NUMERIC, SYMBOLIC, AND GEOMETRIC COMPUTATION

Numerical Methods

Pennsylvania State University – University Park; Jesse L Barlow; ***Numerical Solution of Eigenvalue Problems and Related Least Squares Problems*****; (CCR-9424435 A000); $48,387; 12 months. (Joint support with the Computational Mathematics Program)**

This research seeks to improve the accuracy of methods to solve some particular eigenvalue problems. The first is the classical symmetric eigenvalue problem. Recent results have shown that there is a large class of symmetric eigenvalue problems for which small structured perturbations result in small changes in the eigenvalues in the relative sense. This class of matrices is called "well-behaved". The problem of finding a necessary and sufficient condition for a matrix to be "well-behaved" is being investigated. A number of related issues have to be considered, including: analysis of methods for updating indefinite eigenvalue problems; investigation of methods for updating the ULV and ULLV approximations to the singular value decomposition and generalized singular value decomposition; and development of analysis of methods for computing the sparse generalized singular value decomposition. The last two issues are extremely important in the solution of ill-posed least squares problems and total least squares problems. The implications of derived results for these problems are being investigated.

University of Colorado – Boulder; Elizabeth Bradley; ***NSF Young Investigator (NYI) Award: New Approaches to Engineering Design: Controlled Chaos and Computer Automation*****; (CCR-9357740 A002); $71,763; 12 months.**

This project explores two new approaches to engineering design. Each of these threads is composed of several synergistic subprojects; these subprojects combine analytical mathematics, numerical simulation, symbolic reasoning, and physical experiments. The first approach is to actively use chaos to improve the designs of various engineering systems. One example of this is causing gases to burn more effectively by induction of chaotic mixing in a combustion chamber. A small, well-placed obstruction can interact with the inflow and with the chamber's geometry to cause large effects: chaos's symptomatic "sensitive dependence on initial conditions." These effects are tested both experimentally and with computational fluid dynamic simulations. Another example is the use of chaos to broaden the capture range of a phase-locked loop circuit. The second approach to improving engineering design is through computer automation. The ultimate goal of this endeavor is a suite of programs that explores different high-level analysis and design paradigms. Such tools would not only streamline an engineer's problem-solving task, but actually amplify creativity. The first step is a program that autonomously constructs mathematical models from information about a system, presented in a variety of forms and formats: measurements made directly on the physical device; a user's observations described to the program in varying degrees of precision, symbolically or graphically; partial models and hypotheses suggested by a user; and general mathematical theory that is encoded in the program's knowledge base.

Cornell University; James H Bramble and L. B Wahlbin; ***Algorithms and Numerical Analysis for Partial Differential and Integral Equations*****; (DMS-9311406 A001); $105,000; 12 months. (Joint support with the Computational Mathematics Program and the Applied Mathematics Program)**

The project studies new techniques and methods of analysis of behavior in existing approximation methods, and introduce and analyze new algorithms for the numerical approximation of various problems. Specific areas to be considered include: (1) preconditioned iterative methods for fast solution of resulting algebraic equations, (2) finite element methods in domains with curved boundaries and interfaces, (3) local behavior of finite element methods in differential and integral equation problems with singularities, and (4) superconvergence phenomena in differential and integral equations. Numerical experimentation and examples play important roles in the discovery and elucidation of various numerical methods. Of course, practical application is a motivating factor for the problems studied. One of the aims of the work is to develop a deeper understanding of many existing methods, improve them or develop new ways of treating old and new problems. This kind of understanding is central to the design of accurate and efficient algorithms for the use in present and future computer environments. Various questions concerning the practical solution of problems of interest in engineering and science are pursued. One aim is to construct methods that are faster and more accurate than existing ones. A second aim is to invent and study techniques for the solution of problems heretofore beyond the scope of even the most powerful computers. Areas of application in which the studies are important are structural mechanics, fluid dynamics, groundwater flow and electromagnetic theory.

University of Kansas ; Ralph Byers; *Numerical Linear Algebra and Control*; (CCR-9404425 A000); $37,475; 12 months.

This project studies existence, uniqueness and numerical methods for calculating a smoothly varying singular value decomposition of a smooth matrix valued function. The smooth singular value decomposition has applications in differential algebraic equations including time dependent optimal control problems for descriptor systems. Preliminary work with real analytic functions is to be extended to a larger class of smooth functions and more efficient numerical methods for tracking all of or part of a smoothly varying singular value decomposition are being investigated. This project is also developing numerical methods for calculating the controllability radius, regularity radius, and other distances of interest in computational control. It is developing efficient, provably reliable, numerically stable methods. Success here will generalize to a means of estimating the distance from a generic matrix pencil to an algebraic variety of nongeneric pencils and to general condition estimators.

University of Iowa; James F Cremer; *Research Initiation Award (RIA): A Problem Solving Environment for Mechanical System Simulation*; (CCR-9309679 A003); $25,873; 12 months.

This project involves experimental research to develop a problem solving environment for mechanical system simulation. Specifically, the research develops software tools that facilitate rapid, high-level creation of mechanical system simulators. These tools are used to generate simulators for a variety of applications, including real-time vehicle simulation, legged locomotion and robotics, and investigation of collision and contact problems. There is a great interest in the development of problem solving environments (PSEs) for engineering and science problems. One of the key challenges lies in developing computer science techniques that enable integration of supporting technologies such as computer algebra systems, numerical analysis libraries, geometric modeling systems, and object-oriented programming systems. This research attacks the problem by concentrating on one well-defined but rich domain, rigid-body dynamics simulation. The project has two specific goals: (1) advance the state of the art in mechanical system simulation by making it easier to create and modify dynamics simulators, and (2) develop a software architecture and software tools that extend from this domain to more general problem solving environments. Use of the software tools to generate dynamics simulators for a number of different applications demonstrate the power of the approach.

Massachusetts Institute of Technology; Alan S Edelman; *Numerical Methods for the Nonlinear Eigenvalue Problems in High Performance Materials Design*; (CCR-9404326 A000); $66,835; 12 months.

The objective of this project is to develop adaptive numerical methods for the first principles prediction of the properties of technologically important materials. These materials may be characterized as having complex structures and compositions, large numbers of particles (> 100) and little or no symmetry. The methods being investigated include a suite of iterative, acceleration, and minimization schemes for the nonlinear eigenvalue problem and accompanying elliptic problem arising in first principles prediction of material properties. This suite includes the eigenvalue iterative methods of Rayleigh-Ritz and Longsine and McCormick; minimization methods such us conjugate gradient, steepest descent, and the trace minimization method by Sameh and Wisniewski; and multilevel methods such as multigrid and fast multipole method. These methods will be used with adaptive grid to exploit the underlying dynamical, localized structure inherent in electronic wave functions. Modern parallel architectures will be used to reduce the computational time and memory costs. The various components of this project will be developed through the close collaboration of researchers from chemistry, physics, computer science, and numerical analysis.

University of Kentucky; Graeme Fairweather and Bernard Bialecki; *Orthogonal Spline Collocation Methods for Partial Differential Equations*; (CCR-9403461 A001); $0; 12 months.

This project is concerned with the development of software implementing new matrix decomposition algorithms for solving the systems of linear algebraic equations arising when orthogonal spline collocation (that is, spline collocation at Gauss points) is applied to separable, second order, linear problems on rectangular regions. These algorithms have application in the solution of nonseparable boundary value problems, problems on general regions, and time dependent problems. The success of matrix decomposition algorithms depends on knowledge of the eigenvalues and eigenvectors of matrices arising in corresponding two-point boundary value problems in one space dimension. Knowledge of such an eigensystem with respect to one coordinate variable reduces the original two-dimensional discrete problem to solving a collection of independent discrete two-point boundary value problems with respect to the other coordinate variable. A software package is developed implementing orthogonal spline collocation algorithms with piecewise polynomials of arbitrary order on nonuniform partitions in each coordinate direction. The package includes, as a special case, a fast Fourier transform solver for piecewise Hermite bicubic orthogonal spline collocation for Poisson's equation in various coordinate systems.

University of Colorado – Boulder; Carlos A Felippa; *High-Performance Computational Methods for Coupled Field Problems*; (ECS-9217394 A004); $900,000; 12 months. (Joint support

with the Magnetospheric Physics Program Program, the Physical Oceanography Program, the Solar-Terrestrial Program, the Computational Engineering Program, the Materials Engineering Program, the Solid Mechanics Program, and the Computational Mathematics Program)

This project is a collaboration between applied mathematics, astrophysics, computer and computational science, engineering, and geophysical sciences, to develop parallel algorithms for problems relating to Coupled Fields and Coherent Structures and Geophysical and Astrophysical Fluid Dynamics (GAFD) Turbulence. The common denominator of the various application areas are performance measures, massive data sets, and the visualization of multi-terabyte data sets.

Rensselaer Polytechnic Institute; Joseph E Flaherty and Boleslaw K Szymanski; ***Domain Specific Parallel Adaptive Scientific Computation*****; (CCR-9216053 A002); $40,000; 12 months.**

This project investigates domain specific parallel computation for the adaptive solution of partial differential equations. The decomposition of parallel programs is achieved with the aid of a family of annotation languages that enable the user to annotate programs written in various programming languages. The synthesis of parallel computation relies on the description of an overall computation done in a simple configuration language in terms of interactions of programs and their fragments created by annotations. The decomposition by annotations and synthesis through configuration simplify the process of (1) determining the grain size for efficient parallel processing, (2) data distribution, and (3) run time optimization.

University of Illinois – Urbana; Efstratios Gallopoulos, Kyle Gallivan, and Randall Bramley; ***Collaborative Research: Hierarchically Parallel Algorithms for Portable and Scalable Performance*****; (CCR-9120105 A003); $8,250; 0 months.**

The goal of this research is to develop parallel sparse system solvers for symmetric indefinite and non-symmetric linear systems such as those occurring in computational fluid dynamics, develop parallel techniques for solving time-dependent problems, and construct a rapid prototyping environment for developing and experimenting with algorithms in sparse matrix computations on shared and distributed memory multiprocessors. In particular, the following are examined: (1) parallel solution schemes for solving Stokes-like linear problems arising in CFD and other augmented Lagrangian problems such as interior point methods of linear programming, (2) incomplete Newton methods with Krylov or row projection iterative solvers for the inner iteration, (3) solution of time-dependent problems using high-order parallel methods in time, (4) defining and developing sparse matrix primitives analogous to the highly effective BLAS-3's for dense computations, and (5) implementing sparse factorization and solution schemes. The goal is portable efficiency and scalability, by exploiting parallelism on multiple levels. This in turn allows the work to be used across a wide spectrum of existing and future computer architectures, instead of simply a particular machine.

Stanford University; Gene H Golub; ***Computational Methods in Linear Algebra Using the Theory of Moments*****; (CCR-9505393 A000); $89,958; 12 months. (Joint support with the Computational Mathematics Program)**

Numerical methods are developed for solving large scale matrix problems arising in applications. These applications are quite diverse and include such areas as statistical modeling and quantum chromodynamics (QCD). The basic tool for these computations comes from the classical theory of moments and numerical quadrature. These problems are equivalent to estimating upper and lower bounds for a quadratic form. One area of particular interest is computing the generalized cross validation parameter. This technique is used in solving ill-posed least squares problems by regularization methods. A numerical procedure is developed which enables one to analyze very large data sets. Also, a method for computing a parameter which is of importance in solving ill-conditioned sparse least squares problems is developed. The basic objective of this research is to develop new and robust algorithms for solving very large scale linear problems.

Brown University; David Gottlieb; ***High Order Methods for Time Dependent Equations*****; (DMS-9500814 A000); $69,755; 12 months. (Joint support with the Computational Mathematics Program and the Applied Mathematics Program)**

The project entails research in long term integrations of genuinely time dependent partial differential equations. It involves the development and application of high order finite differences and finite element schemes as well as spectral methods. The methods to be developed and applied are suitable for problems in several space dimensions with complicated geometries. A major consideration in developing and assessing high order methods for long term integrations is their scalability. Based on the experience gained already in parallelizing ENO codes, a further effort to parallelize spectral and finite element based ENO codes is being undertaken. The research has two components, theory and applications, those components are linked together. The theory is motivated by the type of applications under investigation and the applications use the theoretical developments. It has been shown that in order to numerically simulate complicated flows that change in time, high order methods are necessary. However those methods, because of their high accuracy, are less robust. The research deals with the issue of the successful implementations of high order methods. This involved theoretical issues (as solving the 100 years old Gibbs Phenomenon) as well as more applied issues. On the applied side, the problem of mixing enhancement by interactions of Shock waves and hydrogen jets are being studied. This entails the simulation of an air shock passing through an hydrogen jet in high Mach numbers. High order methods are mandatory here since the process of interest is the mixing and combustion inside the jets. The current codes, Spectral and ENO are to be modified to handle more general cases. Parallel versions of ENO and spectral methods are being applied now and will be further modified.

University of North Carolina – Chapel Hill; John H Halton; *Sequential Monte Carlo Techniques for the Solution of Large Linear and Non-Linear Systems*; (CCR-9322102 A001); $69,708; 12 months.

Almost all mathematical problems in science and engineering are approximated by linear and non-linear systems of integral and/or partial differential equations, which vary widely in number, form, and character. Since analytical solutions do not exist for most problems of interest, numerical approximation techniques, such as finite element and finite difference methods, are widely used, ultimately resulting in a system of linear or non-linear algebraic equations, which must then be solved. In the realistic representation of practical applications over large and/or heterogeneous domains, such systems may contain m=104 to 107 unknowns. For non-linear or transient problems, the system requires the repetitive solution of corresponding linearized problems for changing parameters. Direct solution methods often cannot be used because of excessive storage and time requirements (the latter are O(m3)). Iterative methods (such as multigrid, conjugate gradients, SSOR, orthomin, and GMRES), which take time O(m2) per iteration, are almost universally applied. Another candidate for solving very large linear systems is the Monte Carlo method, which takes time O(m) per iteration; but the high variances of the estimates and the very slow convergence has tended to eliminate it from consideration. The sequential Monte Carlo method is a promising modification which shows guaranteed convergence. This method is applied to broad classes of large systems of linear and non- linear equations. Preliminary computations show promisingly large improvements in speed and efficiency over both plain Monte Carlo and deterministic methods.

University of Michigan – Ann Arbor; Janis P Hardwick and Quentin F Stout; *Postdoc: Use Parallel Computers to Help Solve Computationally Intensive Problems in Statistical Design and Analysis*; (ASC-9504041 A000); $46,200; 24 months. (Joint support with the New Technologies Program)

This project concerns the use of parallel computers to help solve computationally intensive problems in statistical design and analysis. The designs considered are sequential, meaning that a design parameters can be altered during the experiment in response to the observations already gathered. Such designs can offer significant cost benefits, but are insufficiently utilized due to the complex analyses they require and the fact they are complicated to conduct. This research attacks these difficulties by considering procedures that are significantly easier to conduct, yet nearly as optimal. The computations are still a major hurdle, especially because the problem one needs to solve require combining sequential designs and computationally intensive bootstrapping.

North Carolina State University – Raleigh; Ilse Ipsen; *Relative Perturbation Techniques for Eigenvalue and Singular Value Decompositions*; (CCR-9400921 A001); $79,707; 12 months. (Joint support with the Computational Mathematics Program)

This project develops perturbation techniques for deriving bounds on the relative error of singular values and eigenvalues, as well as bounds on the error angles of singular vectors and eigenvectors in terms of a relative gap. Deflation and convergence criteria based on these bounds have the potential to lead to highly accurate and efficient QR-type and Jacobi algorithms for computing eigenvalue, singular value and URV decompositions. In the context of the singular value decomposition of a matrix B, a class of perturbations is investigated which represents all possible perturbations that do not change the rank of B. In particular, it includes componentwise relative perturbations of bidiagonal and biacyclic matrices, and perturbations that annihilate an offdiagonal block in a block triangular matrix. So far, many existing relative perturbations bounds have been derived for singular values and vectors of bidiagonal matrices from general results for this class of perturbations. Also, new perturbation results have been proved for singular values and vectors of biacyclic, triangular and shifted triangular matrices. These results are extended to the generalized Hermitian eigenvalue problem, and to the eigenvalue problems for structured and non-Hermitian matrices.

University of Utah; Chris Johnson; *NSF Young Investigator (NYI) Award: Quantitative Inverse Electrocardiography*; (CCR-9458064 A001); $100,000; 12 months.

The goal of this project is to bring together expertise in geometrical modeling, numerical analysis, large scale computing, and scientific visualization applied to problems in medicine—computational medicine—to interactively investigate bioelectric fields and provide the ability to design bioelectric devices. Every year, 500,000 people die suddenly due to abnormalities in their heart's electrical system (cardiac arrhythmias) and/or coronary artery disease. Traditional electrograms (ECGs) show damage that already has occurred in the heart; consequently physicians currently treat many life- threatening disorders of the heart's rhythm after they occur. This project seeks to equip physicians with a noninvasive and accurate means of determining the changes within the heart's electrical system that signal the onset of disease much earlier and allow them to treat the disease prior to significant damage to the heart. To accommodate efficient design and optimization, a computational steering package is developed which allows the user to design bioelectric devices and measure their effectiveness in an interactive graphical environment. Using interactive graphical input devices, engineers are able to design devices, place them directly into the computer model, and automatically change parameters and boundary conditions as well as the mesh discretization level needed for an accurate finite element solution. Instead of the typical simulation mode – manually setting input parameters, computing results, storing data off to disk, visualizing the results via a separate visualization package, then starting again at the beginning – software is developed to "close the loop" and allow the visualization to help guide (steer) the design and computation phases of the simulation. Not only are specific results on bioelectric field problems significant, but this general approach is applicable to many other engineering and scientific problems, and the computational infrastructure developed is broadly useful to many other researchers.

