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Lawrence Livermore Laboratory

SURVEY OF APPLIED AND COMPUTATIONAL
MATHEMATICS AT LLL

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FOREWORD

This survey of applied and computational mathematics was prepared at the request of G. D. Dorough, LLL Associate Director for Scientific Support. The material given in Chapter 2 was contributed by many people. The major contributors are listed below.

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This report was compiled and edited by J. Chang, M. Ekstrom, and F. Fritsch. Because of the multiple-source contributions in Chapter 2, there is some non-uniformity in style and technical detail among the various topics. Certain smaller individual efforts have not been included because of limited general interest or possibly as a result of the ignorance of the editors. We apologize for such unavoidable omissions and for failure to identify all individuals whose work is represented here. Constructive comments are welcomed.

SURVEY OF APPLIED AND COMPUTATIONAL MATHEMATICS AT LLL

ABSTRACT

This report is a summary of current activities in applied and computational mathematics at the Lawrence Livermore Laboratory. It is evident from our survey that there is a very broad spectrum of research and development in this area of mathematics here. However, only a small percentage of the total effort is directly involved with fundamental research.

We recommend that the Laboratory adopt a formal policy to establish and support a research program in applied and computational mathematics. Coordination of related efforts is needed, and steps toward this are recommended. In addition, a study of interactions between mathematical methods and computer architectures is necessary for the Laboratory's ever increasing requirement for computational capability.

CHAPTER 1

INTRODUCTION

Conservatively speaking, the Lawrence Livermore Laboratory spends at least 15% of its budget on computational problem solving.* Research and development (R/D) efforts associated with these activities are conducted in support of a large number of scientific and technological applications by various divisions of the Laboratory. Because the overall research activity of the Laboratory is characterized by the direct coupling of physical modeling with experimental research, fundamental advances in applied and computational mathematics are essential to Laboratory programs. Despite the lack of an organized program coordinating individual research efforts in applied and computational mathematics, there is considerable depth and breadth in this

*The Computation Department budget for the fiscal year of 1976 is approximately \$14 million. To this should be added another \$15 million for the programmatic manpower costs as estimated in this survey (Table 2). Of this \$14 million, approximately \$200 000 supports applied mathematics research and \$130 000 supports computer science research. The remaining amount constitutes the necessary operating costs (no capital equipment costs) for maintaining the computer center and providing services to the various LLL programs.

area of the Laboratory's research. There is also cross-fertilization of ideas among the scientific programs.

This report is a summary of current activities in applied and computational mathematics at LLL. The research in computer science will not be discussed and may be presented in a future survey. Since the majority of the mathematical research is performed by individuals associated with specific areas of application, this summary is presented in the context of these applications. The research can be divided into two broad categories: simulation of physical systems and analysis of experimental data.

The simulation of a physical system involves the representation of relevant physical processes by a set of mathematical equations. For systems of interest to the Laboratory these mathematical models (i.e., equations) must be solved numerically on large-scale computers. Historically these computational problems have always pressed the limits of the available computing capacity, both in terms of available computational algorithms and facilities; and there is no reason to expect this to change in the future. Programmatic needs have always required the inclusion of as much detail of the physical processes as is consistent with the computing capacity. This is an evolutionary process that stimulates the continued development of new numerical methods in hydrodynamics, chemical kinetics and transport theory, and solution of general ordinary and partial differential equation systems.

The second principal use of applied and computational mathematics at LLL is in the analysis of experimental data. Modern scientific experiments are usually expensive to perform and require complex methods of data acquisition and analysis. Mathematical techniques are necessary to maximize the yield of desirable information from experimental data and to aid in the design of experiments. This work is oriented toward the development of advanced statistical processing techniques, including stochastic system modeling, applied estimation, and pattern recognition.

A survey of applied and computational mathematical activities in various areas of application constitutes the bulk of this report. The order in which these activities are presented is that of decreasing effort level. Estimates of the levels of effort in full-time equivalents (FTE'S) for the various activities are given in Table 2. In the concluding section common threads among the areas are identified, and an argument is presented for support for a coordinated research program in applied and computational mathematics at LLL.

