the equivalent facilities are available by using system components within the LAN. Nevertheless, the total performance of the computing facility should reflect that available from 5M workstations, i.e., reduced function workstations should not degrade total system performance appreciably. In particular, the megabyte of RAM and MIPS processing rate and the megabyte of storage can be provided within the LAN and need not necessarily characterize each workstation, e.g., the LAN could include one or more multi-MIPS, multi-megabyte processors and a file server incorporating a large disk system. The megapixel and megabit transmission rate requirements, however, are very workstation specific.

The megapixel requirement means that the product of the veritical and horizontal resolutions and the bits per pixel exceed one million. For example, 1024 x 1024 resolution with 8 bits of color provides 8 megapixels. In association with the megapixel criterion, the display should be bit-mapped, and the software should support multiple display windows and a 'mouse' for both interactive graphics and a menu/token driven environment.

Although not an explicit requirement, virtual memory is almost mandatory to meet the many demands that will be placed on these systems. Because routine numerical applications require 4 megabytes of memory, total system memory demand will be very large. Real memory systems must be carefully considered if reduced function workstations are included. Further, if the local system is to be used for program development for production systems accessible through the network gateways, the memory capacity and performance of the local system must be a significant fraction of the production system so that reasonable testing can be performed locally. This is particularly applicable to memory capacity because memory restrictions play a more significant role in algorithm and program design than the other elements of the 5M criteria.

Use of secondary, or low-end, workstations for production computations should be anticipated, and their performance capabilities should not be significantly less than the high-end workstations. For scientific applications, the floating-point performance available to a workstation should be sufficient for the users to observe actual performance of at least .1 MFLOPS, and the floating-point characteristics should be consistent with those of the IEEE floating-point standard. A floating-point coprocessor or other provision for hardware floating-point will probably be necessary to achieve these speeds.

The software system should support both menu/token and command driven environments, bit-mapped interactive graphics, multiple display windows, a language-independent program development system, both internal and external (using the network gateways) messaging, network support for the most commonly used network protocols (e.g., X.25 and TCP/IP), and file transfer and program portability with the systems routinely available through the network gateways. Program portability should be a primary consideration in system and compiler selection.

The program development system should be language independent and provide full-function editing capabilities, a file/program management facility, a symbolic debugging facility, and a program performance analysis facility. The program development system cannot be assessed in the limited context of the workstation and its LAN. Although much of the program development will be for the workstation, much will be for remote systems.

The system should provide 'expert' compilers that support program portability not only in terms of language syntax and semantics but also program performance. This requirement is more stringent than simple conformance to specific language standards. The compilers must encourage and guide program development in directions that will result in acceptable performance both on the local system and vector systems available through the network gateways. By implication, the workstation must provide sufficient performance and memory capacity for this type of use.

APPENDIX C
LETTERS AND POSITION PAPERS

THE MATHEMATICS OF SCIENTIFIC COMPUTATION

I. INTRODUCTION:

The Department of Defense, as one of the largest users of computation, perhaps the largest, must be vitally concerned with the quality of that computation. In particular, there is great sensitivity in terms of the accuracy, efficiency, and cost associated with the scientific calculations that DOD does in its own laboratories, in the design and operational activities of the services, and in DOD-sponsored research and development work. As dependencies on large calculations grow, the quality of computation becomes an increasingly important matter. We have seen quality considerations catch up on a number of U.S. private sector technologies and products in a frightening fashion. We must be sure this does not occur in a field as important to DOD as scientific computation.

Large computer application programs have a number of levels at which one must be concerned. The software codes must be well-structured and modular to allow for efficient building, merging, and repair (correction and debugging). If possible, some form of either validation for correctness or testing must be built into the programming as it is being constructed. The algorithms chosen to be used for the unraveling of the equations and for their solving must be as close to optimum as possible from the point of view of minimum use of machine instructions and optimal transfers of data from large storage to fast storage and then to the execution units.

Before any of these can be done, however, there must be adequate assurance that the physical and mathematical problems have been correctly posed; that, in fact, there are solutions and something of their qualitative character is understood. And, at the very base of a useful calculation, the phenomena itself, whether one of physics and chemistry or of the operation or design of systems, or a logistics problem, must be satisfactorialy understood and formulated.