University of Minnesota – Twin Cities; Vipin Kumar; *Highly Parallel Direct Solvers for Sparse Linear Systems*; (CCR-9423082 A000); $67,313; 12 months.

Direct methods for solving sparse linear systems are important because of their generality and robustness. For linear systems arising in certain applications, such as linear programming and some structural engineering applications, they are the only feasible methods for numerical factorization. This project is developing a scalable parallel direct solver for solving sparse symmetric-positive definite(SPD) systems of linear equations, and is investigating its utility and effectiveness in the context of linear programming problems and least square problems. A highly parallel formulation of the factorization phase of the direct solver for SPD systems has been developed. This is being extended to the other three phases (ordering, symbolic factorization and triangular system solving) of a complete scalable parallel direct solver. Parallel formulations are being investigated on a variety of hardware platforms, including traditional MPPs such as CM5 and Cray T3D, as well as clusters of DEC and IBM workstations. The parallel algorithms are being implemented in a portable form using a programming library that supports collective communication, and will be made available to researchers and practitioners elsewhere.

Michigan State University; Tien-Yien Li; *Homotopy Algorithms for Solving Sparse Polynomial Systems*; (DMS-9504953 A000); $67,000; 36 months. (Joint support with the Computational Mathematics Program)

Recently, it has been proved that modeling the sparse structure of a polynomial system by its Newton polytopes leads to a major computational breakthrough in solving polynomial systems by homotopy methods. The "random product homotopy" approach undertaken in the project intends to construct a start system for the homotopy in random product form with its Newton polytopes containing those of the target system. On the other hand, the "polyhedral homotopy" based on an elegant formula for computing the mixed volume can find all zeros of a polynomial system by following much fewer, in most occasions the exact amount of, homotopy curves. Polynomial systems occur everywhere in mathematics, science and technology. Very small systems are easily solved by hand, but larger systems cannot reliably be so solved, if at all. The project aims to implement a portable solver using the latest in polynomial system solving algorithms and capable of being incorporated into applications programs. Research is being carried out to advance the state of the art and our understanding of polynomial systems; additionally, various application areas will be studied, such as kinematics, control theory, geometric modelling, and biochemistry in which problems reducible to polynomial system solving arise.

University of Notre Dame; Andrew Lumsdaine; *CAREER: High-Performance Computing for Computational Engineering*; (CCR-9502710 A000); $113,249; 36 months.

The primary emphasis of this Career Development Plan is the coordinated development of research and education programs in high-performance computing for computational science and engineering.

Research Plan: The main goals of high-performance computing are high-performance, scalability, and portability. To attain these objectives for modern scientific and engineering applications, new hardware paradigms, new software methodologies, and new numerical algorithms are needed. Moreover, the interdependencies between hardware, software, algorithm, and application have an essential bearing on performance, scalability, and portability and must also be well understood. This work is an inclusive effort to create a substantial, unified base of understanding about high-performance computing for scientific and engineering applications that can be broadly applied. The specific objectives of this work are to: (1) Develop and analyze high-performance, portable, computational kernels and numerical libraries that are capable of exploiting modern computing architectures and operating systems, such as symmetric multiprocessors, multi-threaded operating systems, and gigabit networks; (2) Develop and analyze prototype object-based and object-oriented scalable software libraries for high-performance computing and for computational scientific and engineering applications; (3) Develop and analyze new algorithms for maximizing the scalability of stationary and time-dependent problems; (4) Apply the new algorithms and software libraries to real, substantial, computational science and engineering applications.

Education Plan: Because of the increasing importance of computational science and engineering, it is important that computer scientists (and indeed, scientists and engineers in general) understand the intricacies and inter-relationships inherent to high-performance computing. A graduate course in numerical computing has already been developed and incorporated into the graduate core curriculum in the Computer Science and Engineering program at the University of Notre Dame. Building on this course, new graduate-level courses in high-performance computing will continue to be introduced. At the undergraduate level, a senior elective in high-performance computing is being introduced, and there will be continued effort to support and direct undergraduate research.

University of Colorado – Boulder; Thomas A Manteuffel, Stephen McCormick, and Thomas F Russell; *Multilevel and Algebraic Iterative Methods in Large-Scale Computation*; (DMS-9312752 A001); $150,000; 12 months. (Joint support with the Computational Mathematics Program and the Applied Mathematics Program)

The project continues to develop numerical methods for solving problems of flows in porous media and to develop and analyze fast algorithms for partial differential equations, for computational fluid dynamics, and for several linear algebra problems. Specifically, the problems are: (a) develop fast parallel numerical methods for the solution of the Boltzmann equation used to model the transport of neutral and charged particles in 1 and 3 spatial dimensions; (b) develop multilevel zonal techniques for large scale computational fluid dynamics applications on parallel computers; (c) study discretization and solution techniques for fluid flows in porous media that involve complex geometry with heterogeneous material properties; (d) develop a new methodology for the solution of systems of partial differential equations by introducing new dependent variables and forming a least-squares functional. In each case, the work exploits and extends multi-level computational techniques. These projects are focused on important applications, such as calculating radiation doses for cancer treatment, ion implantation for semiconductor development, global weather modeling, fluid flow over airfoils and through rocket nozzles, oil recovery and contaminant transport in subsurface water supplies. They reflect the growing recognition that effective numerical modeling of physical phenomena involves several stages — formulation of the mathematical model, transforming the model into a discrete problem, and developing algorithms for the numerical solution of the discrete problem on advanced computers — none of which should be attempted without consideration for the others. Each project examines all components of the process, reformulating the model and discretization when necessary to yield discrete problems that can be efficiently solved numerically on parallel computers.

College of William and Mary; Roy Mathias; *Numerical Linear Algebra: Accuracy and Parallelism*; (DMS-9504795 A000); $62,000; 36 months. (Joint support with the Computational Mathematics Program and the Applied Mathematics Program)

The project studies the accuracy of parallel algorithms for finding the eigenvalues and eigenvectors of linear systems and develops efficient parallel algorithms for eigenvalue problems, especially the nonsymmetric case. The first part of the project focuses on analysing the accuracy of parallel algorithms — in particular (1) parallel prefix type algorithms (2) Jacobi algorithms for the (possibly generalized) symmetric eigenvalue and singular value problems (3) implementations of the Hessenberg QR algorithm. The question of accuracy is important, though little work has been done on it, because some parallel algorithms can be much less accurate than the corresponding serial algorithm — so much so that the results that they produce are meaningless. The second part of the project seeks efficient parallel algorithms for the nonsymmetric eigenvalue problem and to improve the efficiency of the parallel algorithms for the symmetric eigenvalue problem. The nonsymmetric case is especially important as there is no algorithm for this problem that can properly exploit the capabilities of a parallel computer. Parallel algorithms are widely used and studied because they allow one to solve a computational problem in much less time than if one were to use a serial algorithm. As parallel computing becomes increasing common it is important to have parallel algorithms that are both accurate and efficient. The goal of this project is to provide such algorithms for problems in numerical linear algebra. Eigenproblems arise naturally in every area of science and technology, so effective algorithms to solve them have broad impact.

North Carolina State University – Raleigh; Carl D Meyer and William J Stewart; *Computational Methods in Markov Chains*; (CCR-9413309 A000); $70,969; 12 months.

This project emphasizes practical as well as theoretical aspects surrounding the application and implementation of algorithms for computing stationary probabilities of discrete Markov chains. Special attention is devoted to applications in which discrete models are used to understand and analyze the dynamics of large systems comprised of a collection of loosely coupled subsystems such as in the study of queuing models and networks, telecommunications, computer performance evaluation, stochastic automata networks, and economic modeling and forecasting. Algorithmic facets concern the development and analysis of parallel multilevel methods based on aggregation/disaggregation techniques—both direct and iterative—and some of these techniques are applied to problems involving stochastic automata networks. An architectural aspect involves the identification of features of vector and parallel computers that are best suited for implementing Markov chain algorithms. Theoretical components involve studying stability properties of Markov chains. These ideas are then used to generate error analyses aimed at understanding the convergence and stability properties of multilevel aggregation/disaggregation algorithms.

Texas A&M University; Paul Nelson, Marvin L Adams, and G. Donald Allen; *Novel Computational Approaches to the Transport Equation*; (CCR-9302782 A001); $105,660; 12 months. (Joint support with the Computational Engineering Program and the Computational Mathematics Program)

This project is directed toward computational solution of the linear particle transport equation, which usually is termed simply the "transport equation." This equation historically has provided a major challenge to the state-of-the-art computer hardware available at any given time. More specifically, the project is directed toward spatial approximations to this equation, because new approaches and better basic understanding in this area seem essential to permit the solution of the transport equation in the complex material arrangements underlying some of the emerging applications of this equation (e.g., identification of underground waste locations for environmental restoration). A certain abstract model (CLOF methods) of one-dimensional spatial approximations in particle transport is being extended and applied, as follows: a massively parallel code is being developed for a general class of one-dimensional spatial approximations; the model is being extended to multiple (two or more) spatial dimensions; a code that permits computational determination of the order of accuracy of an arbitrary two-dimensional CLOF is being developed; the CLOF methods that have the very desirable property of satisfying the diffusion limit are being characterized. The corner-balance method, which is a novel spatial approximation that seems to enjoy several properties that are highly desirable for multidimensional calculations, is being extended to the three-dimensional setting, initially for parallelepiped cells, and subsequently for meshes composed of cells that are general (convex) polyhedra.

University of Maryland – College Park; Dianne P O'Leary and Gilbert W Stewart; *Numerical Methods for Ill-Posed Problems and Markov Chains*; (CCR-9503126 A000); $71,443; 12 months. (Joint support with the Computational Mathematics Program and the Applied Mathematics Program)

This project concerns two topics in numerical linear algebra: the numerical treatment of Markov chains and regularization of ill-posed linear systems. The topics share common features: singular or nearly singular matrices; use of iterative methods for large-scale problems; interesting problems in matrix perturbation; and connections with infinite dimensional problems. The computation of the steady-state vector of a Markov chain as well as other important quantities are being investigated. In particular, algorithms are being developed and analyzed for calculating mean first passage times and for computing the recurrence matrix of M/G/1 type queues. In addition aggregation methods with overlapping blocks and the behavior of chains with sluggish transients are being considered. When ill-posed problems are discretized they result in ill-conditioned linear systems which must be regularized to yield accurate solutions. There are three main goals in this work. The first is to prove the folk theorem that if the components of the data vector with respect to the singular vectors decay sufficiently fast then the conjugate gradient iteration will produce a regularizing set of solutions. The second is to treat problems with errors in the matrix by a regularized total-least-squares approach. The third is to further understand preconditioning strategies for iterative solution methods.

University of California – San Diego; Maria E Ong; *Numerical Methods for the Nonlinear Eigenvalue Problems in High Performance Materials Design*; (CCR-9403864 A000); $49,054; 12 months.

The objective of this project is to develop adaptive numerical methods for the first principles prediction of the properties of technologically important materials. These materials may be characterized as having complex structures and compositions, large numbers of particles (> 100) and little or no symmetry. The methods being investigated include a suite of iterative, acceleration, and minimization schemes for the nonlinear eigenvalue problem and accompanying elliptic problem arising in first principles prediction of material properties. This suite includes the eigenvalue iterative methods of Rayleigh-Ritz and Longsine and McCormick; minimization methods such us conjugate gradient, steepest descent, and the trace minimization method by Sameh and Wisniewski; and multilevel methods such as multigrid and fast multipole method. These methods are being used with adaptive grid to exploit the underlying dynamical, localized structure inherent in electronic wave functions. Modern parallel architectures are being used to reduce the computational time and memory costs. The various components of this project are being developed through the close collaboration of researchers from chemistry, physics, computer science, and numerical analysis.

University of California – Los Angeles; Stanley J Osher and

Bjorn Engquist; *Development, Analysis, and Applications for Numerical Methods for Nonlinear Partial Differential Equations*; (DMS-9404942 A001); $125,000; 12 months. (Joint support with the Computational Mathematics Program and the Applied Mathematics Program)

The project studies the development, analysis, and applications of numerical methods for nonlinear partial differential equations. The three main topics addressed are: (1) high resolution methods, including shock capturing, front capturing, numerical homogenization, and particle methods, (2) multiscale analysis applied to these and other related problems, and (3) fast methods for linear evolution equations based on multiscale analysis and high frequency asymptotics. Engineering and physical applications studied include combustion, fluid dynamics, crystal growth, Stefan problems, microwave scattering, and reacting gases. These innovative numerical methods are used to simulate real world problems in the areas of aeronautics, oil recovery, materials science, and environmental science. Transition to industrial and military application is made in the above areas, as well as in low observables, semiconductor device modelling, and shape recognition. These methods are applicable wherever the phenomena to be studied have sharp changes of state variables or are beyond the resolving capabilities of standard methods.

University of Minnesota – Twin Cities; Haesun Park and J. Ben Rosen; *Solution of Structured Total Least Norm and Parameter Estimation Problems*; (CCR-9509085 A000); $70,306; 12 months. (Joint support with the Computational Mathematics Program)

A solution to an over determined linear system, where there may be errors in both the data matrix and the target vector, is required in many important applications in sciences and engineering. Recently, a new technique called Structured Total Least Norm (STLN) has been developed for obtaining the solution that preserves any affine structure, after the data are perturbed to account for the errors. It also permits the error to be minimized in various norms. The STLN algorithm is being investigated and developed into an efficient and practical solution method for many applications. Its computational performance is being studied and a more complete convergence theory is under development. Significant algorithmic and computational improvements are being made in order to efficiently handle large-scale problems and special structures. A particular study is being conducted to apply the STLN method to the model reduction by Hankel norm approximation problem. The effect of different norms are being explored. The STLN algorithm is being extended to solve more general problems where the structured matrix is a differentiable function of parameters to be estimated, and its performance is to be compared to other parameter estimation methods such as Prony's method.

University of Minnesota – Twin Cities; Linda Petzold, Robert T Tranquillo, and J. Ben Rosen; *Multi-Disciplinary Challenge (MDC) Award: A High-Performance Problem-Solving Environment for Optimization and Control of Chemical and Biological Processes*; (CCR-9527151 A000); $550,000; 12 months.

The primary goal of this research is the development of a high-performance problem solving environment (PSE) for the optimization and control of chemical and biological processes, with initial emphasis on bioengineering applications. The optimization and control of such processes requires the repetitive solution of time-dependent partial differential equations (PDEs) in two or three spatial dimensions. The computational requirements of this problem, which must be solved interactively, can only be met by the use of massively parallel computers. Such a comprehensive and powerful PSE does not currently exist, and its development presents significant computational and computer science challenges. The initial application is the design and optimization of a small diameter bioartificial artery. Over 600,000 surgical procedures for blood vessel replacement are conducted in the U.S. annually, many involving synthetic polymer substitutes for small diameter blood vessels that fail due to lack of biocompatability, which is not an issue for bioartificial arteries. A PDE model based on continuum mechanical theory that describes the distribution of cells, fibers, and stresses in a tissue will be used to simulate the evolving compaction of a bioartificial artery. Optimization of the ultimate properties of the bioartificial artery is sought, in particular the ability to withstand pulsatile arterial pressure. PDE systems of a similar mathematical structure commonly arise as models for chemical processes with a need for their control and optimization. The project includes collaboration with and input from scientists and engineers at several industrial and government laboratories with applications in chemical processing. To optimize or control a process described by PDEs, the original time interval is divided into subintervals in a multiple- shooting type approach. The PDEs on each subinterval are discretized in space via parallel adaptive finite el ement methods to give a large system of differential algebraic equations (DAEs). Parameters or control variables are then optimized, subject to state and control variable and continuity constraints (equality and inequality) using large-scale nonlinear programming techniques. Extensive knowledge and research experience in adaptive methods for PDEs, DAEs, large-scale optimization, parallel computing, computing environments, and chemical and biological processes, are required to successfully develop such a PSE. The reaerch team members cover this broad range of required expertise, and have a successful record of collaboration with each other.

Old Dominion University ; Alex Pothen; *Parallel Sparse Matrix Computations*; (CCR-9412698 A000); $50,000; 12 months.

This project investigates the design, implementation, and analysis of algorithms for several problems that arise in the solution of large, sparse systems of equations and least squares problems on high-performance parallel computers. The irregular nature of the memory access required by sparse matrix algorithms makes good performance difficult to achieve. Innovative algorithmic approaches capable of better exploiting concurrency than the traditional sequential approaches, and careful implementations that exploit the memory hierarchy are essential to obtain good performance. The following problems are being investigated: (1) An algebraic approach to the partitioning problem that arises in partitioning data and computation on parallel computers, and in computing nested dissection orderings, (2) The problem of reordering sparse matrices to minimize profile with applications to computing incomplete factorization preconditioners (3) The product-form-inverse approach to the solution of sparse triangular systems on parallel computers, (4) The solution of rank-deficient least-squares problems on sequential and parallel computers.

Purdue University; John R Rice; ***ARPA-NSF Workshop: Scalable Scientific Software Libraries and Problem Solving Environments, Purdue University September 25-27, l995*****; (CCR-9523243 A000); $5,000; 12 months.**

This workshop addressed issues in building problem solving environments (PSEs) for partial differential equation (PDE) based applications and, more concretely, initiating a development of a set of common community standards for the components of scaleable PDE libraries. There is no natural forum for establishing such standards and yet they are essential to progress in building PSEs for PDE based applications. The size and complexity of these software systems require that builders be able to use components developed by other groups. The results of this workshop are of three types: (1) A proceedings which compiles the material presented at the workshop, (2) a workshop overview paper to be submitted to IEEE Computational Science and Engineering, and (3) A series of smaller follow-on meetings of a group of five to ten people who will specify, analyze, and propose community standards for components of scalable PDE libraries. These standards, will build on existing standards from sub-areas such as linear algebra (ScaLAPAK) and parallel computing (e.g., HPF, MPI).