CHAPTER 2

SURVEY OF MATHEMATICAL ACTIVITIES

Numerical Hydrodynamics

Most of the computer time at LLL is used to solve numerical simulation models of physical systems. Significantly more than half of this time is consumed by models of physical systems that evolve in time; in most cases, the modeled systems consist of one or more fluids interacting. Each model usually includes additional physics such as particle transport, precipitation, and material strength, but the common element is hydrodynamics.

Hydrodynamics comprises the laws of conservation of mass, momentum, and energy that govern the motion of fluids. These laws generally take the form of partial differential equations; the numerical models at LLL usually consist of finite-difference approximations to these partial differential equations. Other numerical techniques such as Fourier transforms and finite elements are also used, but to a lesser degree at present.

The conservation laws are referred to a coordinate system (a mesh) that may change position with time. In one extreme, the coordinate system moves with the local fluid velocity; this is called the Lagrangian formulation. In the Eulerian formulation, the mesh remains fixed in time and the fluid moves through it. When the mesh moves, but with a different velocity than the fluid, we have the continuous rezone formulation. Other formulations are CEL (combined Eulerian - Lagrangian) and FLAG (Free-Lagrangian).

The Lagrangian formulas may include slide lines to permit the relative motion of different parts of the fluids to take place. Pure Eulerian formulations have limited value for most problems of interest at LLL; the multi-fluid Eulerian formulation permits different fluids separated by Lagrangian lines to interact and to evolve on the same mesh.

Most hydrodynamics models deal with compressible fluids, and shocks are automatically taken into account by an artificial viscosity such as that of von Neumann and Richtmyer.

Most models used a finite difference approximation that is explicit in time; some work is being done on implicit models.

The codes listed below are classified as hydrocodes because each one involves a hydrodynamic model to some extent. At first glance, it appears that

we have an inordinate number of hydrocodes and that there is an enormous duplication of effort. However, most of these codes contain numerical models of additional physical processes, and the hydrodynamic model is usually tailored to match the rest of the model. In some cases, the hydrodynamic model is only a small fraction of the entire code.

Most of the hydrocodes in use were developed at LLL; only three (WONDYNG, TUTU2 and RAD9) originated outside LLL. All codes are running on the CDC 7600 (LTSS system) computers*, and those noted are also running on the CDC STAR-100 Computers.

All codes are time-dependent — we have grouped them according to their spatial characteristics. Some remarks on the future will be found at the end of this section.

Finally, we note that this is an incomplete list. Each of the codes represents a significant investment in person-years, and is more or less a production code. There are, however, many other hydrocodes around the lab for the investigation of new techniques — some of these codes no doubt will be listed in a future report.

Unfortunately many of the hydrocodes at LLL may not be described in an unclassified document such as this, but will be discussed in a separate report. It should be noted that the major effort in code development has centered around this class of calculations; and the hydrocodes listed below have benefited much from such research.

LLL Hydrocodes

Except as noted, the codes in Table 1 are all time-dependent, compressible, explicit, finite difference, numerical hydrodynamics codes. These methods use a von Neumann-Richtmyer-like artificial viscosity (q) for shock calculations.

* Reference to a company or product name does not imply approval or recommendation of the product by the University of California or the U. S. Energy Research & Development Administration to the exclusion of others that may be suitable.

Table 1. Hydrocodes at LLL.