Part of this whole process lies within the scope of the mathematical sciences and part lies without. Those activities which depend on the linguistic aspects of programming or on the architectural concepts and structures of the operating systems or the hardware are the realm of the computer scientist even for very large application programs. However, the mathematical parts--the problem formulation and its qualitative analysis, the translation into numerical methods, and the selection of an optimum algorithm--all depend heavily on the background that the linguistic and architectural components contribute.

In this spirit, we propose a new initiative in mathematical research that takes as a major goal the improvement of large scale scientific computing. There have been notable endeavors of this kind in past years; we do not mean to work in uncharted territory:

- The Fast Fourier Transform began in an attempt to solve a problem in low temperature physics. A thorough understanding of its uses, the formulation of problems to take advantage of its capabilities, a search for best algorithms, and their efficient programming on many machine systems has followed. It is now a sine qua non in signal processing and has revolutionized data handling and analysis.

- The nonlinear partial differential equations of transonic flow have been a mathematical and computing target for over thirty-five years. Increased knowledge of the physical phenomena, understanding of the qualitative behavior of solutions, new numerical approaches and algorithms that take advantage of these and of machine structure have now produced fuel-saving airfoil designs that are appearing on military and commercial aircraft.

- Linear programming came out of W.W. II naval logistics. It has become a money-saving and labor-saving mathematical tool, an essential part of military logistics and operations and of design. The improvement of large software codes has gone hand-in-hand with a deepening understanding of the mathematical structure, complexity, and limitations of linear programming algorithms. In very recent years, a new approach, the elliptic method and a new estimate on the linear nature of the simplex method, have stimulated further mathematical study.

Examples such as these abound; they show very well that the most effective of the large software packages for important scientific calculations are firmly based on well thought-through mathematical analysis and numerical methods.

II. AREAS OF RESEARCH:

Scientific computation depends on discrete approximations to the equations that describe the physical phenomena. Asymptotic or other perturbation approximations often provide invaluable insights into the nature of nonlinear behavior and are of great help in designing efficient numerical methods.

The origins of methods for finding approximate solutions of an initial or boundary value problem can often be found in the mathematical analysis of the system. For example, the finite element method for solving elliptic boundary value problems draws heavily upon the variational framework in which the basic issues of existence, uniqueness, continuity with respect to data, and regularity of solutions are addressed. This interaction between the approximation methods and the underlying analysis is an important component of the whole study.

A major challenge is the development of comprehensive theories for the nonlinear problems arising for elliptic problems (nonlinear elasticity, the static semiconductor equations), parabolic problems (nonlinear diffusion and transport, combustion), and hyperbolic problems (wave motion on ocean surfaces, ground motion, shocks, entropy inequalities). A study of the questions of well-posedness and regularity is of fundamental importance in laying the groundwork for sound methods for the approximation of solutions. Support of this area is currently inadequate in view of the importance of these problems.

There are many other areas in which more analysis is needed in computational mathematics: solution-adaptive methods need considerable attention at present. These methods use information about approximate solutions developed at initial stages to refine and modify the framework of the approximation itself. The adaptation should be incorporated into the approximation process at a fundamental stage and should be done in an optimal way. Research into the developement of approximate methods for problems with different time and length scales and problems with singularities or roughness in coefficients or data requires more analysis. Another challenging area arises from parameter dependent problems. The question of solution stability typically involves examination of the solution manifold, which for many complex problems is accessible only by computation. The comparison of the solution manifold of the discrete problem with that of the original problem is an important incompletely explored question. These and many other research areas require a closer tie between the computational methods under development and the analytical tools applicable to these problems.

A related topic in which further research is needed to support the development of computational mathematics concerns implementation of the computational methods by a computer architecture. With the advent of "vector," "array," "systolic," and "parallel" processing, it is evident that the architectural issues in the development of computational methods are becoming increasingly important. In fact, we must be able to resolve the interplay between the methods and the computers on which they are to be implemented in order to be successful. Thus, we should consider computation as a path from a partial differential equation to a discretionization method to a method for solving the resulting linear algebra, then the "mapping" of these to the computational process on a computing engine. We need to address the relative merits for scientific computing of massively parallel architectures, systolic architectures, data-flow machines, machines with reconfigurable communication networks, computers with a few, powerful processors. These machines must be matched to the computational tasks for which they are best suited.