University of Texas – Austin; Gregory J Rodin, J. Tinsley Oden, Robert A van de Geijn, and James C Browne; ***Application of High Performance Computational Methods to Micromechanical Characteristics of Composite Material*****; (ECS-9422707 A000); $422,825; 12 months. (Joint support with the New Technologies Program, the Software Engineering Program, the Operating Systems and Systems Software Program, the Computational Engineering Program, and the Solid Mechanics Program)**

Design of composite materials to have desired properties is a task of great engineering significance. Presently this is usually accomplished through trial and error laboratory synthesis and ad hoc analysis with the result that non-optimal design is commonplace. The dramatic increase in computational power available for mathematical modeling and simulation raises the possibility that computationally-based design can play a significant and complementary role to laboratory development of composite materials, as has been the case in other engineering design problems. The computational problem is to determine the overall properties (not necessarily linear elastic) of the composite material from the constituent properties. The goal of this research is to create a toolbox of computational components with which engineers can design and analyze composite materials directly form the microstructural level. The approach taken is to adapt the emerging methods for high performance parallel computation, being developed for computational modeling in other domains, to micromechanical analysis of composite materials. The application of large-scale computation to this calls of problems has been impeded by the fact that neither available computation power nor available computational methods were adequate for realistic micromechanical models. The methods to be adapted in this project are: (i) parallel adaptive finite element and boundary element methods for computational fluide dynamics and acoustics, and (ii) parallel fast multipole methods emerging form many-particle dynamics. The most significant properties of these methods are: Superalgebraic convergence rates, permitting effective simulations with models requiring a minimum computational effort to achieve acceptable accuracy's. Amenability to common infrastructure for efficient parallel implementation. Natural applicability to micromechanical modeling of composite materials since they perform similar roles in their current domains. The methods are complementary in their domains of application to composite materials. The development of the methods and of the toolbox will be empirical and example driven.

Carnegie Mellon University; Armistead G Russell, Peter A Steenkiste, Bernd Bruegge, and Gregory J McRae; ***A Distributed Computational System for Large Scale Environmental Modeling*****; (CCR-9217365 A005, A006); $156,250; 0 months. (Joint support with the EPA-DIST COMP SYS FOR LARGE SC Program)**

A premise of this Grand Challenge Application project is that high performance computing environments and numerical experimentation play vital roles both in unraveling the complex physics and chemistry occurring in the environment, but also in shaping the design of cost effective public policies. Distributed heterogeneous computing systems offer the potential to revolutionize the current approach to environmental modeling. Research is carried out to improve the models, their mapping onto advanced architectures, and to create a flexible software environment that enbables more widespread use of the tools.

University of Minnesota – Twin Cities; Youcef Saad; ***CS&E Postdoctoral Associate: Parallel Iterative Methods and Preconditioners for the Large, Sparse, Symmetric Eigenvalue Problem*****; (ASC-9504038 A000); $46,200; 24 months. (Joint support with the New Technologies Program)**

The numerical solution of the large, sparse, symmetric eigenvalue problem is required by many scientific and engineering applications, such as electronic structure calculations. Iterative methods, the only means of meeting these demands, are faced with two challenges. The first involves degenerate or pathologically close eigenvalues, and the second involves matrices of very large size that may not stored. Parallel computing and preconditioning are powerful ways for improving the performance of iterative methods. This proposal has three major goals. First, to extend the parallel preconditioned eigenvalue methods that are used in atomic structure calculations to the complex molecular structure calculations in solid state physics. Second, to extend the existing eigenvalue codes to solve for large number of eigenvalues of very large matrices. Third, to explore further the eigenvalue preconditioning, with application to molecular structure matrices resulting from finite difference/element discretization techniques. Preconditioning for large matrices that cannot be stored are also being examined. Finally, work on domain decomposition preconditioners is continued on both the aforementioned application and on arbitrary matrices. Domain partitioning ideas is being tested in combination with a coarse solve correction on a properly chosen small system. The aggregation/disaggregation technique is being investigated for creating the small system.

University of Minnesota – Twin Cities; Youcef Saad; ***Massively Parallel Preconditioners for Krylov Subspace Methods*****; (CCR-9214116 A002); $59,737; 12 months.**

The goal of this research is to investigate highly parallel preconditioning techniques for solving general large sparse linear systems of equations. Of particular interest are linear systems that arise from the discretization of partial differential equations on unstructured grids. The investigation focuses on efficient preconditioners which scale well when the number of processors is very large. In this situation, the standard incomplete factorization preconditioners are not satisfactory. The project investigates a number of non-standard alternatives which emphasize approximations based on "high level of accuracy." These are similar to ILU factorizations with high level of fill-in. Many of the highly parallel preconditioners, suffer from the disadvantage that they entail a larger number of iterations than standard preconditioners to achieve convergence. This often outweighs any potential gains arising from the higher degree of parallelism. However, recent experience suggests that increasing the accuracy of the preconditioner is a good strategy for achieving faster execution by reducing the number of iterations. The use of multi-coloring techniques is also investigated.

University of California – Berkeley; James A Sethian and Alexandre J Chorin; ***Computational Techniques from Geometry and Statistical Physics Applied to Fluid Mechanics and Interface Problems*****; (DMS-9504950 A000); $210,413; 12 months. (Joint support with the Computational Mathematics Program and the Applied Mathematics Program)**

This project studies the motion of singularities in solutions of differential equations, in particular, the motion of interfaces as described by level-set methods and applied to problems in interface motion, and the motion of vortices in three space dimensions, as described by vortex methods and other Lagrangian techniques. The interface techniques exploit Hamilton-Jacobi methodology coupled to upwind schemes for hyperbolic solvers; new work focuses on developing fast methods, methods for multiple interfaces, and the incorporation of effects of visibility, surface diffusion, and reflection/re-emission in surface profile motion. The vortex motion through Lagrangian methods develops machinery from renormalization methods and polymer analysis from statistical physics applied to fluid phenomena through linkage with Shenoy-Williams methodology, and Kosterlitz-Thouless formulations. Methods are being developed to follow the motion of interfaces and vortices. Such problems arise in flows of materials, for instance, and whenever the places where objects or materials meet or end change with time. These are common situations throughout science and engineering. The work is applied to a number of areas. In etching, deposition, and lithography in the manufacture of microelectronic components, the work is used to analyze process steps leading to higher yield and efficiency of electronic devices. In image enhancement, segmentation, and recognition applied to medical imaging, the work leads towards automatic software for recognizing cardiac data in CT and MRI scans. In grid generation, the techniques are used to develop new techniques for building grids around complex bodies, as required in aircraft and engine design. The Lagrangian and vortex particle work focuses on generation of large turbulent structures in wakes, motions of polymers in superfluids, and fundamentals of superconductivity.

Rensselaer Polytechnic Institute; Robert L Spilker, Mark H Holmes, Boleslaw K Szymanski, Mark S Shephard, and Joseph E Flaherty; ***Understanding Human Joint Mechanics through Advanced Computational Models*****; (DMS-9318184 A003); $468,000; 12 months. (Joint support with the Bio-**

engineering Program, the New Technologies Program, and the Computational Mathematics Program)

The objective of this research is to develop and demonstrate the capability for predicting, by computer simulation the ground motion of large basins during strong earthquakes, and to use this capability to study the seismic response of the Greater Los Angeles Basin. The research seeks to: (1) Develop three-dimensional models of large-scale, heterogeneous basins that take into account earthquake source, propagation path, and site conditions; (2) Develop nonlinear models for sedimentary basins that experience sufficiently strong ground motion; (3) Develop unstructured mesh methods and associated fast parallel solvers, enabling the study of much larger basins; (4) Develop software tools for the automatic mapping of the computations associated with large unstructured mesh problems on parallel computers; (5) Characterize the computation and communication requirements of unstructured mesh problems, and make a set of recommendations for the design of future parallel systems. While the work is motivated by an interest in gaining a better understanding of strong seismic motion in large basins, the algorithms and software tools developed will be applicable to a wide range of applications that require unstructured meshes.

University of Utah; Frank Stenger and Kris Sikorski; ***Sinc Algorithm Development and Studies*****; (CCR-9307602 A001); $70,101; 12 months.**

This project investigates SINC methods for ODES. The following tasks are undertaken; (1) develop a SINC ODE-IVP (sequential and/or parallel) program package for solving ordinary differential equation initial value problems, (2) develop a (sequential and/or parallel) program package to evaluate multidimensional convolution integrals, (3) write a program package which uses the Maple program to reduce a partial differential or integral equation to a system of algebraic equations, based on SINC derivative and/or SINC convolution collocation, (4) write program packages, based on SINC derivative and/or SINC convolution collocation, to solve problems which are important for ongoing research at the University of Utah (the forward problem Maxwell equations, with variable permeability and permittivity, but with constant conductivity; the solution, based on SINC convolution collocation, of the integral equation formulation of a scalar conservation law problem in two and three dimensions), and (5) comparison studies of the complexity and stability of SINC and classical methods, especially in areas in which one can expect SINC methods to have advantages over classical methods, such as for problems with singularities, problems over unbounded regions, boundary layer problems, stiff problems, and computationally intensive problems such as the solution of the above cited Maxwell equations.

North Carolina State University – Raleigh; William J Stewart and Carl D Meyer; ***A Workshop on the Numerical Solution of Markov Chains, January 16–18, 1995, North Carolina State University, Raleigh, North Carolina*****; (CCR-9413252 A000); $10,000; 12 months. (Joint support with the Computational Mathematics Program)**

This grant supported a workshop on Numerical Solution of Markov Chains. The area is of current high research activity and wide applicability. The workshop brought together three groups of researchers working in this field: applied probabilists, numerical analysts, and system engineers. The goals of the workshop included:

- To foster co-operation among diverse researchers, to minimize unnecessary duplication and to identify new long- term research objectives.
- To bring up-to-date and to inform researchers who work in one branch of this area, the work being undertaken in different areas.
- To produce a comprehensive set of proceedings that will become a significant reference work.
- To launch a repository of numerical examples that arise in Markov chain applications, and to couple it with sparse matrix manipulation procedures and well-tested and robust numerical solution methods.

University of Minnesota – Twin Cities; Michael R Taaffe and Bruce Schmeiser; ***Correlated Decomposition for Analyzing Dynamic Stochastic Systems*****; (DMI-9300058 A002); $142,400; 12 months. (Joint support with the Operation Research Program and the Production Systems Program)**

This research is concurrent with creating methodology and software for efficiently analyzing models of manufacturing systems, including complexities such as assembly, blocking, and time dependence. Efficient analysis is obtained by combining the speed and efficiency of queueing network approximations with the details and generality of computer simulation experimentation. The combined approach, which is referred to as Correlated-Decomposition Approximation and Simulation (CDAS), allows the strengths and weaknesses of these two methodologies to complement each other. The approximations and simulation work together by using the approximations as control varieties and the newly developed more general biased-control varieties, for the simulation. The goal is to improve analysis efficiency by two or three orders of magnitude compared to ordinary simulation experiments. The combined CDAS methodology analyzes the behavior of large complex manufacturing systems in a matter of seconds or minutes rather than the hours or days that simulation alone can require and to do so with accuracy beyond that possible in present queueing network approximation software.

Columbia University; Joseph F Traub; *Average Case and Probabilistic Setting of Information-Based Complexity*; (CCR-9420543 A000); $148,056; 12 months.

Problems with only partial or contaminated information arise in many disciplines: computer science, physics and chemistry, control theory, statistics, prediction and estimation, scientific and engineering computation, geophysics, decision theory, and finance. Furthermore, this information is often expensive to obtain. The goal of information-based complexity is to create a computational complexity theory for problems with partial, contaminated, and priced information, and to apply the results to solving specific problems in varied disciplines. The prime foci of this project are the following: (1) Breaking Intractability: Many problems in science, engineering, and even finance, deal with functions that have a large number, d, of variables. However, typical multivariate problems are intractable in the worst case deterministic setting. The only way to break intractability is to weaken the assurance by switching to another setting. Randomized, average case, and probabilistic settings continue to be studied. In particular, it has been proven that multivariate integration and approximation are both strongly tractable on the average. The proof is non- constructive; the problem of how to sample in d dimensions to achieve strong tractability is being addressed. (2) Software Development and Testing: Theoretical investigations have led to algorithms for important problems such as high dimensional integration. To make these methods widely available, software is being developed and tested. Since these methods contain a large amount of inherent parallelism, the implementation is being done on a workstation network. Testing is also planned on parallel computers. Real-world problems are used for testing. (3) Probabilistic Complexity of Piece-Wise Smooth Functions: Piece-wise smooth functions arise in diverse areas of science and technology such as computer vision, image and signal processing, scientific computation, meteorology, seismology, and to mography. Because of negative results of the worst-case setting these problems are being studied in the probabilistic setting. New algorithms for integration, approximation, and detection of singular points are being studied and implemented.

Cornell University; Lloyd N Trefethen; *Non-Normal Matrices and Operators: Analysis, Computations, Applications*; (DMS-9500975 A000); $96,500; 12 months. (Joint support with the Computational Mathematics Program and the Applied Mathematics Program)

The project concerns problems involving highly non-normal matrices and operators. Approximately speaking, this means matrices and operators whose eigenvectors or eigenfunctions are far from orthogonal. Most matrices and operators that arise in applications are normal or close to normal, but the highly non-normal cases constitute an important minority, one that has been poorly handled by traditional methods based on eigenvalues. The emphasis of this project is on methods that avoid the use of eigenvalues. Some of these make use instead of certain sets in the complex plane known as pseudospectra, defined in terms of perturbations of the spectrum or equivalently as regions bounded by level curves of the norm of the resolvent. The applications investigated fall in three areas: numerical solution of non-self-adjoint partial differential equations; iterative solution of large-scale matrix problems; and fluid dynamics, specifically hydrodynamic stability and transition to turbulence. This work is connected with some major ongoing developments in science and engineering. One is a basic change in the prevailing view of how fluid flows become unstable and eventually turbulent, with potential applications across many branches of mechanical, aeronautical, and civil engineering as well as in meteorology, geophysics, and other scientific fields. A second, less accessible to the public but still of great importance, is the great shift underway in computational science from "direct" to faster "iterative" methods for solving large-scale linear algebra problems.

Carnegie Mellon University; Noel J Walkington; *Construction and Analysis of Algorithms for Degenerate Variational and Parabolic Problems*; (DMS-9504492 A000); $67,000; 36 months. (Joint support with the Computational Mathematics Program and the Applied Mathematics Program)

This project investigates physical problems involving phase changes and their numerical approximation. In general these problems exhibit one of two distinct traits; either the solutions take on the character of a free boundary problem where the unknown boundary separates the phases, or the phases are finely interspersed. The former are modeled by degenerate parabolic equations. While the theory for these equations is well developed, this is not the case with the discrete theory for their numerical approximation. For example, optimal rates have only recently been established for convergence of the classical Stefan problem in a dual Sobolev space; however, rates of convergence of the energy in the space of integrable functions is still an open question. Even less is known about approximations of the mean curvature equation that arises, for example, when the interface between the phases has more structure. The project also studies the approximation of problems that exhibit fine phase mixtures. Because these problems involve structures that are much finer than any feasible mesh, the research utilizes the recent theory of Young measures to characterize the fine scale behavior. This theory shows that the fine scale behavior is far from random and in many cases can be characterized by a the (macroscopic) Young measure. The project studies and analyzes algorithms that approximate the Young measure. The projec also develops efficient ways to computationally model problems arising in the environmental and material sciences. One interesting feature of these problems is that they often exhibit interfaces where different materials meet. For example, when modeling the spread of pollutants, the single most important quantity is the location and motion of the interface between the pollutant and the clean environment. Problems in the material sciences often involve very fine scal e phenomena involving interfaces between different phases of the same material. This phenomenon is ubiquitous, being observable, for example, in most metals. However, the fine scales also present many obstacles when analyzing such materials. The projectr develops the computational tools to circumvent these problems, providing another step towards the automation of the design and development of modern (and traditional) materials.

Fordham University; Arthur G Werschulz; ***Complexity of Differential and Integral Equations*****; (CCR-9500850 A000); $77,073; 36 months.**

This project continues investigation of the computational complexity of differential and integral equations. New problems to be studied include the following: (1) Problems with singular data. Special attention is paid to problems on domains having corner singularities, problems whose coefficient data has known singularities, and problems for which the forcing function has a singularity of a given type. (2) Exterior problems. The research concentrates on the Helmholtz problem on exterior domains, which arise in scattering theory. (3) Further work on mixed derivative spaces. The research concentrates on problems, as well as the possible optimality of finite element methods. (4) Stochastic differential equations. These problems arise in many areas, such as science, engineering, and finance. Nothing is known about their complexity. The complexity of optimal algorithms for such problems is being studied.

New York University; Olof B Widlund; ***Iterative Substructuring Methods for Elliptic Problems and Related Algorithms*****; (CCR-9503408 A000); $70,000; 12 months.**

The development of numerical methods for large algebraic systems is central in the development of efficient codes for computational fluid dynamics, elasticity, and other core problems of continuum mechanics. Many other tasks in such codes parallelize relatively easily. The importance of the algebraic system solvers is therefore increasing with the appearance of parallel and distributed computing systems, with a substantial number of fast processors, each with relatively large memory. The development of improved methods will, together with more powerful computer systems, make it possible to carry out simulations in three dimensions, with quite high resolution, relatively easily. Work will continue in developing iterative substructuring and other domain decomposition methods for increasingly difficult elliptic problems. Domain decomposition algorithms are iterative methods, often of conjugate gradient type, for the parallel solution of the large linear, or nonlinear, systems of algebraic equations that arise when partial differential equations are discretized by finite elements, finite differences, or spectral methods. In each iteration step, local problems representing the restriction of the original problem to a potentially large number of subregions are solved approximately. The subregions, which can be allocated to individual processors of a parallel computer, form a decomposition of the entire domain of the problem. In addition, the inclusion of a coarse subproblem often substantially increases the efficiency of the preconditioner. In this study, which combines mathematical analysis with the design and numerical testing of algorithms, a special emphasis is on the study of spectral elements and other high order finite element methods, on nonconforming methods such as the mortar finite elements, and on the difficulties which are related to distorted subregions or elements.