Code name	Principal contact(s)	Division	Remarks
One-Space-Dimensional Lagrangian Codes			
KO	J. Woodruff	B	Contains material strength and porous models.
	M. Wilkins	H	
UKTOF	E. McCauley	NTE	Contains material strength.
WONDYNG	E. McCauley	NTE	
SOC	C. Snell	K	Contains material strength.
One-Space-Dimensional Eulerian Codes			
PUFL	B. Germain	K	1 1/2-dimensional with Lagrange boundary, multiphase.
1D2FAZ	W. Comfort	K	Multiphase flow.
LIP	J. Fleck	T	Implicit formulation.
Two-Space-Dimensional Lagrangian Codes			
HEMP	P. Brown	B	Contains material strength, slide lines, triangular zone, two-way slide lines.
	M. Wilkins	H	
LASNEX	G. Zimmerman	A	STAR.
OOZE	R. Barton	B	Continuous rezone.
TENSOR	P. Brown	B	Contains material strength, slide lines.
	V. Kransky	B	
	D. Burton	K	
TUTU2	E. McCauley	NTE	
LASDNIX	J. Fleck	T	
Two-Space-Dimensional Eulerian Codes			
TEULER	A. Buckingham	H	Turbulence models and viscosity, STAR implicit as well as explicit.
MAITAI	W. McCauley	H	Multifluid, multiphase, viscosity.
ANIMAL	I. Lindemuth	A	Implicit, toroidal geometry.
KRAKEN	R. DeBar	T	Multifluid.
RAD9	M. Cunningham	K	Multifluid.
ABMAC	J. Viecelli	T	Incompressible, multifluid, viscosity, no q.
GEM	J. Viecelli	T	Generalized mesh, viscosity.
GEMINI	L. Edwards	H	Generalized mesh, viscosity, interior rigid bodies.

Table 1 (cont.)

Code name	Principal contact(s)	Division	Remarks
FOURD	J. Fleck	T	Uses Fourier Transform, linearized hydro, plane geometry.
2D2FAZ	W. Comfort	K	Multiphase, no q.
ZAM2	M. MacCracken	G	Multiphase, incompressible, 2-dimensional Atmospheric Simulation Model with eddy viscosity.
URBMET	R. Bornstein	G	Plane geometry.
Two-Space-Dimensional Coupled-Eulerian Lagrangian Codes			
CEL	L. Edwards	H	Can use HEMP for Lagrange.
CHAMP	L. Edwards	H	CEL plus multifluid Eulerian, HEMP Lagrange.
Three-Space-Dimensional Codes			
HEMP3D	M. Wilkins	H	Lagrangian, material strength.
TOKU	J. Wilson	B	Eulerian.

Future Needs

The codes listed are all more or less production codes; there are a number of current investigations not mentioned that concern improvements in techniques, new methods, etc.

Some areas that require work and should be investigated are:

- Better numerical techniques for handling shocks not resolved by the mesh.
- Work on implicit and semi-implicit methods.
- Multiphase techniques, e.g., chemical reactions, combustion, vapor bubbles in a liquid, liquid droplets in a vapor.
- Higher order differencing methods in particular applications.
- Finite element methods for both compressible and incompressible cases on one, two, and three space dimensions.
- Comparison of finite element and finite difference solutions.
- Equation-of-state formulation implementation.
- Other *new* techniques for solving systems of partial differential equations.
- Graphic display of two- and three-dimensional solutions.

- Interactive graphics.
- Links from code to code.
- Vectorization techniques.
- Each of the codes listed requires a generator to specify initial conditions (materials, mesh, geometry, etc.) and boundary conditions. Each code also requires editing facilities to produce results in human-readable form such as numbers and pictures. Work is needed on generation and interpretation of results, particularly in the three-dimensional case.
- Mesh generators.

Chemical Kinetics and Transport Phenomena

Physical systems involving coupled chemical kinetics and dynamic transport processes are the central areas of research for many programs at LLL. For example, processes of this type constitute the focal point of theoretical analysis in tropospheric and stratospheric pollution modeling, *in-situ* coal gasification, *in-situ* oil shale retorting, chemical laser, and general combustion research. Complementary to this is the research program on the basic theory of chemical kinetics. The theoretical models for these systems are usually represented by a set of coupled nonlinear partial differential equations describing some conservation laws for the physical variables of interest, such as the number density of chemical species, temperature, pressure, etc. These systems of partial differential equations are similar in structure yet often differ in their mathematical properties. This is the result of differences in the physical domain of interest and the approximations representing the detailed molecular and atomic processes. Nevertheless, the underlying similarities do serve to identify certain common interest in computational mathematics.