III. FUNDING MODE:

We propose that this initiative, The Mathematics of Scientific Computation, be managed as a coordinated program through the three services mathematical sciences basic research groups. At present, each of these groups has a very small base program that covers some of these topics. These efforts require substantial broadening in terms of particular problem coverage and technique development. These base programs are inadequate in terms of the problems they can cover; we are asking for a major expansion of these efforts. In addition, there are excellent researchers in the fields we have mentioned who are not now supported and who are capable of making excellent contributions.

We propose that funding for this research initiative be, for the most part, concentrated at a number of research centers. A few of these exist at present at which there are a large enough group of researchers, post-docs, and graduate students plus the necessary computation facilities to provide in-depth study on one or several of the problem areas. One purpose of funding in a focussed fashion is to establish other centers of excellent research work in these computation fields so that, as new application topics arise in DOD technological requirements, these groups will be available. Unlike other work in mathematics, the problems, the methods, and the implementation of trials and tests of codes do require group activity.

It is our estimate that at a full scale strength of twenty-five people (five researchers, five post-docs, and fifteen graduate students) at each center would cost on the order of .9-1.1 million dollars per year. We propose the establishment of six new centers in the next three years. These would not be established with block "center funds" but rather as a set of separate research contracts aimed at particular applications or technique development problems. Thus, the contracting and reviewing procedures would be the ones usually employed with 6.1 funding.

Finally, recent reviews of the 6.1 research funding by external groups (the Bennett Committee of the DOD-University Forum; the David Committee of the NAS/NRC) have concluded that the base programs in the mathematical sciences, while generally and seriously underfunded, are of high quality and represent a solid contribution to DOD. For this reason we are requesting that the program described here be a new effort, complimenting and adding to research now underway.

Hirsh Cohen
June 11, 1984

For: Ad hoc mathematics advisory group to the DOD-University Forum.

STANFORD UNIVERSITY
STANFORD, CALIFORNIA 94305

Gene H. Golub
Professor and Chairman
DEPARTMENT OF COMPUTER SCIENCE

Telephone:
(415) 497-3124

September 10, 1984

Dr. John Connolly
Office of Advanced Scientific Computing
National Science Foundation
Washington, D.C. 20550

Dear Dr. Connolly:

Many thanks for making your excellent presentation at the SIAM meeting in Seattle. I am sure we all found it interesting to hear of NSF's initiative in supercomputing.

My colleagues and I, however, are quite concerned about certain aspects of this project. In particular, we feel that it is still not completely understood how to use supercomputers in their most effective manner. In particular, there is still a need for developing new (or possibly re-examining old) algorithms which will take advantage of all the power of these computers. It is important that the numerical analysis/scientific computing community be involved in this, since we have the greatest expertise in devising and analyzing numerical algorithms which are relevant to scientific computing.

In a similar vein, I think it also important that the computer science community have some association with this project. We see increasingly that simply having a supercomputer is not sufficient to accomplish large scale computation. A supercomputer environment can easily degenerate and the supercomputer would not be of great use if one does not have excellent means of communications and supporting systems software.

As you can see, I feel that supercomputers should involve a larger scientific community than was initially envisioned. There is a lot of expertise now in developing numerical software and in developing computer systems. It think it is important these these communities be also taken in account in the supercomputer initiative.

Yours sincerely,

Gene Golub

Gene H. Golub

CC: Jack Dongarra
Dr. John Polking
Kent Curtis
Dr. Bruce Barn
Dr. M. Ciment

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HIRSH G. COHEN
PRESIDENT

REPLY TO:
IBM RESEARCH CENTER
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YORKTOWN HEIGHTS, NY 10598

December 6, 1984

Dr. John C. Polking
Division Director
Division of Mathematical Sciences
National Science Foundation
Washington, D.C. 20550

Dear John,

I don't know where you stand on shaping the mathematics of computation initiative but I thought you might find the enclosed statement useful.