University of Texas – Austin; David M Young and David R Kincaid; ***Interative Algorithms and Software for Parallel Architectures for Partial Differential Equations*****; (CCR-9504954 A000); $56,371; 12 months.**

The objectives of this project are (1) to carry out research on iterative algorithms for solving large sparse systems of linear algebraic equations with emphasis on systems arising from problems involving partial differential equations and on the use of parallel computers, (2) to develop research-oriented prototype software based on the algorithms, and (3) to test the algorithms and software on a range of problems. Among the algorithms to be considered are parallel alternating-type methods, periodically generated iterative methods, rational iterative methods, and iterative methods for solving large sparse nonsymmetric linear systems.

Pennsylvania State University – University Park; Hongyuan Zha; ***Research Initiation Award (RIA): The Canonical Correlations: Numerical Algorithms and Extensions*****; (CCR-9308399 A003); $22,447; 12 months.**

The goal of this research is to carry out the perturbation analysis of structured (e.g.Toeplitz) matrix pairs and to analyze the convergence behavior of the numerical algorithm in connection with constructing efficient preconditioners. Numerical algorithms are developed for updating and downdating problems associated with canonical correlations when data points are added or deleted. Theories and algorithms are developed for the following extensions of canonical correlations: canonical correlations with a general bilinear form, canonical correlations with linear equality constraints, canonical correlations of several data sets. This research is expected to yield new concepts in matrix decompositions and numerical linear algebra and statistical computation, and facilitate and further spread the use of canonical correlation analysis in the general scientific community.

University of Texas – San Antonio; Xiaodong Zhang; *Research at Undergraduate Institutions (RUI): High Performance Parallel/Distributed Computing for Numerical Algorithms, Software and Scientific Applications*; (CCR-9400719 A000); $66,815; 24 months.

This project focuses on three important problem areas in high performance parallel/distributed computing: 1) designing, analyzing, implementing and testing several groups of structured methods for solutions of large sparse nonlinear systems of equations on parallel and distributed systems; 2) applying numerical algorithms to solve large real-world problems; and 3) studying execution patterns of scientific application programs for effective parallel program and architecture design.

Louisiana State University – Baton Rouge; Hong Zhang-Sun; *VPW: Waveform Relaxation Method*; (HRD-9550154 A000); $107,738; 12 months. (Joint support with the Visiting Professorships for Women Program)

The advent of new generation of massively parallel computers has caused previously efficient numerical algorithms to be reexamined. Massively parallel computers are comprised of many hundreds, sometimes thousands of processors. For a numerical algorithm to fully exploit the power of such machines it must be able to be 'decomposed' into largely independent pieces which can be distributed across the available computer processors. The waveform relaxation method is such a method for solving systems of ordinary differential equations and time-dependent partial differential equations. In addition to its advantages in parallel processing, it also allows different integration step sizes to be used for different subsystems, resulting in substantial savings in computation for some applications. The theoretical and experimental studies suggest that the waveform relaxation method has a great potential for developing reliable, scalable efficient parallel algorithms for solving a wide range of differential equations. The objective of this research is to further investigate the nature of the waveform relaxation method, and develop fast scalable parallel algorithms for solving certain type of ordinary differential equations and time-dependent partial differential equations. The long term goal of this research is to make the developed algorithms applicable to real-world computational problems, such as the real time integration of torpedo or missile trajectories, modeling of earthquake effects on buildings, and simulation of fluid-structure interaction. This work will involve the algorithm design, theoretical analysis with a possible focus on the search of optimal convergence rate, and numerical testing on sequential and parallel computers. Interactive activities include: teaching a course at the graduate level on numerical linear algebra, numerical partial differential equation, or on parallel numerical computation; and leading an interdisciplinary research seminar seri es on scientific computation and applications to which both local and national researchers will be invited to participate.

Symbolic and Algebraic Computation

Purdue University ; Chandrajit Bajaj; *Geometric and Solid Modeling with Algebraic Surfaces*; (CCR-9222467 A003); $78,101; 12 months. (Joint support with the Computer Systems Architecture Program)

The numerous approaches in computational geometry have been largely theoretical and deal with discrete and combinatorial structures such as point sets, lines, polygons, polyhedra and at most general arrangement of hyperplanes. This project considers the design and implementation of efficient algorithms for an arbitrary arrangement of algebraic curves and surfaces and specifically compact solids bounded by curved algebraic surface patches. The class of algebraic surfaces, a subset of arbitrary analytic surfaces, provides enough generality to accurately model almost all complex rigid objects. Additionally, algebraic curves and surfaces have compact storage representation and form a class which is complete under all common operations required by a geometric modeling system. Finally, representing physical objects with algebraic surfaces encompasses all prior modeling approaches. The research thrusts of this project are: (1) the design of efficient algorithms for basic operations on algebraic surfaces (these manipulations include intersection, parameterization, Ck-interpolation, and approximation), and (2) the design of efficient algorithms for basic manipulations on solids bounded by algebraic surface patches (these manipulations include: boolean set operations, convex hull, decomposition, convolution, offset, blending, and smoothing operations).

City University of New York – City College; Gilbert Baumslag; *Computational Group Theory*; (DMS-9103098 A005); $260,000; 12 months. (Joint support with the Computational Mathematics Program and the Algebra & Number Theory Program)

The objectives of this research activity are as follows: (1) to develop some very general, all purpose, algorithms to help study groups given by generators and defining relations, (2) to compile computer-generated libraries of examples, references and the like, pertaining to the general subject combinatorial group theory, and (3) to provide a vehicle for the dissemination of new results and advances in the field. In the main, the program that developed is designed to provide information about a wide variety of properties of groups. Combinatorial group theory is important in abstract algebra, and with close connections to topology, logic and wide variety of other disciplines as well. Its study leads to an understanding of structures underlying many aspects of science.

Barnard College; David A Bayer; ***Computational Methods in Algebraic Geometry and Topology*****; (DMS-9501723 A000); $90,000; 36 months. (Joint support with the Computational Mathematics Program and the Algebra & Number Theory Program)**

This project investigates methods for computing in both algebraic geometry and topology. In algebraic geometry the focus is on the connections between toric varieties and integer programming. In topology the focus is on methods to compute on 3-manifolds. The project seeks to use the interplay between topology and algebraic geometry such as the interpretation of the Haken normal surface as a Hilbert basis for a polyhedral cone. Finally a goal is to develop virtual reality software for direct manipulation of 3-manifolds.

University of California – Berkeley; John F Canny; ***A Toolkit for Non-linear Algebra*****; (CCR-9320588 A001); $103,390; 12 months. (Joint support with the Computational Mathematics Program and the Algebra & Number Theory Program)**

This project undertakes the implementation of an algebraic-geometric toolkit, written in C, which can solve systems of equations over the complex numbers, and inequalities over the reals. There are many applications of such a toolkit, since problems from many branches of science and engineering can be formulated using systems of polynomial equations and inequalities. By several well-known theorems, in particular, Tarski's theorem for the reals, it is possible to solve such problems in principle. But the worst case bounds are exponential or doubly-exponential in the number of variables, and no practical system has appeared that can deal with more than a few special cases. On the other hand, systems of polynomials may have a special structure, a kind of sparseness, that implies a complexity (measured by the algebraic degree) much lower than the worst case. Indeed, most of the important applications are of this type. Very recently, algorithms have been developed that can exploit this structure. This realization is a strong motivation for developing the toolkit at this time. In addition, there have been improvements in algorithms for sign determination and symbolic-numeric computation, and it is felt that these methods are now advanced enough to warrant implementation.

California Institute of Technology; K. Mani Chandy, James C Pool, Daniel I Meiron, John H Seinfeld, and Steven E Koonin; ***Multi-Disciplinary Challenge (MDC) Award: Integration of Symbolic Computing with Framework of Classes and Problem-Solving Archetypes*****; (CCR-9527130 A000); $600,000; 12 months.**

The goal of this project is to help scientists and engineers carry out computational tasks more effectively by doing research on:

- The integration of symbolic and numeric computation to facilitate problem specification, exploration and result verification.
- Hierarchies of reusable computational abstractions organized in libraries with well-defined navigational structures.
- Exploiting commercial standards and tools for object-request brokers, compound documents, and collaboration infrastructure.

The project takes a novel approach to problem-solving environments (PSEs). Its focus is on the entire process of problem-solving from initial conception, symbolic specification, solution, visualization, comparison with experimental data, and feed back. The project focuses on problem-solving environments, not merely programming environments. This focus leads to research on reusable abstractions at all levels of problem-solving. Important abstractions include the problem-solving method itself, method-specific abstractions for sequential and parallel program design, reasoning and debugging, performance analysis and tuning, and frameworks for class libraries. PSEs are more useful when they are more specific. However, rather than build one problem- solving environment for one class of user, application domain, programming language and machine, this project aims at the basic research that will enable us to develop tools for building specific PSEs. To use a metaphor, rather than doing research on workbenches we want to do research on machine tools that can be used to build workbenches. Traditional PSEs deal with extending a workstation environment whereas this project is concerned with developing structured collaborative environments for problem-solving. Scientists and engineers collaborate when they solve problems, and they share much more than code. PSEs based on collaboration also provide object-request brokering and compound multimedia document interfaces. Since this vision is both novel and ambitious, a critical aspect of the project is leveraging methods and tools developed for scientific, commercial and home-computing applications.

Wichita State University; Shang-Ching Chou; ***Automated Generation of Human-Readable Proofs in Geometry*****; (CCR-9420857 A000); $68,713; 12 months.**

This project continues investigation of automatic generation of proofs of theorems in geometry. The emphasis is on short and human-readable proofs. For this, the newly discovered area method and new methods based on other geometrical concepts, such as full angles and trigonometric functions, are being developed. Extension of these techniques are being sought to geometric inequalities as well as to non-Euclidean and higher- dimensional geometries. The techniques are being implemented in a system with a sophisticated graphics display.

Northeastern University; Gene Cooperman and Larry A Finkelstein; *Applications of Group Theory to Large Scale Computation*; (CCR-9509783 A000); $66,000; 12 months.

This project addresses computational issues for finite groups that are currently beyond the scope of current algorithms and existing technology. The groups are represented either as permutation groups or as matrix groups defined over finite fields. The questions of interest concern both group theoretic structure and applications of the group theory. A central motivation for the research is the construction of permutation representations for matrix groups defined over finite fields. This is an important part of a large-scale international effort to develop a suite of computational tools for performing matrix group computations. The tools to be developed have application to problems in the physical sciences, engineering, and those parts of mathematics dealing with high dimensional matrix representations of groups. A second research area concerns computational techniques for solving the minimum word problem for finite groups. This problem arises in many contexts, such as routing in interconnection networks and coding theory, and is known to be computationally difficult. The research will lead to new algorithms which use group automorphisms to prune the search tree of possible solutions. A third research area is the development of a software architecture to bring parallel computers to bear on large scale problems in computational group theory, such as the construction of very large matrix and permutation representations. Such as integrated, interactive environment will enable researchers to quickly overcome the initial learning barrier for effective use of parallelism. They will be able to combine readily available networks of workstations at their home site (such as student labs), with an already familiar interactive language, such as GAP or LISP.

University of South Carolina – Columbia; Karel Culik; *Finite Automata Methods in Image Compression and Manipulation*; (CCR-9417384 A000); $65,000; 12 months. (Joint support with the Theory of Computing Program)

A new method for image description, compression, and manipulation based on finite automata is studied. A Weighted Finite Automaton (WFA) computes a real function on 0,1,... n. For n = 2, such a function can be interpreted as the grayscale function specifying an image. The most important application of WFA is the new image-compression method based on the WFA inference algorithm. This method can be classified as a fractal compression method, but it is different and performs considerably better than the previous fractal methods for image compression. It produces an excellent compression size to quality ratio for the widest variety of images. The current image-data compression software performs well; however, it does not reach the full potential of WFA for image compression. One of the main goals of this project is to optimize the compression algorithm to make it faster and to produce better quality regenerated images for the same compression rate. Weighted Finite Transducers (WFT) are a tool for the description and implementation of image transformations. The project is investigating the WFT and their applications, their efficient implementation, and the design of inference algorithms for WFT.

University of California – Berkeley; Richard J Fateman; *Topics in the Representation and Manipulation of Mathematical Knowledge*; (CCR-9214963 A002); $65,000; 12 months.

This project investigates computer technology in support of the representation and manipulation of mathematical notation by the computer. The long-term goal is to produce a consistent and constructive representation of a substantial, useful class of engineering and applied mathematics, driven by the needs of significant applications. Key issues to examine include the use of multiple representations, and the encoding of geometric, algebraic, logical, algorithmic, and physical relations in symbolic mathematical computation. The specific topics to study include: (1) developing new algorithms and representations for manipulation of functions of a complex variable correctly and with some generality (In particular both correct manipulations and proofs in analysis must account for branch cuts.), (2) providing a computing framework for dealing with mathematical derivations, theorem proving, and manipulation, (3) providing a practical approach to a bounded-time version of the zero-equivalence problem for algebraic expressions, and (4) exploring of parallel algorithms for basic polynomial algorithms and pattern-directed transformations.

University of Tennessee – Knoxville; Jay I Frankel; *The Use of Symbolic Computation for Solving Nonlinear and Integro-Differential Equations*; (CCR-9320385 A001); $5,000; 0 months.

The goal of this work is to develop an accurate numerical method which employs symbolic computation for solving linear and nonlinear multivariable integral and integro-differential equations of mathematical physics. When possible, a posteriori (and a priori) error estimates are sought to evaluate the effectiveness and accuracy of the projection methods used for obtaining the numeric solution. Projection methods such as collocation using different sets of basis functions on either a global or local basis are developed to obtain accurate and reliable results. Symbolic computation permits previously insurmountable analytic manipulations to be performed for purposes of (1) developing expansion based solution methods, and (2) establishing error estimates and convergence rates. The major contribution of the investigation are twofold; (1) to exploit the development of symbolic manipulation for augmenting analytic, numeric, and graphic computation in support of solving and analyzing nonlinear integral and integro-differential equations of mathematical physics, and (2) to investigate, extend, and develop the recent formulation of Kumar and Sloan for scientific computation of multivariable Hammerstein-Fredholm equations.

University of Illinois – Urbana; Daniel R Grayson; *A Software System for Algebraic Geometry Research*; (DMS-9210807 A002); $74,850; 12 months. (Joint support with the Computational Mathematics Program and the Algebra & Number Theory Program)

This award supports the development of a computer software system enabling large scale research computing projects dealing with systems of polynomial equations in many variables. The result of the project are a usable and efficient computer program, which executes the Groebner basis algorithm for computing standard bases and syzygies of ideals and modules over polynomial rings. Improvements over the existing program, Macaulay, include the addition of a good programming language for the user, the ability to work over more general coefficient rings, and increased speed of execution. This project is in the general area of commutative algebra and the computer-aided computational aspects of this field. There is a growing interest in using computers to answer theoretical questions in algebra and conversely, algebra is quite useful for the development of algorithms. This project makes use of both the theory and practice of symbolic calculations to solve real problems in commutative algebra.

University of Southern California; Ming-Deh Huang; *Computational Number Theory and Computational Algebraic Geometry*; (CCR-9412383 A000); $64,857; 12 months.

This research explores the rich and potentially fruitful interplay between number theory and algebraic geometry to investigate computational problems in number theory, with emphasis on: discrete logarithms over various groups, which is a fundamental problem of cryptographic significance; polynomial congruences modulo primes, including the univariate and multivariate cases; small nonresidues in finite fields; efficient algorithms for computing with curves over finite fields, with emphasis on fundamental arithmetical problems on curves which are important for applications in computational number theory, cryptography and coding theory; applying the results obtained to public-key cryptography, coding theory, and other areas as well.

University of Southern California; Douglas J Ierardi; *Studies in Computational Algebra and Algebraic Geometry*; (CCR-9402819 A000); $74,780; 24 months.

Ideas from algebraic and arithmetic geometry have contributed to recent advances in symbolic algebraic computation, computational number theory, and in the effective geometry of real semi-algebraic sets. In motion-planning and modeling, the reintroduction of classical methods of elimination theory including multivariate resultants, u- resultants and Chow forms have aided in the design of efficient parallelizable algorithms. In number theory, rational points on abelian varieties defined over finite fields have provided a rich new source of groups with arithmetic properties that can be exploited in the design of new algorithms. This study addresses computational problems for which algebraic and algebro- geometric methods have had significant impact. The research further explores the applications of multivariate resultants to problems involving algebraic curves over finite fields and their Jacobians. These methods have been successfully applied in designing factorization-free algorithms which have achieved order-of-magnitude improvements performance in computing arithmetic properties of curves. Methods of elimination theory that have been used to explore the structure of semi-algebraic sets and to construct solutions to systems of polynomial inequalities are also studied. Such methods have been successfully applied to the design of theoretically efficient solutions to very general problems in solid modeling and algorithmic motion-planning. This research focuses these methods on somewhat more constrained problems from manufacturing and from molecular modeling involving topological polyhedra with low degree surfaces in low dimensional spaces where algebraic tools, together with the basic paradigms of computational geometry, provide a framework for the design of both theoretically efficient and potentially practical algorithms.