In the absence of chemical kinetics many of the relevant transport processes can be dealt with by techniques and codes described in the preceding section (Hydrodynamics). The inclusion of chemical kinetics not only increases considerably the number of equations to be solved (often by factors of 2 to 20), but introduces greater nonlinearity and the so-called stiffness problems to the equations. Stiffness refers to the presence of processes with widely differing time scales (e.g., by factors of 10^3 to 10^{10}) and, in general, necessarily adds considerable computational cost to the numerical model. Any

special treatment of the difficulty must be compatible with at least some of the existing hydrodynamic techniques, or totally new solution methods must be constructed for the complete physical model. Some of the treatments developed at LLL are described in the following sections.

Pure Chemical Kinetics System

The identification and analysis of a proper and relevant chemical kinetics reaction scheme is fundamental to all studies on coupled kinetics and transport systems. For any system the importance of known and hypothetical reactions, the level of complexity in reaction schemes, and the level of accuracy desired for individual reaction rate coefficients must be studied. This can be achieved through numerical solution of the relevant nonequilibrium chemical kinetics rate equations under various constraints. To this end many programs have been constructed. At LLL both general solution techniques and specific application-type programs have been developed.

Such a program consists of a kinetics data library, data search routine, kinetics equation writer, equation solver, and sensitivity analyzer.¹⁻⁴

Kinetics Data Library — In the course of pollution studies in the upper atmosphere and urban environment, an extensive collection of chemical reactions has been gathered. This library contains a large portion of the currently available data on photochemical kinetics, including both neutral and charged species as well as radicals. The library is, and should be, constantly updated. Chemical kinetics pertinent to other systems of interest could be incorporated if justified by demand.

Data Search Routine — Given any particular chemical species, the routine will search the library and list all the pertinent reactions as well as the evaluated current kinetic rate data and catalogue number. With the information, the researcher can choose a specific reaction for further investigation.

Kinetic Equation Writer — After selecting all the appropriate reactions by catalogue number, the researcher can instruct the program to write the corresponding system of differential equations. The program automatically lists the equations and writes a daughter program.

Equation Solver — Using a reliable state-of-the-art numerical differential equation solver, the time-dependent solution for any given initial state is obtained with internal error estimation at every step of the integration.

Sensitivity Analysis — This program analyzes the sensitivity of the above solution to the uncertainties in input parameters, such as concentration of initial species, reaction rate coefficients, etc. The output from this program indicates the results of these uncertainties.

This versatile program could be used to test the significance of any reaction, reaction rate, or impurity in a complex chemical system.

On a more fundamental level, an active area in computational chemistry is the theoretical derivation of reaction rate coefficients. In principle it is possible to compute the potential energy surface for each molecule and then carry through a systematic series of collision trajectory calculations to obtain the collision cross section, the reaction probability, and hence the reaction rate coefficients. At present such an elaborate sequence of calculations is still difficult, mostly because of the absence of efficient algorithms for the necessary quantum chemical calculations. Once such computational techniques are established, many of the more difficult kinetics work in the laboratory may be circumvented.

Models of the Stratosphere and Regional Air Quality Models

In recent years LLL has developed several models of the atmosphere, both as a tool for basic research in atmospheric science and for applied research in atmospheric pollution.^{5,6} Each describes not only the relevant atmospheric motion but also the photochemistry of active pollutants. The stratospheric model is global in structure while the urban pollution model is regional in scope. All models derive the principal transport coefficients from actual meteorological data while the reactive pollutant concentrations are computed from basic chemical kinetics theory. These models usually include 10 to 20 nonlinear partial differential equations with a rather large physical domain of interest. Consequently almost all of the classical difficulties in the numerical solution of partial differential equations are present, e.g., stiffness, size of the system, nonlinearity, accuracy requirements, and computation cost. With each advance in solution technique the system can be expanded to include more chemical detail or more resolution. As a result, the development of better computational techniques for these models is necessary as long as there is a need for better accuracy and more detail.