As will be obvious, I prepared it for use in our dealings with DOD. It became a part of a report on 6.1 Research submitted by Ivan Bennett's committee for the DOD-University Forum. Some of the comments and ideas may be useful to you.

I'm also sending a copy of a letter I sent to Ivan Bennett to reinforce the proposal.

I hope these are useful. I'm sending copies to Werner Rheinboldt.

Sincerely yours,

Hirsh Cohen

Hirsh Cohen

/emk

Enclosures

cc: W. Rheinboldt

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December 4, 1984

Dr. Werner C. Rheinboldt
University of Pittsburgh
Faculty of Arts and Sciences
Department of Mathematics and Statistics
Andrew W. Mellon Professor of Mathematics
Pittsburgh, PA 15260

Dear Werner:

I enjoyed very much the workshop on Computational Mathematics. I was very impressed by the quality and diversity of the participants. I feel that the program might be presented to the Science Foundation as an initiative very much on the lines of the Experimental Computing Program of the Division of Computer Science. That means that each grant would be for a 5 year initial period and there would be 3 or 4 new grants every year until a sufficient level is reached. Industrial participation should be sought. I see three natural points of contact:

1) Summer employment for graduate students within industrial research groups
2) 1 year or shorter visits by industrial researchers to university computational research groups.
3) Visits by members of university researchers to industrial research groups

Obviously, industry is a good source of computers as gifts or at greatly reduced prices.

Originally the NSF experimental computation initiative was to be jointly with the Department of Defense but after the inception of the program the D.O.D. pulled out. Now is the time I feel to approach the D.O.D. for joining this program, but by no means should the NSF part of the program be contingient on D.O.D. participation.

Whatever plans are developed I would presume would be submitted to the Advisory Board of the Mathematics Division for their endorsement.

With warmest regards,

Peter

Peter D. Lax

National Aeronautics and
Space Administration

Ames Research Center
Moffett Field, California 94035

NASA

Reply to Attn of: D:200-1

March 7, 1985

Dr. Werner C. Rheinboldt
Andrew W. Mellon Professor
of Mathematics
Department of Mathematics and Statistics
Faculty of Arts and Sciences
University of Pittsburgh
Pittsburgh, PA 15260

Dear Werner:

I appreciate receiving from you a draft of the Report of the Panel on Future Directions in Computational Mathematics, Algorithms, and Scientific Software. Your study certainly is a timely one. Research advances in these discipline areas are changing the way the country does business in a wide range of technical areas. We at Ames have participated in that revolution for fifteen years and expect the same rate of progress to continue for the foreseeable future.

I will be very interested to see how the Panel recommendations are received by NSF. While I realize it is outside your charter, I would be interested to hear any ideas you and the Panel have on what additional steps Ames can take to advance computational mathematics.

Best regards,

Bill

William F. Ballhaus, Jr.
Director

The University of Michigan
Computing Center
1075 Beal Avenue
Ann Arbor, Michigan 48104

March 12, 1985

Professor Werner Rheinboldt
Department of Mathematics
University of Pittsburgh
Pittsburgh, PA 15260

Dear Professor Rheinboldt:

The enclosed description of computing facilities for mathematical computation evolved from a series of messages exchanged between Gregory Marks, Special Assistant to the Vice-Provost for Information Technology, Professors Ridgway Scott, William Martin, and Richard Phillips, and me.

The "5M" criterion was developed within the College of Engineering and is basically a model of its current activity in workstation design. For example, the College has had great success in using Macs as reduced function workstations attached to Apollo rings with the computing capability obtained from the Apollos.

Traditionally, floating-point performance and quality have been given little attention in comparison to the more general hardware features and software. Because the systems under consideration are specifically for mathematical computation, it is appropriate perhaps that the floating-point characteristics of the hardware be more carefully examined in this case.

We have taken the liberty of devoting at least some space to the software systems for the workstations, but our specifications remain quite incomplete.

I hope that our description will be helpful.

Sincerely,

Leonard J Harding

Leonard J Harding

LJH:mft

Enclosure

cc: Professor Bernard Galler