Rensselaer Polytechnic Institute; Erich L Kaltofen; *Efficient Computer Algorithms for Symbolic Mathematics*; (CCR-9319776 A001); $72,353; 12 months. (Joint support with the Algebra & Number Theory Program)

This project continues research in design, analysis, and implementation of efficient algorithms for several basic computer algebra problems. The parallel time complexity of solving linear systems with a minimum number of processors is further investigated. New sequential and parallel randomized algorithms for sparse linear systems are explored, and polynomial-time algorithms that make irreducible polynomials factorizable via substitution of the variables by monomials are sought. Another research direction is how to handle imprecise data in the course of symbolic computation. The allowance of floating point coefficients in a symbolic (i.e., parameterized model) is considered crucial for a symbolic approach to real-world problem solving.

In particular, the question of computing in polynomial-time the nearest singular Toeplitz matrix for a given Toeplitz matrix, and the nearest pair of polynomials with a common divisor for a given pair of relatively prime polynomials, is a starting point for the theory of precision-tolerant symbolic computation. Ultimately, the problem of factoring over the complex numbers a minimally perturbed version of an absolutely irreducible curve is attacked. Algorithm implementation is done using the DSC system for distributing a symbolic computation over a network of workstations.

University of Oregon – Eugene; William M Kantor; *Groups, Algorithms, and Geometries*; (DMS-9301308 A002); $65,150; 12 months. (Joint support with the Theory of Computing Program, the Computational Mathematics Program, and the Algebra & Number Theory Program)

This project addresses groups, algorithms and geometries. Probabilistic and asymptotic properties of finite groups are studied: the nature of random elements, or of random subgroups, of a given permutation group. Some results obtained are applied to algorithmic questions concerning permutation groups. The study of polynomial-time and parallel (complexity class NC) group-theoretic algorithms continues. Additional new practical group-theoretic algorithms are obtained, in some cases based on methods developed in polynomial-time situations. All of this work makes detailed use of the classification and properties of finite groups. Some of these algorithms depend on geometric methods. Other geometric projects are continued including investigations into the number of planes, designs, generalized quadrangles, or other geometries, based upon special properties of their automorphism groups. This project is in the general area of finite group theory and the computer-aided computational aspects of this field. There is a growing interest in using computers to answer theoretical questions in algebra and conversely, algebra is quite useful for the development of algorithms. This project makes use of both the theory and practice of symbolic calculations to solve real problems in group theory.

New Mexico State University; Reinhard C Laubenbacher and David R Finston; *Mathematical Sciences REU Site: Computational Algebraic Geometry*; (DMS-9415268 A000); $12,000; 12 months. (Joint support with the Computational Mathematics Program and the Algebra & Number Theory Program)

The purpose is to organizes a five-day symposium on Groebner bases and convex polytopes, featuring a series of ten lectures by Professor Bernd Sturmfels describing some of the central results about Groebner bases of toric ideals and their application to problems in integer programming and statistics. These lectures are complemented by a concurrent contributed paper session. Polynomial equations are important in algebraic geometry and commutative algebra. Moreover, many scientific, economic and engineering problems can be modeled by polynomial equations, and polynomials arise in computational statistics, integer programming, and a variety of other optimization problems. The theory of Groebner bases provides the foundation for many algorithms used in the analysis of such equations. So the theory plays a significant role not just in basic research but also in the solution of problems of strategic interest. Increasingly, this theory is becoming part of the standard curriculum at US universities. Thus, the subject the conference is of interest to students, teachers and researchers in several disciplines, including mathematics, engineering, computer science, and operations research.

University of North Carolina – Chapel Hill; Dinesh Manocha; *Numeric and Symbolic Methods for Polynomial Manipulation*; (CCR-9319957 A001); $64,249; 12 months.

Algorithms for symbolic and numeric manipulation of polynomial systems are needed for basic symbolic, numeric and geometric computations and their application to problems in graphics, geometric modeling, robotics, vision and engineering. This research takes a three-fold approach to these problems using multipolynomial resultants: (1) Develop better algorithms for symbolic resultant computation and solving nonlinear polynomial equations using resultants and matrix computations. Algorithms are being developed in the context of exact arithmetic as well as floating point arithmetic. It involves better formulations of resultants in terms of matrices and determinants and use of symbolic and numeric algorithms making use of the matrix formulation. (2) Specialize these algorithms to applications in computer graphics, geometric modeling and robotics by making use of the specific polynomial systems arising in these applications. (3) Develop a library of routines, ELIMPACK, for symbolic resultant computation and finding roots of polynomial equations (in exact and floating point arithmetic). This package is of great utility to symbolic computation, numerical computation, geometric applications and the engineering community. The results also help in understanding the complexity of geometric problems described in terms of polynomial equations.

University of Georgia; Carl Pomerance, Andrew Granville, and Helmut Maier; *Topics in Analytic and Algorithmic Number Theory*; (DMS-9206784 A003); $92,000; 12 months. (Joint support with the Computational Mathematics Program and the Algebra & Number Theory Program)

This research addresses problems in analytic, computational, and additive number theory. Work continues on integer factoring algorithms, in particular the number field sieve. Size of the coefficients of cyclotomic polynomials and irregularities in the distribution of primes is addressed. Work also occurs on the distributions of the primes as well as sieve theory. This is research in the field of number theory. Number theory starts with the whole numbers and questions such as the divisibility of one whole number by another. It is among the oldest fields of mathematics and it was originally pursued for purely aesthetic reasons. Within the last half century, it has become an essential tool in developing new algorithms for computer science and new error correcting codes for electronics.

University of Delaware; B. David Saunders and Bobby F Caviness; *East Coast Computer Algebra Day, University of Delaware Newark, Delaware, April 8, l995*; (CCR-9505363 A000); $9,880; 6 months.

This meeting was addressed by invited speakers who have made outstanding contributions to the field of computer algebra. The speakers anchored the meeting and helped attract participants from the computer algebra or computational scientific/engineering communities from the eastern half of the US. The invited talks and poster sessions contributed by the community covered the breadth of computer algebra: algorithms, software, and applications. The principle theme of this l995 meeting was applications. The purpose of this meeting was to stimulate interest in and to enhance understanding of the technical aspects of computer algebra, by providing a way for those in the region who are active or interested in becoming more active in computer algebra to meet with each other in an inexpensive and easily accessible way.

Ohio State University; Akos Seress; *Efficient Computation in Finite Groups*; (CCR-9503430 A000); $30,369; 12 months.

This project continues research in the area of efficient manipulation of finite groups and estimation of their parameters. Algorithms for finite groups and their associated Cayley graphs have a wide range of applications in mathematics and computer science. These applications range from problems related to the classification of finite simple groups to the mixing rate of Markov chains, the design of interconnection networks for large interacting arrays of CPU's, the graph isomorphism problem (of relevance to chemical documentation), and group-based cryptography (such as DES). The principal consumers of the expected results will be the areas of computational group theory and the complexity theory of algorithms; but applications arise in the other areas mentioned as well.

North Carolina State University – Raleigh; Michael Singer; *Symbolic Computation and Differential Equations*; (CCR-9322433 A000); $86,558; 36 months.

This project develops symbolic algorithms to determine the algebraic structure of solutions of differential equations. In particular, the research includes the following: (i) Refine and extend algorithms for computing Galois groups of linear differential equations and algorithms for solving these equations in terms of classes of special functions; (ii) Develop algorithms to decide various properties of the Galois group. For example, give an algorithm to calculate the dimension of the group; (iii) Construct linear differential equations with a given Galois group; (iv) Develop improved algorithms to factor linear differential equations; and (v) Find first integrals of nonlinear systems of differential equations.

University of New Mexico; Stanly L Steinberg; *IMACS Applied Computer Algebra Meeting, Albuquerque, NM*; (CCR-9521541 A000); $9,000; 6 months.

IMACS Applied Computer Algebra Meeting, Albuquerque, NM, May 16-19, l995. This meeting focused on the applications of computer algebra systems (CAS) in engineering, applied mathematics, pure mathematics, and education. It was the first international meeting of this type. This meeting was particularly timely because of the great strides made in using deep computer algebra results like the Grobner Basis and quantifier-elimination algorithms and their generalizations to produce significant results in differential equations, in the analysis and implementation of discrete methods for differential equations, to control theory, and to many other areas. The use of computer-algebra techniques is growing rapidly in most if not all engineering and science areas and thus the dissemination of the latest techniques is important and are not covered by disciplinary meetings.

Cornell University; Michael E Stillman; *A Software System for Algebraic Geometry Research*; (DMS-9210805 A002); $75,000; 12 months. (Joint support with the Computational Mathematics Program and the Algebra & Number Theory Program)

This award supports the development of a computer software system enabling large scale research computing projects dealing with systems of polynomial equations in many variables. The result of the project is a usable and efficient computer program, which executes the Groebner basis algorithm for computing standard bases and syzygies of ideals and modules over polynomial rings. Improvements over the existing program, Macaulay, include the addition of a good programming language for the user, the ability to work over more general coefficients rings, and increased speed of execution. This project is in the general area of commutative algebra and the computer-aided computational aspects of this field. There is a growing interest in using computers to answer theoretical questions in algebra and conversely, algebra is quite useful for the development of algorithms. This project makes use of both the theory and practice of symbolic calculations to solve real problems in commutative algebra.

Rutgers University – New Brunswick; Wolmer V Vasconcelos; ***Studies in Commutative Algebra and Its Applications to Computational Algebra*****; (DMS-9500786 A000); $60,000; 12 months. (Joint support with the Computational Mathematics Program and the Algebra & Number Theory Program)**

This project concerns the study of Cohen-Macaulay structures, in algebra, combinatorics, and geometry, and is driven by their wide presence and the opportunities offered in issues of computational complexity. The project investigates invariants of blowup algebras for their role in deciding the property of Cohen-Macaulay; contributes to the ongoing process of algebraization of tangent and secant algebras; studies the role of various measures of complexity in the processing of basic operations of computational algebra; and develops methods and algorithms that facilitate the efficient processing in large scale computations in geometry. This project is in the general area of computational algebra and the computer-aided computational aspects of this field. There is a growing interest in using computers to answer theoretical questions in algebra and conversely, algebra is quite useful for the development of algorithms. This research will not only aid in the development of computer programs in commutative algebra but will influence the development of computer programs in other areas. One aspect of this project concerns the development of a computer program which will solve systems of polynomial equations. This is significant in manufacturing both for modeling and for the development of robots.

Kent State University; Paul S Wang; ***High-Performance and System Integration for Symbolic and Numeric Computation*****; (CCR-9201800 A002, A003); $54,040; 12 months.**

The first goal of this project is to develop and implement parallel algorithms for symbolic polynomial factorization. The past work on "pfactor" is extended, and parallel linear and quadratic p-lifting techniques are investigated. The second goal is to investigate the integration of numeric, symbolic, and graphic techniques. A distributed paradigm is devised to interface loosely coupled scientific and mathematical computation components. The vision is to develop scientific computation systems consisting of multiple autonomous compute servers running on different hosts. Each compute server in such a system supplies a single or a set of related services such as polynomial factorization, solution of linear or nonlinear equations, automatic code generation from symbolic programs, or graphic display of mathematical functions, just to name a few services.

Kent State University; Paul S Wang; ***SymbolicNet – An Internet Information Service for the Symbolic Computation Research Community*****; (CCR-9423696 A000); $23,354; 12 months.**

The project addresses a critical need in the symbolic and algebraic computation (SAC) community: the easy and speedy dissemination and access of research information on the Internet. The Institute for Computational Mathematics (ICM) at Kent State University has been operating a gateway (symbolic@mcs.kent.edu) to the Internet electronic bulletin board for the SAC community for a number of years. This project expands this service with a World-Wide Web server to form an organizational framework for SymbolicNet—a facility to be established that, through the use of WWW, Gopher, FTP, WAIS, automated subscription, and e-mail distribution, will provide a rang of useful information services for the SAC community. Cooperation with appropriate information services at other sites will also be important.

Kent State University; Paul S Wang; ***Efficient Algorithms and System Interface for Scientific Computation*****; (CCR-9503650 A000); $105,000; 24 months.**

This project focuses on three related areas:

(1) No-missing-term p-adic lifting — Establishing a faster algorithm for recovering final results in multivariate polynomial operations such as GCD (Greatest Common Divisor) and factoring. The lifting method is most effective when the polynomials involved are sparse, containing just a few of all possible terms.

(2) Function Evaluation Optimization and Applications — Speeding up the repeated evaluation of functions in closed-form formulas through the application of recurrence relations. Nested recurrences called "chain of recurrences" will be derived by symbolic computation and applied to increase the evaluation speed of formulas at regular intervals. Application in interactive graphical visualization will be made.

(3) Interfacing Distributed Scientific Systems — Seeking to establish an efficient and standardized protocol to connect different autonomous systems for scientific computation. Such a protocol is necessary to build distributed "problem solving environments".

By exploiting sparseness and solving systems of linear equations, the p-adic lifting procedure of item (1) will be investigated. Feasibility will be studied. Algorithms will be specified, implemented and applied. For area (2), automatic generation of chain of recurrences (CR) for functions of one or more variables will be implemented, and tested for speed and effectiveness. The numeric properties of CRs will be studied. The technique will be applied to speed up interactive graphical visualization of mathematical functions. For area (3), an efficient and flexible protocol(called MP) will be designed. Libraries in C will support the protocol.

Yale University; Kenneth M Yip; ***NSF Young Investigator (NYI) Award: Computational Mechanics Workbench*****; (ECS-9357773 A002); $25,000; 12 months. (Joint support with the Knowledge Models and Cognitive Systems Program and the Computational Engineering Program)**

This project develops a category of intelligent computational tools for scientists and engineers. Given a high-level specification of a physical problem in terms of nonlinear partial differential equations, these tools are able to automatically: (1) simplify that equations by asymptotic techniques, (2) prepare numerical simulation experiments for the simplified model, (3) monitor and control the experiments, (4) interpret the results in high-level terms, and (5) derive qualitative predictions form the model by approximate analytical methods.

Temple University; Doron Zeilberger; ***Combinatorics, Special Functions, and Computer Algebra*****; (DMS-9500646 A000); $40,000; 12 months. (Joint support with the Computational Mathematics Program and the Algebra & Number Theory Program)**

This project investigates problems in the areas of algebraic combinatorics, the theory of special functions, and computer algebra. One direction of this project is a continuation of the research program on the use of computer algebra for computerized proofs of identities in combinatorics and the theory of special functions. Other goals of this project include the development of a general theory of permutation statistics, the study of holonomic aspects of combinatorial statistical mechanics, and the extension of methods developed in the principal investigator's recent proof of the alternating sign matrix conjecture to other, still open, problems in this area. Because both special functions and combinatorics are so prevalent in the natural sciences, this research has many potential applications to both science and technology, as well as to pure mathematics. This research is in the general area of combinatorics. Combinatorics attempts to find efficient methods to study how discrete collections of objects can be arranged. The behavior of discrete systems is extremely important to modern communications. For example, the design of large networks, such as those occurring in telephone systems, and the design of algorithms in computer science deal with discrete sets of objects, and this makes use of combinatorial research.

Ohio State University; Feng Zhao; ***Research Initiation Award (RIA): Intelligent Computing in Automating the Design and Control of Complex Physical Systems*****; (CCR-9308639 A001); $5,000; 0 months.**

Computationally simulating complex physical systems in engineering design has become a common practice. Yet most of today's simulations rely on extensive numerical computations. Nonlinear physical systems can exhibit extremely complex behaviors that defy human analysis and pure numerical simulations. The analysis and design for these systems are limited by the available computational power and the system complexities. This research project will develop powerful computer simulation technologies for the analysis and design of nonlinear control systems. Programmable primitives will be developed for constructing simulations and synthesizing high-performance controllers. Hybrid computation will be explored for integrating symbolic and numerical methods with AI reasoning and representation techniques in (1) manipulating and visualizing the dynamics of physical systems based on a phase-space representation, and (2) guiding the execution of numerical computations. The expected results of this research is to expand the scope of what current numerical simulation programs or state-of-the-art knowledge-based systems can do in solving pressing scientific and engineering problems.

Ohio State University; Feng Zhao; ***Intelligent Simulation Methods for Dynamical Systems*****; (CCR-9457802 A001); $100,000; 12 months.**

This project investigates new computational methods for prototyping physical systems with desired dynamical behaviors, with expected applications in design and control engineering. It develops a computational environment for visualizing and manipulating dynamics of physical systems through a combination of numerical and symbolic computations. More specifically, this project studies (1) automated characterization of dynamical systems through analytic and geometric analysis, and (2) techniques for interactive synthesis, optimization, and visualization of dynamics, for example, "computational scissors" that cut-and-paste vector fields and shape the desired dynamical properties (e.g. stability regions) for a complex system that is otherwise difficult to design.

Computational Geometry

Duke University; Pankaj Agarwal; ***NSF Young Investigator (NYI) Award: Geometric Algorithms and Their Applications*****; (CCR-9357814 A003); $32,500; 12 months.**

Computational geometry has provided efficient algorithms for geometric problems in several applied areas including graphics, robotics, CAD, and geographic data processing. The project continues studying these problems and explores new areas where computational geometry can play an important role. Work on problems involving arrangements of surfaces, dynamic data structures, geometric optimization, interaction detection, and multi-dimensional searching is pursued. There is a special emphasis on higher dimensional problems.