In recent years these models have been developed under pressure for immediate application to many regional and national programs, such as the San Francisco Bay Area Air Quality Assessment⁶, the impact of ozone of exhaust from supersonic transport,⁷ nitrogen from nuclear war,⁸ and chlorine from halocarbons.⁹ With the publication of first generation models it is now possible to re-examine their structure. The numerical schemes in current models are not sufficiently flexible to allow quick modification of the computer code to suit the advances in physical theory. It is also desirable to study in detail the numerical accuracy of various schemes as they apply to real problems. Faster solution methods are necessary, corresponding to the needs of real time applications.

Computational Modeling of Flow in Porous Media

The flow of gases and liquids in underground porous media is important to a number of LLL programs. Among these are: nuclear containment, where high-pressure superheated steam from a nuclear cavity condenses in surrounding rocks; geothermal wells, where the flow consists of high-pressure saturated water and steam; and the LLL *in-situ* coal gasification program, where gases, tars, and condensing and evaporating steam flow through, and react with, a packed bed of rubblized coal.

Despite the diverse nature of their constituents, all of these flows take place in porous media, i.e., solids containing connecting voids. On a small scale the structure of these media is quite irregular, with void spaces made up of randomly connected cracks and holes. Since detailed flow calculations on this scale would be impossible, the simplifying assumption is made that each porous medium is locally homogeneous, the flow being determined entirely by local porosity and permeability and by the viscosities of the fluids.

Flows of this type are governed by Darcy's law, an empirically derived relation that replaces the usual momentum equation and which states that the fluid velocity is proportional to the local pressure gradient. This has the effect of converting the advection terms that appear in the mass and energy conservation equations into diffusion-like terms. Under these assumptions, all of the above flows are described by coupled systems of time-dependent nonlinear diffusion equations, complicated by multiphase effects when condensible fluids are present, and by chemical reactions in the case of coal gasification.

At present one-dimensional models describing gas flow and chemical kinetics in a coal bed are being compared with experimental results in coal gasification programs.¹⁰ Complementary codes describing the flow of multiphase, multicomponent fluids in porous media have been very successful in describing some experiments. A unification of these two sets of codes would then contain the essential multiphase, multicomponent flow found in *in-situ* coal gasification processes. Such unification will require modification of current numerical schemes. This, together with the desire to expand to two-dimensional models for more realistic simulations, indicates the need for considerable research in this area.

Combustion Research Program

During the past year LLL began a program of theoretical combustion research. This research is directed toward a wide variety of applications, ranging from analysis and understanding of fundamental physical processes to engineering design computer models for specific applications.¹¹⁻¹³

The principal goal of the combustion research program is to develop computer programs that can be used to analyse and design practical combustion systems. The specific requirements of these programs depend somewhat on the particular systems to which they are applied. Thus, the needs of a computer model for a turbine combustor may be slightly different from those for an internal combustion engine model. Despite such variations, the same physics is important in nearly all combustors. As a result, the present approach has been to develop a simple numerical model for each physics subsystem. Concurrently, various geometrical configurations appropriate to specific combustors are examined. The geometry is then combined with the necessary physics models to construct a simple computer model of that combustor. Specific components of the resulting model can be refined as needed.

In most combustors the important physics systems that must be included are the chemical kinetics of burning, the hydrodynamics of fluid motion, energy production and transfer, and energy losses to the combustor walls. Since the great majority of practical combustors produce a strongly turbulent environment, turbulence must also be included in any complete description. Since turbulence couples hydrodynamics, energy transfer, and chemical kinetics, a unified treatment of these processes is necessary.

This is a developing program with significant importance not only in actual applications but in creating new areas of computational mathematics. The nature of all real combustors will require the investigation of three-dimensional hydrodynamics. This alone could consume many years of intensive computational experimentation, not to mention the search for suitable numerical methods for the coupled turbulence and chemical kinetic systems.