Carnegie Mellon University; David Baraff; *Research Initiation Award (RIA): Non-Interpenetrating Rigid Body Simulation*; (CCR-9308353 A002); $22,514; 12 months. (Joint support with the Computer Systems Architecture Program)

The ability to realistically simulate the motion behavior of physical objects has become an area of great importance in science, engineering, training and planning. Realistic simulation requires accurately modeling the behavior and interactions of contacting objects. In particular, it is necessary to be able to simulate the same non-interpenetrating motion that real-world objects undergo. An important subset of physical simulation is simulations where all objects are modeled as being perfectly rigid. The abstraction of a perfectly rigid body, though physically unobtainable, is an excellent and reasonable approximation for many real-world applications in robotics and computer graphics. Even with the rigid-body assumption, simulation is made difficult by the need to deal with complex surface geometries and contact phenomena such as friction. This project aims at extending the capabilities of current physical simulation systems that model contact and collision between systems of rigid bodies and explore practical uses for simulation systems. Specifically, the investigation centers on the development of new geometrical algorithms that allow for simulations with greater levels of geometric complexity, and the extension of computational complexity bounds and algorithms for the problem of contact with friction. This project is also exploring using non-interpenetration constraints to aid in interactive computer-aided design and modeling applications.

Princeton University; Bernard M Chazelle and David P Dobkin; *The Design and Analysis of Geometric Algorithms*; (CCR-9301254 A003); $152,219; 12 months.

The project investigates problems within three broad areas of computational geometry: (1) design and implementation of efficient and robust geometric primitives, (2) algorithmic complexity of multidimensional searching and (3) mathematical tools (e.g. discrepancy theory) for randomized (and derandomized) geometric algorithms. These areas cover the spectrum from practical considerations which arise when implementing and debugging geometric algorithms to theoretical questions arising in algorithm design and lower bound proofs. Tools continue to be built which can ultimately be used to produce and share geometric software.

Middlebury College; Matthew T Dickerson; *Research at Undergraduate Institutions (RUI): Proximity Problems with Applications to Greedy and Minimum Weight Triangulations*; (CCR-9301714 A001); $4,266; 0 months.

This project investigates greedy triangulations and related proximity problems with a specific concern for the development of efficient algorithms. Topics under study include: new algorithms for the greedy triangulation in two and three dimensions; data structures for testing edge-compatibility in higher dimensional triangulations; properties of higher dimensional greedy triangulations; algorithms for near-neighbor enumeration in higher dimensions; and new alternate triangulation methods for approximating the minimum-weight triangulation. Both worst-case and expected-case algorithms are being explored. The primary concern is with sequential algorithms in Euclidean space, but parallel algorithms and other distance metrics may also be investigated. Undergraduate students are involved in the project.

Johns Hopkins University; Michael T Goodrich; *Constructing, Maintaining, and Searching Geometric Structures*; (CCR-9300079 A002); $44,989; 12 months.

This project investigates the construction and maintenance of geometric structures, as well as methods for efficiently searching in such structures. This involves studying known computational geometry problems which are as yet unsolved, new computational geometry problems dealing with the dynamic maintenance of geometric structures, and new computational geometry problems arising from applications in computer graphics and computer vision. The algorithms developed are for sequential and parallel models of computation.

Stanford University; Leonidas Guibas; *Geometric Algorithms and Applications*; (CCR-9215219 A002); $92,456; 12 months.

As the application of computers to the physical world widens, there is an increasing need for computers to deal with the physical attributes of objects, such as their geometry. The relatively young field of Computational Geometry has made impressive strides in providing an algorithmic foundation for the solution to many geometric problems in computer graphics, computer vision, robotics, and many other application areas. This project undertakes research in the design and analysis of geometric algorithms in a variety of areas including Voronoi diagrams and Delaunay triangulations, the computation of arrangements or parts thereof, and visibility and intersection problems. The robustness issue in geometric computing is also addressed. The goal is to extend the current methods of computational geometry to deal more effectively with problems in spaces of higher dimension (three or more) and involving objects of higher algebraic complexity(curved, as opposed to straight).

Purdue University; Christoph Hoffmann and Elisha Sacks; ***Spatial Geometric Constraint Solving Using Constructive Geometry and Homotopy Continuation*****; (CCR-9505745 A000); $77,288; 12 months.**

The project develops the theory and implementation of a practical spatial geometric constraint solver that integrates symbolic methods from constructive geometry with numerical methods from homotopy continuation theory. Geometric constraint solvers are a key component in modern Mechanical Computer-Aided Design systems, and offer a critical technology for increased productivity, rapid response manufacturing, and agile manufacturing. Effective solvers exist for planar constraints, but spatial problems of moderate size exceed the capabilities of many research solvers. The solver being developed will cover the broad class of problems specified by distance, angle, and incidence constraints among points, lines, and planes. It will solve small problems interactively and problems of moderate size in a few seconds. Using a constraint graph whose nodes represent elements and whose edges represent constraints, a constraint analysis will decompose the constraint problem into a series of small construction problems that can be solved efficiently using preprocessing. Elementary constructions will be carried out algebraically, more complex construction steps by homotopy continuation. The hybrid algorithm combines the robustness and completeness of symbolic methods with the uniformity and efficiency of numerical methods.

Northwestern University; D. T Lee; ***Bi-Criteria Optimization, Geometric Location & Related Problems*****; (CCR-9309743 A003, A004); $82,151; 12 months.**

Optimization problems that arise in computational geometry and other related areas are investigated in this project. Special emphasis is placed on bi-criteria optimization problems and geometric location problems. In a communication network, the two important criteria that are of great practical implications are the communication delay and total cost. In path planning routing, the two important criteria are the total length and the number of bends. Optimization problems concerning two criteria either simultaneously or in lexicographical order are studied. Among those to be studied are weighted farthest neighbor Voronoi diagram construction for a set of point sites, a new class of geometric problems, called the capacitated path problem, in which the obstacles have capacities and the cost of a path avoiding these obstacles is a function of the length of the path and the capacities of the obstacles visited by the path, and routing problems with multiple source-destination pairs such that these paths do not cross and yet their total length is to be minimized. The goals of this research are to apply geometric techniques to tackle these new classes of optimization problems, and to identify problems that can (or cannot) benefit from the underlying geometric properties.

Yale University; Laszlo Lovasz; ***Algorithms in Convex Geometry and their Applications in Combinatorial Optimization*****; (CCR-9402916 A001); $76,468; 12 months. (Joint support with the Theory of Computing Program and the Geometric Analysis Program)**

This project investigates the problems of volume computation, sampling from geometric domains, integer programming, and some basic yet not well understood problems such as containment between convex bodies. The goals are to develop new algorithms, to test implementations and, parallel to this, to explore theoretical bounds on the efficiency of algorithms. The main tool in the design of these algorithms is randomization, in particular random walks and Markov chains.

Carnegie Mellon University; Gary L Miller; ***Algorithm Design and Implementation for Parallel Scientific Computation*****; (CCR-9505472 A000); $106,647; 12 months. (Joint support with the New Technologies Program)**

This project applies parallel algorithm design theory to problems arising from scientific problems governed by partial differential equations. Most of the effort is restricted to solving combinatorial algorithmic problems including mesh generation and partitioning. This project develops algorithms and code for the solution of scientific problems that are highly unstructured and whose solution may be rapidly changing with time. Thus, the emphasis is on parallel mesh generation algorithms that will run on parallel machines in conjunction with the system solvers. The project also continues to improve the parallel efficiency of linear system solvers and will extend the work on combinatorial approaches to the construction of good preconditioners for linear system solvers. These are used to speedup the convergence rate of iterative methods. A central approach taken by this project for the design of new algorithms for problems such as mesh generation and preconditioner construction is to use the fact that the underlying graphs for these problems have small separators that can be quickly found. Under prior projects partially supported by NSF, algorithms were discovered and developed to partition, for instance, finite element meshes into roughly two equal size pieces by removing a small number of elements. This work is referred to as the geometric approach to separators. The geometric approach quickly produces provably good partitions for finite element meshes. This project intends to show how the role of mesh generation methods and separator technology can be reversed. In particular, good mesh generation methods are being developed which use the separator technology. This technology will also be used in the construction of good iterative methods for solving these underlying systems. Further improvements are being made in the geometric separator algorithms via experimental and analytic methods. Relationships between the geometric method and other known algorithms and methods, such as spectral, are being investigated.

State University of New York – Stony Brook; Joseph S. B Mitchell and Esther M Arkin; *Algorithmic Studies in Applied Geometry*; (CCR-9504192 A000); $90,000; 12 months.

This investigation has three major objectives: (1) to add new algorithms and methodologies to the repertoire of computational geometry techniques, including new approximation methods and new algorithms that are simpler and easier to implement than existing ones; (2) to formulate precise algorithmic versions of a large body of geometric problems from allied fields, in such a way that the methods of computational geometry can be applied successfully and so that the community of largely theoretical computational geometers can be properly exposed to the more practical applications of the field (allied fields include cartography, computer vision, computer-aided design, graphics, manufacturing, etc); and (3) to disseminate methodologies of computational geometry to applied researchers who work in allied fields but who have been largely unaware of progress in computational geometry, particularly since it has been construed as a primarily theoretical instrument. The third objective is accomplished through discussions of research directions with contacts in industrial research labs and through publishing papers for conferences and in journals whose readership includes a breadth of engineering disciplines.

University of Maryland – College Park; David M. Mount; *Geometric Tools and Applications*; (CCR-9310705 A001); $13,116; 0 months.

The goal of this research is the design, analysis, and implementation of algorithms and data structures for a collection of geometric computational tools. These tools are chosen to directly address existing computational problems in application areas including data compression, molecular biology, geographic information systems, and computational fluid dynamics. In particular the following areas are considered. (1) Practical algorithms and data structures for nearest neighbor searching in high dimensions, and applications to problems in data compression. (2) Algorithms and data structures for detecting intersections and simulating the motion of a set of moving objects in two and three dimensional space. (3) Construction and maintenance of triangulations with specified shape requirements and applications to geographic information systems and mesh generation in computational fluid dynamics. Emphasis is on practical, implementable solutions to these problems, and both theoretical and empirical analyses of their performance.

Smith College; Joseph O'Rourke and Ileana Streinu; *Research at Undergraduate Institutions (RUI): Visibility, 3D, and Other Topics in Computational Geometry*; (CCR-9421670 A000); $46,735; 12 months.

The focus of computational geometry is designing algorithms for solving geometric problems. These arise in a number of application contexts, such as graphics, robotics, medical imaging, and manufacturing. The project's concentrations touch on all these application areas. A number of visibility questions are being examined, including covering regions with floodlights, and the structure of visibility graphs. Several of the problems being explored involve three dimensions: reconstruction from parallel slices (and its application to graphics morphing), computing diameters and centerpoints of sets (with applications to pattern recognition), and motion planning configuration spaces (application to robotics). Fundamental questions in the theory of arrangements are being addressed. Several problems arising from the manufacturing community are being tackled, including that of scheduling a punching tool to create a hole in a sheet of metal of a prescribed shape. Female undergraduate students are engaged in all aspects of the research, and several useful software packages are being produced and distributed.

Purdue University ; Jorg Peters; *NSF Young Investigator (NYI) Award: Surface Splines Over Irregular Meshes*; (CCR-9457806 A001, A002); $67,500; 12 months.

Models of die casts in manufacturing, level sets of complicated functions, deposition fronts in simulation, pleasing shapes in animation, fast prototyping, and visualization of interactions in a virtual world have one thing in common: the need for efficient representations of smooth surfaces. At present, some of our understanding and use of scientific results is handicapped by the fact that the standard representation used for the task, tensor-product B-splines, can only model a small subset of these surfaces naturally and efficiently, namely surfaces that allow for a regular, checker-board arrangement of its pieces. Free-form surface splines extend the spline paradigm and techniques to cover also irregular arrangements. In extending, they preserve the intuitive generation of the surface from the control mesh by a process of cutting with hyperplanes, also known as corner cutting or subdivision. So far only first-order, tangent continuous surface splines exist. Extension to higher-order continuity is both of fundamental and practical interest. The fundamental aspect consists of a new theory that arises when synthesizing surfaces from pieces using massive computing power in contrast to analyzing surfaces as in classical Gaussian differential geometry. The goal of this research is to develop a general framework for surface splines and to use the representation to optimize the shape of surfaces with respect to various cost functions. The immediate goal is the derivation of curvature-continuous surface splines and to find tools to adjust the variation of curvature, an important quality criterion for surfaces. Since the challenge is considerably greater than the definition of first-order surface splines over irregular meshes, progress requires heavy use of symbolic computation and graphics for quality assessment.

New York University; Richard Pollack, Janos Pach, and Micha Sharir; *Studies of Geometric Algorithms and Their Applicatins*; (CCR-9424398 A000); $107,151; 12 months.

The relatively new field of computational geometry has developed at an accelerating rate in the past few years. The problems that it encompasses cover a wide range of applications, such as motion planning and computer graphics, and their solution often involves the use of sophisticated techniques drawn from many branches of mathematics and theoretical computer science. Prior work includes extensive contributions to many basic and applied problems in the area, including motion planning, hidden surface removal and related visibility problems, combinatorial and algebraic analysis of arrangements of curves and algebraic surfaces, randomized algorithms for linear programming and other optimization problems, etc. The purpose of this research is to continue the work in these fields and to extend it into new core areas in computational geometry. A major portion of the research is devoted to the study of arrangements of curves and surfaces. Specifically, the following problems are being studied: 1. Combinatorial and algorithmic problems related to substructures (lower envelopes, single cells, zones, etc.) in arrangements of surfaces in higher dimensions. 2. Related algorithms in real algebraic geometry for computing cells and road maps in semi-algebraic sets. 3. Combinatorial and algorithmic problems involving planar arrangements of segments or curves (also known as "geometric graphs". A theme that is manifest in this work is the rich cross-fertilization between basic research in computational geometry and the various application areas, where problems in one area motivate the study of new basic problems whose solution in turn finds applications in many other areas. Another theme is the strong connection between the combinatorial analysis of substructures in arrangements and the design of corresponding efficient algorithms for constructing and utilizing these structures. Often the efficiency of such an algorithm crucially depends on the size of the structure to be computed, and most of the algorithm design has to be devoted to the combinatorial analysis of the complexity of that structure. These considerations are reflected in the work being done.

University of California – Berkeley; Raimund Seidel; *Presidential Young Investigator (PYI) Award: Randomized Geometric Algorithms and Data Structures*; (CCR-9058440 A005); $54,500; 6 months. (Joint support with the Special Programs Program)

This project investigates the possible use of randomization in the design of algorithms and data structures for geometric problems that involve a large number of objects, with a particular emphasis on various aspects of the so-called higher-dimensional point location problem. The goal is to design data structures that permit the rapid location of a query point in a polyhedral partition of d- space. Various range query problems which consider possible tradeoffs between preprocessing time, space usage, query time, and randomization are also investigated.

New York University; Micha Sharir, Janos Pach, and Richard Pollack; *Studies of Geometric Algorithms and Their Applications*; (CCR-9122103 A004); $13,100; 6 months.

This project investigates the geometric structure and develops efficient geometric algorithms for the following areas: (1) Arrangements and configurations, including the complexity of a single cell, zones and envelopes, space partitions, and arrangements of lines in space; (2) Geometric algorithms for robot motion planning, including motion planning for various systems with 3 degrees of freedom, motion planning based on generalized voronoi diagrams in 3 space, and extremal placements and high-clearance motion; (3) Visibility problems in three dimensions, including output-sensitive hidden surface removal, and ray shooting and tracing; (4) Randomized techniques in geometry, including design and analysis of randomized geometric algorithms, epsilon-nets, and derandomization of geometric algorithms; and (5) Applications and related problems, including k-sets in arrangements, union of geometric objects, geometric optimization, layout of graphs in the plane, incidence and distance problems, and transversal problems. A theme in many of the investigated research areas is the study of problems in higher dimensional space and involving curved objects (rather than flat objects in 2 or 3 dimensions). Such problems are much harder to tackle than problems traditionally studied in computational geometry, but are essential for many applications (such as those mentioned above). Another theme is the rich cross-fertilization between basic research in computational geometry and the various application areas, where problems in one area motivate the study of new basic problems whose solution in turn finds applications in many other areas. As the algorithms and techniques become more refined and efficient, they are implemented to test their pragmatic feasibility.

New York University; Micha Sharir and Jacob T Schwartz; *Implementation and Experimentation with New Geometric Algorithms for Motion Planning*; (CCR-9311127 A001); $78,887; 12 months.

Exact combinatorial solutions to the motion planning problem in robotics, which use precise computational geometry techniques, especially for systems with few degrees of freedom, tend to be more robust than heuristic or approximating solutions; they can achieve performance that is theoretically faster than that of naive solutions by an order of magnitude or more, and it is therefore desirable to test their pragmatic feasibility in real systems context, both to complete the somewhat abstract algorithm variants typical of theoretical developments in computational geometry, and to show that they indeed perform well in practice. This project undertakes the development of an 'industrial-strength' motion planning system for bodies translating in 3-dimensional polyhedral environments. This system utilizes efficient and precise geometric algorithms obtained through ongoing theoretical work, whose worst-case complexity attains the best theoretical bounds known for the problem, and also turn out to be very efficient in practice.

Washington University; Subhash Suri; ***Approximation Algorithms in Computational Geometry*****; (CCR-9501494 A000); $39,078; 12 months.**

This project investigates the topic of approximation algorithms in computational geometry, with focus on the following two problems: polyhedral surface modeling and Euclidean shortest paths. In surface modeling, one tries to construct a polyhedral model of a complex surface, based on a set of unordered sample points. The computational complexity of constructing and manipulating the model depends on its number of vertices and faces, and therefore a natural optimization goal is to minimize these features in the model without exceeding a prespecified error tolerance. The project studies various surface-modeling problems within the formal framework of computational geometry, and analyzes the issues of computational complexity. The problem of computing shortest paths is central to robotics and autonomous navigation. The research investigates efficient approximation algorithms for shortest path problems in two and three dimensions. In two dimensions, the query version of the shortest path problem is studied: preprocess a set of polygonal obstacles so that given two points p and q, the distance between them can be determined in polylogarithmic time. In three dimensions, the goal is to design simpler and more practical alternatives to the exact algorithms for shortest paths among polyhedral solids or on a polyhedral surface.