Oil Shale Retort Modeling

A computer model is being developed to simulate the processes involved in the co-current vertical retorting of a rubblized bed of oil shale. Such a model is needed to predict *in-situ* retorting rates and oil yields for the design criteria for commercial *in-situ* retorting, and to suggest basic process changes for significant improvements in yield and cost.

The governing equations in the model are the conservation and continuity equations for a fixed-bed chemical reactor. These equations address the following processes:

- Axial transport of heat and mass in the downward flowing gas.
- Heat transfer between the gas stream and shale particles.
- Endothermic decomposition of organic material (kerogen) that results in the formation of oil, hydrocarbon gas, and carbonaceous residue.
- Endothermic decomposition of carbonate materials (dolomite and calcite).
- Endothermic reaction of carbonaceous residue with carbon dioxide evolving from decomposition of carbonate minerals.
- Exothermic reaction of carbonaceous residue with oxygen diffusing into the spent shale.
- Exothermic reaction of carbon monoxide, hydrocarbon gas, and oil vapor with oxygen in the gas stream.

Simplification of the governing equations can be achieved since the thermal capacity of the solid is much greater than that of the gas and, therefore, gaseous transients are negligible. With this approximation the reduced governing equations are hyperbolic with the characteristics parallel to the coordinate lines. The method of characteristics is then used to integrate the equations. Integration along the characteristics is performed with a stiffly stable, second-order, linear, multistep method formulated by Gear.¹⁴ Trapezoidal rule is used to start the integration.

Further developments of computation techniques are totally dependent on the mathematical model of the physical processes. As more is known about the competing processes in oil shale retorting experiments, additional physical mechanisms may necessitate changes in the character and type of the governing partial differential equations, with accompanying changes in solution methods. Consequently the relevant mathematical research in computational modeling must consider not only the eventual multidimensionality of the problem but also the continued evolution of the characteristics of the governing equations.

Laser Optics and Related Problems

Theoretical Atomic and Molecular Physics

The main efforts in theoretical atomic and molecular physics described here involve theoretical support for gas laser development. These lasers will be used in future applications for laser fusion, laser isotope separation, and laser photochemistry. Support of the gas laser effort includes understanding the basic process and the many possible loss mechanisms. Potential energy curves must be computed, interpreted, and used to study dynamic effects. Since most of the candidate laser systems are electron beam or photolytically pumped, the study of electron-atom, electron-molecule, and heavy particle scattering is of prime importance. Currently under study in support of the Laser Isotope Separation Program is the uranium atom: effects of intense fields, multi-photon effects, coherence, saturation, etc.

The basic approach for solving theoretical problems is to utilize the Laboratory's empirical modeling philosophy; i.e., semi-empirical models are developed that include theoretical models normalized with experimental results. Our recent studies on the uranium atom provide a good example. Hartree-Fock calculations were used to determine starting parameters of a nonlinear optimization process for parametrizing experimentally observed atomic spectra.

The research can be divided into six areas: atomic and molecular structure, dynamics, electron scattering and photoionization, kinetics photon physics, and data analysis. Atomic and molecular structure studies include prediction, calculation, and interpretation of energy levels and complex potential energy surfaces.¹⁵ In some cases, large matrices (10^6 to 10^7 matrix elements) must be formed, manipulated, and diagonalized. Spectral sparse matrix techniques¹⁶ and theoretical approaches¹⁷ have been developed for these applications. The area of dynamics involves the use of potential