University of Minnesota – Twin Cities; Shanghua Teng; ***CAREER: Geometric Methods for Numerical Computing: Graph Partitioning, Mesh Generation and Parallel Computation*****; (CCR-9502540 A000); $129,935; 36 months.**

This research focuses on the development of geometric methods and their numerical applications. The project involves the design of efficient algorithms for a variety of fundamental problems in parallel geometric and numerical computing and the implementation of these algorithms on both modern supercomputers and workstation clusters. The research has two principal directions. Geometric Methods for Unstructured Mesh Partitioning and Generation: The main theoretical and software question is how to make use of underlying geometric structures and numerical conditions to efficiently generate an unstructured finite element mesh and partition it for subsequent parallel numerical simulations. Parallel Numerical and Scientific Applications: The primary goal is to apply geometric mesh partitioning techniques to the parallel solution of large sparse linear systems, to adaptive and hierarchical computations, to distributed COSMOS circuit simulation, and to dynamic load balancing for parallel N-body simulations. The companion education plan is to design and teach courses in computer science, in the newly introduced Scientific Computation Program at the University of Minnesota, and in the areas that bridge the two. It involves the development of research programs and projects for graduate and undergraduate students who are interested in interdisciplinary research. It also involves the development of summer professional programs for professionals from industry companies, government research labs, and other universities, to initiate the collaboration between universities and industry.

Optimization and Mathematical Programming

Rutgers University – New Brunswick; Farid Alizadeh; ***CAREER: Applications of Convex Programming in Combinatorial Optimization: A Mathematical, Algorithmic and Computational Study*****; (CCR-9501941 A000); $135,000; 36 months.**

The semidefinite programming problem (SDP), including implementation of numerically stable interior point algorithms, mathematical properties of the feasible sets, and in particular applications of SDP in combinatorial optimization are being investigated. First, two versions of the primal-dual interior point SDP algorithm are being implemented. One version is in MATLAB and is intended as an easy to use and change software for small to medium size problems. Another implementation is in FORTRAN 90 and is intended for high performance parallel and vector/pipelined machines and is meant to solve large scale problems. In addition feasibility of active set methods for SDP is being investigated. Next applications of SDP in general 0-1 integer programming problems are being studied. The feasibility of branch and bound SDP techniques which solve an SDP problem at each stage but may require far fewer branchings overall is being investigated. If such an approach is found to be practical, general purpose programs will be developed. In theoretical investigations, the following applications of SDP are being studied: parallel computational complexity of the Lovasz number of graphs, approximation algorithms for the minimum vertex cover problem, applications to the general matching problem, and polyhedrality of the feasible sets of SDPs under affine transformations. The connection of primal–dual method of linear and semidefinite programs to the problem of quadratically constrained quadratic programming is being investigated. In addition, those cones are being investiagted whose associated optimization problem leads to complementarity relations that are bilinear forms; linear programming, quadratically constrained quadratic programming and SDP are examples of such problems. For teaching plans, active participation in helping RUTCOR establish a masters program is planned. Courses in semidefinite programming and in computational biology in graduate school, and a course designed to survey various software available for optimization problems are being developed. At the undergraduate level teaching of courses in the affiliated departments of computer science, mathematics and statistics is expected. Also a textbook on SDP is in preparation.

University of Baltimore; Hossein Arsham; *Research at Undergraduate Institutions (RUI): Optimization of Discrete Event Simulation Models: Single Run Based Approaches*; (CCR-9505732 A000); $23,587; 12 months. (Joint support with the Operating Systems and Systems Software Program and the Theory of Computing Program)

The aim of this project is to obtain new results which can help reduce the time and computational effort required when using the computer simulation models for optimization found in many discrete- event systems. The focus is on the enhancement of the Score Function and Likelihood Ratio methods to provide accurate estimates for derivative and perturbation, respectively. The goals are: improvements the existing variance reduction techniques, theoretical unification, some extensions, and advancements in the practical implementation of these "single run" methods. The project is to develop procedures and algorithms, investigate their accuracy versus execution time behavior, and present numerical results for a wide variety of queuing, inventory, and reliability models.

Carnegie Mellon University; Egon Balas and Gerard Cornuejols; *Polyherdral Methods in Integer and Combinatorial Optimization*; (DMI-9424348 A000); $130,001; 12 months. (Joint support with the Operation Research Program, the Computational Mathematics Program, and the Applied Mathematics Program)

This project continues earlier research in integer and combinatorial optimization problems. The earlier research developed a new approach to solving mixed integer programming problems based on a framework described as 'lift-and-project cuts' within the context of the branch and bound technique. The procedure has been founded to be robust and more efficient than any of the approaches currently used in solving mixed integer programs. The current research is aimed at investigating some other unresolved questions associated with the improved technique. Included in the questions to be resolved are matters related to the characterization of the computational behavior of the algorithm, development of some other new algorithms, and the design and implementation these algorithms to solve a broader class of problems. The lift-and-project cut approach to mixed integer programming has applications to several areas of design, manufacturing, distribution, facility location, and civil infrastructure development. One such application is the optimal design of multi-product batch plants in chemical engineering, where the optimization is concerned with the choice of unit plants sizes for various stages of the process and the batch sizes for the products. Another example is the design of a cost-effective fiber optics network that protects services against the consequences of equipment failure. In the area of civil infrastructure development, one example is the design of a minimum weight truss consisting of a number of specified bars with fixed modal locations, under specified conditions on stresses, bar elongations, and nodal displacement. Another class of problems studied in this research is the generalized traveling salesman problem where the development technique can be used to construct optimal rolling cycles i n a hot strip mill. This research has the potential to significantly enhance the advancement and the understanding of integer and combinatorial optimization problems. Furthermore, several sectors of the economy stand to benefit from the results.

Massachusetts Institute of Technology; Dimitri P Bertsekas; *Laboratory for Information and Decision Systems*; (DMI-9300494 A001); $80,000; 12 months. (Joint support with the Operation Research Program)

Many operations in design, production planning, and resource management encounter optimization problems, that is, mathematical problems of choosing optimally several factors that affect a productivity index. These are problems of considerable computational difficulty that have been extensively investigated. This research focuses on several such problems that arise in practice and have a large scale structure, such as a network or a dynamic system structure. Methodological improvements for the solution of these problems has significant practical impact. The research aims at the understanding of the performance of existing network optimization, linear programming, and nonlinear programming algorithms, and develops algorithms with improved performance for both a serial and a parallel computing environment.

Rice University; Robert E Bixby; *Investigations in Mixed Integer Programming*; (CCR-9407142 A000); $70,000; 12 months.

While recent years have seen remarkable progress in integer programming, both theoretically and practically, most of that progress has come in the solution of pure 0/1 problems. On the other hand, mixed problems, problems with both continuous and discrete variables– usually 0/1 variables–dominate in practice; moreover, practitioners regularly produce instances of these models that cannot be solved using currently available codes. This combination of success in solving pure 0/1 problems and the existing demand for methods to solve difficult real-world mixed problems has received considerable attention in the research community. Nevertheless, general-purpose mixed-integer solvers remain primarily branch-and-bound solvers, and while they often employ rather sophisticated "heuristic" devices, they still use few of the algorithmic ideas implicit in recent theoretical developments. This research will attempt to change that situation by developing a research code including both the standard methods that have been successful in practice, as well as incorporating ideas based upon recent theoretical developments. The focus will be on actually solving real-world instances that arise as general mixed integer programs but cannot currently be solved.

Towson State University; Darush Davani; ***Optimization of Discrete Event Simulation Models: Single-Run-Based Approaches*****; (CCR-9505731 A000); $19,448; 12 months. (Joint support with the Computer Systems Architecture Program and the Theory of Computing Program)**

The aim of this project is to obtain new results which can help reduce the time and computational effort required when using the computer simulation models for optimization found in many discrete- event systems. The focus is on the enhancement of the Score Function and Likelihood Ratio methods to provide accurate estimates for derivative and perturbation, respectively. The goals are: improvements the existing variance reduction techniques, theoretical unification, some extensions, and advancements in the practical implementation of these "single run" methods. The project is to develop procedures and algorithms, investigate their accuracy versus execution time behavior, and present numerical results for a wide variety of queuing, inventory, and reliability models.

University of Wisconsin – Madison; Michael Ferris; ***: Development of Efficient Serial and Parallel Algorithms Based on Mathematical Programming Theory*****; (CCR-9157632 A004); $62,500; 12 months.**

Efficient serial and parallel algorithms, backed by a sound mathematical programming theory, are developed. Emphasis is placed on effective distribution of constraints among parallel processors as well as line-search stabilization techniques for nonlinear complementarity and other problems. Finite termination of algorithms via weak sharp minima and related concepts will are investigated.

Columbia University; Eva K Lee; ***CAREER: Mixed Integer Programming-Parallelism and Applications to Statistical Analysis*****; (CCR-9501584 A000); $133,438; 36 months.**

A major focus of this research is to develop a general purpose "industrial strength" mixed integer programming (MIP) code with parallel distributed computing capability — in particular, a code that allows parallel execution on clusters of personal computers or various types of workstation platforms. A second focus of the research is to explore new applications of mixed integer programming to problems in discriminant analysis. A recently developed MIP model of a problem in discriminant analysis opens up a new avenue for approaching this important area of statistics. The polyhedral structure of this class of problems is being investigated, and efficient computational strategies to solve real instances are being developed. In conjunction with the research plan, a concerted effort is being expended to arouse more interest in mathematical programming (especially integer programming) and its computational aspects among engineering students. New courses/seminars on computational linear algebra, parallel computation and mixed integer programming are planned. In addition, an effort is being made to establish interaction with industry, thereby exposing students to important issues in building and analyzing models for real-world problems and in deriving and assessing solutions.

University of Wisconsin – Madison; Olvi L Mangasarian; ***Applications, Algorithms and Theory of Mathematical Programming*****; (CCR-9322479 A001); $69,993; 12 months. (Joint support with the Computational Mathematics Program and the Applied Mathematics Program)**

Highly promising mathematical programming techniques are applied to medical diagnosis and prognosis as well as to machine learning in general. Five years of experience with a highly accurate system for breast cancer diagnosis, in current use at University of Wisconsin Hospitals, is drawn upon to develop a linear-programming-based prognostic system. Parallel algorithms for the solution of large-scale constrained optimization problems are developed, by distributing ingredients of the problem (constraints, gradients, or/and variables) among parallel processors. Each processor has complete responsibility for varying its own problem ingredients, while allowing the other ingredients to vary in a restricted fashion. The processors share new information computed, then a fast synchronization is performed and the process is repeated. Preliminary algorithm prototypes have been tested successfully with some high parallelization efficiency on publicly available test problems and significant real-world applications. Error bounds are developed for possibly inconsistent systems of inequalities, mathematical programs and complementarity problems. The novel idea here is that the system may be unsolvable, and the bounds are meaningful whether the system is solvable or not. In the latter case, it bounds the distance between the point under consideration, and the set of least error solutions of the system. New mathematical programming approaches to some machine learning problems are studied. In particular a new quadratic programming model for a cascade architecture in neural networks is being studied, as is another one for the inherently difficult problem of minimizing the number of misclassified points by a separating plane.

University of Wisconsin – Madison; Robert R Meyer; *High-Performance Computation of Optimal Network Flows*; (CCR-9306807 A002); $60,750; 12 months.

Historically, parallel computers have focussed on a single mode of parallelism: Multiple-Instruction Multiple-Data (MIMD) or Single-Instruction, Multiple Data (SIMD). Some new computers efficiently implement both paradigms in a single integrated "universal" architecture capable of supporting large numbers of powerful processing nodes in a design scalable to teraflop computation. Clearly, this capability to perform well on both SIMD and MIMD computation is the basis for many future high-performance architectures. This hybrid parallelism is also ideally suited for implementing many algorithms for large-scale mathematical programming, since these methods require powerful individual processors for the solution of optimization subproblems (which may take the form of a medium-sized linear or quadratic program), efficient message passage capabilities for the transfer of subproblem solutions, and efficient synchronization and SIMD-style operations across processors. Proper algorithmic design thus allows the solution of optimization "megaproblems" that were intractable on preceding architectures. This project focuses on network-related optimization problems because such problems arise in a great variety of real world applications for which there are real data as well as problem generators.

Stanford University; Walter Murray and Michael Saunders; *Large-Scale Constrained Optimization*; (DMI-9500668 A000); $100,000; 12 months. (Joint support with the Operation Research Program)

The objective of this research is to develop, study, and implement algorithms for solving large-scale, nonlinear optimization problems. A large-scale optimization problem is characterized by a large number of variables and constraints. Two solution approaches form the focus of the research. These approaches are respectively, the interior point (barrier) method and the sequential quadratic programming (SQP) method. The interest in the interior point method stems from their success on linear programming problems, and some interesting properties that may be of value when certain difficult constraints are encountered. The interior point method can be used to eliminate constraints on the eigenvalues of a matrix. On the other hand, interest in the use of SQP is prompted by the success of the approach on small and medium-sized problems, and the experiences of the investigators on the performance of the technique on two classes of large, practical problems that differ substantially in character. If successful with these approaches, the developed algorithms will be coded into software to facilitate their applications by practitioners. There are several engineering, manufacturing, scientific, and business problems that can be described by large-scale nonlinear optimization models. The algorithms being investigated in this research could open the window to a better understanding of this class of optimization problems. Many problems in various areas of human endeavor stand to benefit from the results of this work.

Northwestern University; Jorge Nocedal; *Numerical Optimization Techniques*; (CCR-9400881 A001); $52,032; 12 months. (Joint support with the Applied Mathematics Program)

This project investigates the design and implementation of algorithms for nonlinear optimization. The research focuses on the solution of large problems, and has two broad objectives. The first is to develop a new algorithm for solving large and unstructured unconstrained optimization problems. This work is motivated by the need of solving large and nonsparse problems efficiently. The new algorithm uses ideas from both Newton methods and variable metric updating, and is tested on large inverse problems arising in weather forecasting. The second objective is to study efficient techniques for handling inequality constraints occurring in nonlinear programming. This research focuses on large problems, and the techniques are designed to be useful in that case. The use of an ellipsoidal-type method is explored. This approach has the advantage of leading readily into a sequence of equality constrained subproblems which can be solved by existing software. An alternative approach, which consists of extending the primal-dual method of linear programming to the nonlinear case, is also explored. The algorithm is posed in the framework of trust region methods, and its relationship with sequential quadratic programming is fully exploited. The two new approaches for handling inequality constraints are tested on a set of large problems, and the treatment of ill-conditioning receives careful consideration.

Johns Hopkins University; Jong-Shi Pang; *Nonsmooth Equations Approach to Optimization and Variational Inequality: Theory and Computation*; (CCR-9213739 A002); $77,160; 12 months.

This project investigates the theory and computation of optimization problems and variational inequalities based on their equivalent formulation as a system of nonsmooth equations.

On the theoretical side, the goal is to gain, through the development of a comprehensive theory for nonsmooth equations via their approximations, a better understanding of the sensitivity, stability, and other instrinsic properties of these mathematical programs. On the computational side, the goal is to develop, relying on generalizations of the classical Newton methods for smooth equations to the nonsmooth context, some robust, globally, and locally quadratically convergent algorithms for solving these mathematical programs. The research is built on work in recent years which has demonstrated the fruitfulness of this nonsmooth-equations approach to variational inequalities, complementarity problems, and nonlinear programs.

Cornell University; James M Renegar; *Issues Relating Linear Programming, Complexity Theory and Numeric Computation*; (CCR-9403580 A000); $122,106; 36 months.

The primary objectives concern the development and analysis of algorithms for linear programming within a complexity theory framework motivated by functional analysis rather than the traditional frameworks motivated by algebra and combinatorics. Special attention is given to issues concerning computer round-off error and inexact data, issues such as how one might use the prior knowledge one has regarding the structure of the problem to be solved in order to efficiently solve the problem using less computational precision than would be needed otherwise. The use of iterative methods for solving the equations that arise when applying interior-point methods is investigated, as is the possibility that the resulting algorithms are (nearly) optimal; optimality is investigated via approximation theory. Perturbation theory for linear programming is being developed. Certain notions which have proven useful in the context of linear programming are being investigated in a more general context involving multi-variate polynomials. It is intended that all of the investigations will be carried out with as much generality as is possible; for example, the cones defining non-negativity will not be required to be polyhedral.

University of Michigan – Ann Arbor; Romesh Saigal; *Studies on Affine Scaling Method*; (CCR-9321550 A000); $56,465; 12 months.

Affine scaling methods form an important class of interior point algorithms for solving a linear programming problem, and there have been some major developments in the convergence and convergence rate theory of these methods. In particular, when the problem may be degenerate, if the step size is less than equal to two thirds of the distance to the boundary, the primal converges to the interior of the optimal face, while the dual to the analytic center of the optimal dual face. Also, by a step selection strategy, these methods have been shown to converge superlinearly. More efficient variants have also been developed. Under this project, four different aspects of these methods are being studied: 1) study of their convergence properties, convergence rates and complexity; 2) study of stable implementations to achieve these higher rates of convergence in computer implementations; 3) study of their connection to Kalman filter and their application to solving stochastic linear programming problems; and, 4) study of their efficient implementations in vector/parallel/distributed computing environments.