energy curves and surfaces. Often the numerical surfaces generated in the structural studies are fit with an analytical function for the dynamic analysis. These surfaces frequently involve three to five atoms (N) that give rise to $3N$ three-dimensional hypersurfaces. These surfaces are used in a classical to fully quantum mechanical description of the interaction between atoms and molecules. Electron scattering and photoionization studies involves solving the numerical wavefunctions¹⁸ in one dimension, diagonalization of complex (imaginary) Hamiltonian matrices¹⁹ and extensive use of expansion techniques for accurate descriptions of functions.^{20,21} Rate equations, often including the effects of intense laser fields, are solved in kinetic analysis. Here the populations of various constituents (atoms and molecules in particular states) are monitored as a function of time, laser intensity, and other parameters that can be experimentally controlled. Inputs to such models include scattering cross section rate constants (i.e., quantities determined by experiment, structure, dynamics, etc.). These kinetic equations are often very stiff and require special techniques for computer study. Photon physics is a new area whose needs have not yet been determined. Data analysis consists of interpretation and modeling of experimental data. Often nonlinear optimization techniques are used to determine empirical parameters describing the experimental processes.

Numerical Calculation of Atmospheric Laser Beam Propagation

One of the major questions addressed in the military application of high-energy lasers, to which the Department of Defense is currently devoting considerable sums of money, is whether the laser energy can be effectively transmitted from laser source to target. The effects that tend to degrade the laser beam can be grouped into two categories; those that originate in the laser system itself and those that originate in the atmospheric medium through which the laser beam propagates.

In the first category we find laser medium inhomogeneities and mirror imperfections that lead to aberrations in the focussed beam, and jitter in the pointing and tracking system that leads to a statistical wander of the focal spot.

In the second category are effects of atmospheric turbulence and thermal lensing. The latter arises from small atmospheric density gradients created by molecular absorption of the laser beam. This molecular heating is nonuniform because of a transverse gradient in beam intensity and because of the

existence of a background wind that arises from natural causes, laser platform motion, and the slowing motion of the laser beam.

While all of these effects are inherently small, they become important when the laser beam is propagated over kilometer distances. A realistic description of atmospheric laser beam propagation requires a complex computer code involving both statistical and deterministic elements and requires the time-dependent solution of hydrodynamic and nonlinear wave equations in three space dimensions.²²

Currently LLL is nearing completion of a comprehensive atmospheric laser propagation code.²³ Copies of this code are being distributed to various Department of Defense contractors. Clearly, as high-energy laser technology advances and deployment of military laser systems is planned, the importance of output from this code will increase. However, the scope of problems that can be handled by this code will most certainly be limited by present generation computers.

LASNEX Code

The LASNEX code is a very general two-dimensional code that is the principal design tool for the LLL effort on the design of a laser fusion pellet. A special variant of the LASNEX code, called LASDNEX,²⁴ has been adapted for laser effects studies that require a low-temperature regime of operation. The latter code has been extensively applied to the study of laser supported detonation (LSD) waves that are generated by an intense pulse of 10.6 μm radiation from a CO_2 laser impinging on a target in an air environment. The main features of LASNEX are its two-dimensional Lagrangian hydrodynamics, a non-equilibrium treatment of plasmas with separate ion and electron temperatures, thermal diffusion of ion and electron energy, either multigroup or equilibrium diffusion of radiation, inverse bremsstrahlung absorption of laser radiation, reflection of laser rays from critical electron density surfaces, special prescriptions for anomalous laser light absorption, treatment of the spontaneous generation of magnetic fields, and thermonuclear burn. The laser light can be followed along Lagrangian grid lines, but when these become distorted it may be necessary to use the ray-trace routine that utilizes geometric optics to follow the true bending of individual trajectories of the laser light resulting from electron density variations. The LASDNEX code uses a Drude model treatment of absorption of laser light in metals at

low temperatures. The code operates in temperature regimes where single ionization is often the maximum encountered. This requires a special nonequilibrium treatment of electron and ion or heavy particle temperatures.²⁴

Magnetic Fusion Energy Research

Large scale digital computers are playing an increasingly important role in magnetic fusion energy research. Only through the use of large numerical models can the complicated physical phenomena in a plasma be adequately described.

MFE computer codes may be divided into several classes:

- Time-dependent macroscopic fluid models
- Time-independent macroscopic fluid models
- Vlasov and particle codes
- Fokker-Planck codes
- Hybrid codes

The following section contains a brief description of each of the above categories accompanied by a summary of relevant computer codes.