Cornell University; Michael J Todd, Yuying Li, Leslie E Trotter, and Robert G Bland; *Computational and Mathematical Investigations in Optimization*; (DMS-9505155 A000); $164,000; 12 months. (Joint support with the Operation Research Program and the Computational Mathematics Program)

This project undertakes broad studies of optimization algorithms and the mathematical theory underlying them. The project covers continuous and discrete optimization algorithms, both exact and approximate, their computational complexity, practical large-scale implementation, performance guarantees (in the case of approximate algorithms), and applications in the physical sciences such as elementary particle tracking, as well as more conventional applications in manufacturing and logistics. Particular investigationss include: (1) a continuation of large-scale computational testing of implementations of minimum-cost network flow algorithms; (2) development and testing of algorithms for large-scale nonlinear minimization problems with bound constraints; (3) performance guarantees for efficient approximation algorithms for machine-scheduling problems with budget constraints and for other combinatorial optimization problems; (4) development of more efficient interior-point methods for convex programming and for linear programming problems where no initial interior feasible solution is known; (5) studies of the polyhedral structure of combinatorial problems in graph theory and partially ordered sets, as well as in applications such as crew scheduling — computational implementation and testing have been an integral aspect of these studies; and (6) further development of complexity theory for continuous nonconvex problems.

These problemss range from modeling through algorithm development and analysis to implementation and testing. Optimization addresses questions like: (1) How do you schedule the production of hundreds of items with varying demands over several months to minimize setup and holding costs, subject to resource limitations and capacities? (2) How do you determine the geometric conformation of a protein (how it "folds") given an approximate en ergy functional for any position?

Indeed, complex systems arising in the engineering, physical, and biological sciences, and in the manufacturing and service industries, involving hundreds to millions of interacting variables, frequently lead to optimization problems when one wishes to control or predict their behavior. The project investigates a number of specific issues related to modeling and algorithm development for a variety of applications, ranging from traditional settings like resource allocation, planning, logistics, and distribution problems to new application areas such as airline crew-scheduling, elementary particle tracking, and shop scheduling. A common thread is the search for efficient methods to solve exactly large-scale instances of such problems, or, if that is not likely to be possible, for efficient algorithms that are guaranteed to obtain a solution that is close to optimal in a precise sense. These algorithms are tested computationally on representative instances of such problems using serial and parallel computers.

Princeton University; Robert J Vanderbei; *Interior-Point Methods for Convex and Semidefinite Programming*; (CCR-9403789 A000); $42,218; 12 months.

Interior-point methods have proven to be efficient for the solution of large, sparse linear and quadratic programming problems. These methods are being extended to cover more general classes of problems. In particular, interior-point technology are being used to create efficient algorithms for the solution of convex programming problems and semidefinite programming problems. The first class is important for general nonlinear optimization and the second has important applications to integer programming.

State University of New York – Stony Brook; David S Warren and I. V Ramakrishnan; *Enhancing the Power and Performance of Tabled Evaluation of Logic Programs*; (CCR-9404921 A001, A002); $169,660; 12 months. (Joint support with the Knowledge Models and Cognitive Systems Program and the Programming Languages and Compilers Program)

This project continues work on the development of XSB system. XSB is a system that integrates logic programming, deductive databases and nonmonotonic reasoning. It uses SLG resolution, a tabled evaluation strategy, to combine Prolog's SLD and deductive databases's bottom up evaluation in a computationally effective way. Current benchmarks show that the XSB system is significantly faster than more traditional approaches to deductive database query evaluation, and shows promise of being very efficient for certain types of nonmonotonic reasoning. In the current project, the XSB implementation will be improved by (1) improving the underlying WAM-based engine to make it more efficient, and (2) developing program transformation techniques to permit XSB programs to be optimized at the source level.

Computational Logic and Theorem Proving

University of Kansas Center for Research Inc; Frank M Brown; *Research on a Theory of Design Change*; (MIP-9526532 A000); $34,709; 12 months. (Joint support with the Design, Tools and Test Program Program)

The mental process of predicting the reasonable consequences of a change in the design of an artifact is an important step in the design process. This research addresses issues in developing a theory of design change. The premise is that the incremental changing of the geometric design of an artifact may be formally explained by logical and mathematical theories, similar to those in automated planning and simulation systems which are used in many fields. Topics being investigated are representation of designs, designer intentions, and constraints. A computational model of the deductive process of changing a design is being developed. The model uses frame laws and default constraints expressed in the modal quantificational logic Z. Other work includes exploring problems of automated deduction of facts in three dimensional geometry, consistency analysis, and developing a taxonomy of appropriate engineering design actions and intents.

University of California – Santa Cruz; Allen Van Gelder; *Practical Algorithms for Problems in Propositional Logic*; (CCR-9503830 A000); $49,273; 12 months.

Problems in propositional logic, such as Boolean satisfiability, are studied from the point of view of developing practical algorithms, although the problems are often NP-complete or co-NP-complete. Such problems are of practical importance in VLSI design verification, test generation, related CAD applications, as well as automated software verification. Many other applications also occur naturally. E.g., higher order theorem provers require a satisfiability checker as a module. Recent hardware advances bring solution of some of these problems within reach. Algorithms are being implemented and tested for performance in typical applications, such as test pattern generation, sequential circuit verification, and program verification. Model search (usually called the Davis-Putnam method) and resolution are two well known, but somewhat conflicting, strategies for solving propositional satisfiability. Model search "succeeds" by discovering a satisfying assignment, whereas resolution "succeeds" by detecting that no such assignment exists. Some work on combining the two ideas in one algorithm has recently appeared. This project investigates more powerful combinations of these methods. Besides resolution, equality recognition can be valuable. The goal is to identify contexts in which resolution, equality recognition, and other inferences can be beneficial in reducing the search space. Equally important is to find efficient implementations, usually requiring advanced data structures. Another goal is the development of application-independent methods. Heuristics described in the literature for particular applications are examined to determine whether the application content can be abstracted away, making the heuristic applicable to a logic problem without knowing its origin.

Columbia University; Donald Goldfarb; ***Algorithms for Mathematical Programming*****; (DMS-9414438 A000); $120,000; 36 months. (Joint support with the Operation Research Program, the Computational Mathematics Program, and the Applied Mathematics Program)**

The objectives of this research are the development, analysis, and implementation of algorithms for solving mathematical programming problems. The focus of this project is on simplex algorithms, interior point algorithms and algorithms that combine interior point and multiplier penalty approaches, with particular emphasis on algorithms that are efficient both in theory and in practice. Specialized algorithms for network flow problems and those that take advantage of the architecture of massively parallel computers are being developed. Since many problems in science and engineering can be formulated as large-scale optimization problems, the development of efficient optimization algorithms under this project will have an impact on fields outside of optimization such as manufacturing (production planning and scheduling), biotechnology (protein folding), civil infrastructure (fleet and crew scheduling and transportation planning), and telecommunications (network design and routing) as well as on the field of optimization itself.

State University of New York – Albany; Deepak Kapur; ***Induction, Proof Management, and Related Research in Automated Deduction*****; (CCR-9303394 A002); $52,645; 12 months.**

The theorem prover Rewrite Rule Laboratory, RRL, and the proof management system Tecton are enhanced to make them useful for applications, especially where analysis of specifications and well-founded ordering play a crucial role in these applications, and large complex proofs often have to be constructed. RRL is a theorem prover based on rewriting techniques and completion which provides support for equational and inductive reasoning. Tecton is a management system, and it provides a menu-driven graphics interface to the theorem prover and emphasized visualization of proofs. Tecton is extended to support a proof command language which provides a user control over proof construction and structuring. Tecton is useful for instructional purposes, for teaching theorem proving, methods for constructing proofs and verification. RRL is extended to enhance its theorem proving capabilities for proving properties by induction. The cover set induction method which has proved quite effective in automating proofs by induction, is further refined. Semantic methods for showing termination of rewrite systems of recursively defined functions, especially those arising in the specification of algorithms and data structures, are studied and further developed. Heuristics for checking the completeness of a cover set designed from a function definition are investigated. Heuristics for automatic lemma generation in RRL are expanded.

University of Wisconsin – Madison; Kenneth Kunen; ***Automated Deduction in Mathematics*****; (CCR-9503445 A000); $120,000; 24 months.**

This research addresses problems in in two major areas: (1) Theorem Proving: Automated deduction is being used to derive mathematical theorems whose proofs would not be feasible without computer assistance. Two facets of this research are: 1a. Search Strategies. This is part of a continuing effort to improve current theorem proving technology. Specific investigations involve: lemma generation, model generation, and linked resolution. 1b. Specific Theorems. New areas of application are being sought out, and well- known open problems involving single axioms for groups and the Robbins algebra problem are being studied. These two facets are closely related. Improvements in theorem prover technology can be applied to proving better theorems. Conversely, proving new theorems gives a way of demonstrating the power of the technology, and failed attempts to prove a theorem can suggest ways in which the technology can be improved. (2) Verification: Here, one uses a computer program to verify existing mathematical theorems. One goal is to develop verification systems far enough so that they could be used as referees for mathematical papers. Concentration is on: (a) The Boyer-Moore prover. This works in finitistic mathematics, and is probably the best known existing verification system. The current system includes the ability to do induction on the ordinal epsilon_0. Extensions of this prover are being examined, with an eye to allowing induction on larger ordinals. (b) A prover for set theory. Within axiomatic set theory (ZFC), one can develop all of mathematics. A verification system based on ZFC is being designed. This system will borrow features already used in the Boyer-Moore prover and other systems, but major new problems will be addressed. One problem is how to encode meta-rules, such as the scheme for transfinite induction. Another is how to allow the user to extend the system by adding type declarations (corresponding to informal mathematical statements such as "from now on, x,y,z will represent real numbers").

State University of New York – Albany; Neil V Murray; ***Implementation and Analysis of Inference Techniques for Classical and Multiple-Valued Logics*****; (CCR-9404338 A000); $45,000;**

12 months.

This project continues a research program in computational logic. The studied areas of research stem directly from an analysis of the structure of formulas in negation normal form and from investigations into multiple-valued logics. The former work led to the development of the deduction rule called path dissolution. The study of dissolution continues, including the study of its properties as an inference mechanism and the development of a portable C++ implementation. For some time it has appeared that dissolution would be a useful tool in the design of prime implicant/implicate algorithms. A new negation normal form (NNF) algorithm, PI, has been developed that can be combined with dissolution for this purpose, and formula classes have been discovered that are hard for CNF/DNF-based methods but that are easy for PI/dissolution. A prototype system has been implemented and is being further developed. These techniques are being extended to multiple-valued logics (MVL's). The work in MVL's also includes the study of annotated logic programming and SLD-style proof procedures, and inference methods for fuzzy logics.

State University of New York – Albany; Paliath Narendran and Deepak Kapur; ***Research on Unification and Related Problems*****; (CCR-9404930 A000); $61,853; 24 months.**

This project investigates unification with a focus on semantic unification where some of the function symbols have semantics associated with them, usually specified in the form of an equational theory. The main objective is to explore decidability and complexity results, and design efficient algorithms in the framework of the constraint paradigm, an approach developed earlier in the study of optimal unification algorithms for associative-commutative theories. In particular, the use of negative constraints and heuristics based on them is being explored to prune the search space. Decidability and complexity issues on various equational disunification problems are also being explored.

University of New Haven; Erik Rosenthal; ***Research at Undergraduate Institutions (RUI): Applications of Classical Inference Techniques to Multiple-Valued Logics and to Prime Implicate Algorithms*****; (CCR-9504349 A000); $50,760; 12 months.**

This project is for research in computational logic. The areas of research stem directly from prior analysis of the structure of formulas in negation normal form. That work raised many questions and led to explorations in several directions. Substantial experimental results at the propositional level, preliminary experimental results at the first order level, and certain theoretical results indicate that the most important of these may be path dissolution, a rule of inference that is strongly complete at the ground level. This project continues exploration of this and related inference mechanisms, largely through experimentation. One major thrust is to further the implementation of the techniques developed earlier. The current first order system ("Dissolver") is a solid platform on which the following techniques may be tested: link selection; computing prime implicants; backtracking; theory links and dissolution; and star chains. While abstract proof-theoretic questions are of interest in their own right, enhancing the performance of Dissolver is an important motivation for the theoretical work in this project. The investigations into multiple-valued logics largely fit the former category; the study of the following issues contributes to the development of Dissolver: dissolution and multiple-valued logics; dissolution, analytic tableaux, and the distributive law; quantifier duplication, proof length, and cycles; algorithms for computing prime implicants; and induction and equality.

SRI International; Natarajan Shankar; ***Interactive Proof Checking*****; (CCR-9300444 A002); $70,370; 12 months.**

Proof construction is a pervasive activity in computing and mathematics. Although techniques for automated reasoning have made it possible to prove theorems with extreme rigor, much of the past effort has been directed towards proving difficult, interesting, and often well-known theorems using general-purpose logics and proof techniques. The application of automated reasoning technology to support formal methods in software engineering has fallen well short of original expectations. The main reason for this failure is the overriding emphasis on automatic theorem proving. A completely new approach is required where the focus must shift from theorems to proofs, and from general-purpose language and inference mechanisms to well-integrated, domain-specific mechanisms. Any sufficiently rich application domain, such as hardware, real-time, concurrent, or fault-tolerant systems, exploits a host of specialized formalisms in order to encode important concepts and methods and to reduce complexity. This project develops multi-modal framework for interactive proof construction to support the use of domain-specific formalisms. The envisaged application is to reason about complex digital systems.

SRI International; Mark E Stickel; ***Research on Automated Deduction*****; (CCR-9408630 A000); $61,306; 12 months.**

The model elimination theorem-proving procedure, like other top-down reasoning procedures, has the defect of repeatedly solving the same goals. The problem can be ameliorated by lemmas or caching, but the "upside-down meta-interpretation" approach to be investigated offers a more comprehensive solution that entails executing the model elimination procedure by a bottom-up reasoning engine, which also enables more control over search strategy. Theory resolution is a framework for incorporating theories into a resolution theorem-proving program, thereby making it unnecessary to resolve directly upon axioms of the theory and improving efficiency. Although many ways of incorporating theories into a resolution theorem prover can be seen as instances of theory resolution, theory resolution provides little guidance on how to incorporate theories. Predicate- and function-matching rules and a multilateral representation for residues in partial theory resolution are being developed as methodologies for using theory resolution. Numerous previously open problems in the theory of quasigroups have been solved recently by automated reasoning systems such as efficient implementations of the Davis-Putnam procedure. In collaboration with other automated deduction researchers and a mathematician expert on the domain, additional effort will be devoted to obtain new results in the theory of quasigroups.

SRI International; Mark E Stickel; ***Travel Support for the l995 Dagstuhl Seminar on Deduction March 20-24, l995, Dagstuhl Seminar Center, Wadern, Germany.*****; (CCR-9500136 A000); $8,375; 6 months.**

An international seminar on deduction organized by Prof. Wolfgang Bibel (Technische Hochschule Darmstadt, Germany), Prof. Koichi Furukawa (Keio University, Japan), and Dr. Mark Stickel (SRI International, Menlo Park, California) was held 20-24 March l995 at the Dagstuhl Seminar Center in Wadern, Germany. About 50 researchers working in the field of automated deduction from around the world were invited to participate.

University of Houston; Rakesh M Verma; ***Computational Aspects of Normalization, Matching and Unification*****; (CCR-9303011 A001); $49,047; 12 months.**

Normalization, matching, and unification are three fundamental computational steps found in virtually all symbolic computation systems. Applications of these operations include term rewriting, functional, equational and logic programming languages, abstract data type specification and verification, automated deduction, code generation, type inferencing, and computer algebra. This project addresses these problems in symbolic computing and the means to design and analyze efficient algorithms for them. Practical algorithms are designed on both sequential and parallel machines. Algorithms which learn efficiently from their history are designed for normalization with respect to several important and useful classes of rewrite systems. Several facets of matching and unification problems are studied from a novel perspective. Algorithms that correlate information from previous match/unify operations are designed for tree pattern matching and its interpreted versions, and subterm unification and its interpreted versions. The practical performance of these algorithms is investigated. This research is useful in enhancing the efficiency of symbolic computation systems as well as provide understanding of the inherent complexities of these operations.

University of Iowa; Hantao Zhang; ***NSF Young Investigator (NYI) Award: High Performance Automated Reasoning and its Applications*****; (CCR-9357851 A002); $42,785; 12 months.**

Reasoning algorithms are used in many application areas of computer science and artificial intelligence, and high performance of reasoning algorithms is indispensable to the successes of these applications. The objectives of this research are to develop high performance reasoning algorithms, and to apply these algorithms in formal verification of hardware and software designs. This research substantially improves the performance of a software system called RRL (Rewrite Rule Laboratory) by adding new reasoning algorithms to it, and by building new applications on the top of it. The research focuses on redundance control of automated deduction and mathematical induction, and efficient representation of data structures. The topics include restricted inference rules, powerful simplification rules, unnecessary computation detection, induction schemata formulation, induction hypotheses handling, and efficient implementations of all the involved algorithms. Practical verification problems are chosen from software and hardware design as test problems for RRL and RRL is enhanced to meet the need of large-scale applications by providing failure- resistant and user-friendly interfaces. Special effort are made on distributing RRL world-wide to the people who are interested in using RRL as either a research tool or a teaching tool in automated reasoning.

University of Iowa; Hantao Zhang; ***High Performance Automated Reasoning*****; (CCR-9504205 A000); $66,095; 12 months.**

Two software systems, RRL (the Rewrite Rule Laboratory) and SATO (SAtisfiability Test Optimized), developed under the past grant, have been successfully used for solving many problems often considered a challenge for automated theorem provers, including several dozens of open problems in quasigroups. The current research will further increase the reasoning power of RRL and SATO. The objectives of this research are to develop new high performance reasoning algorithms, and to apply these algorithms in specification and verification of hardware and software, and in solving open problems in algebra, logic and combinatorics. The research focuses on constraint satisfaction and automated mathematical induction. The topics include efficient constraint propagation, parallel and distributed reasoning, intelligent induction schemata formulation, management of large proofs, and implementation and experimentation of all the involved algorithms. Practical problems will be chosen from software and hardware design verification and combinatorics as test problems for both RRL and SATO. Both systems will be enhanced to meet the need of large-scale applications by providing user-friendly interfaces. Special effort will be made to distribute RRL and SATO to the automated reasoning community worldwide.