Existing Programs

Time-Dependent Macroscopic Fluid Models — The models described below are more commonly known as magnetohydrodynamics (MHD) codes when simulating the fast Alfvén time scale (nanoseconds to microseconds), and transport codes when simulating the diffusion time scale (milliseconds).

- RESTAB (J. A. Dibiase, D. D. Schnack, J. Killeen). The computer program RESTAB solves linearized, time-dependent MHD equations for a compressible plasma with nonzero resistivity, viscosity, and thermal conductivity. It is used to study linear resistive instabilities in a cylindrical geometry. The calculation is one-dimensional. Equations for the magnetic fields, fluid velocities, and temperatures are advanced in time by solving a system of six coupled, implicit difference equations.
- MHDXY, MHDTOR (D. D. Schnack, J. Killeen). These codes solve nonlinear, time-dependent MHD equations in two dimensions, and are used to study the nonlinear evolution of resistive instabilities.

Program MHDXY uses Cartesian coordinates, and MHDTOR is for toroidal geometries. The Alternating Direction Implicit (ADI) method is used on an Eulerian grid.

- MHD (C. H. Finan III, J. Killeen). The program MHD solves the full time-dependent MHD equations in three dimensions, and is used to study nonlinear instabilities and other three-dimensional MHD phenomena. The Douglas-Gunn algorithm in vector-matrix form is used to allow full coupling among the elements of the vectors.
- ANIMAL (I. R. Lindmuth, J. Killeen). The ANIMAL code solves time-dependent two-dimensional, Eulerian MHD equations using the ADI method. Various coordinate systems may be used. A moving grid is implemented where necessary. The program has been used to study the theta pinch and a laser produced plasma.
- RZFLU (D. V. Anderson). Program RZFLU is an explicit, two-dimensional, axisymmetric, multifluid MHD code that solves the full set of fluid equations in the quasi-neutral limit on a moving R-Z grid. Minimal numerical diffusion and arbitrary boundary conditions are features of this code.
- MAGFLU (D. V. Anderson). Program MAGFLU is an explicit, two-dimensional axisymmetric, multifluid MHD code designed to represent large anisotropies in the tensor transport coefficients. A moving orthogonal flux grid is used.
- TRANSPORT (A. A. Mirin, J. Killeen). This code solves the one-dimensional transport equations for toroidal systems in both classical and neoclassical regimes. Circular flux surfaces are assumed, and transport coefficients are based on lowest order expansion in the inverse aspect ratio. The difference scheme is implicit, second order, and iterative.
- TNT (K. D. Marx, A. A. Mirin, J. Killeen, B. E. Kelley). Program TNT solves a system of two-dimensional transport equations in toroidal as well as other geometries. Only the classical transport coefficients are currently available. The ADI difference scheme is used on a fixed nonuniform grid. The equations are linearized and solved iteratively.
- RDBP (R. P. Freis, M. E. Rensink). This multifluid transport code calculates radial profiles of plasma densities and temperatures in mirror confined systems with neutral injection beams. The set of

coupled parabolic equations is solved by an iterative, implicit finite difference algorithm.

Time-Independent Macroscopic Fluid Models — The following models are designed to compute prospective equilibrium plasma configurations and to determine their stability.

- BETA (J. Killeen, S. L. Rompel). This program computes finite beta plasma equilibria in axisymmetric configurations. The magnetic field is derived from a stream function that satisfies a nonlinear, second order partial differential equation. The resulting boundary value problem is solved by the ADI technique.
- ASTEQ (D. V. Anderson, J. Killeen). The ASTEQ program solves the combined Vlasov and plasma equilibria for the Astron device on a R-Z cylindrical domain. A vacuum magnetic field and the fields resulting from the electron layer and plasma are studied. The elliptic equation for the stream function is solved using the ADI technique with iterations.
- TOREQ (D. F. Anderson, J. Killeen). The TOREQ program is similar to ASTEQ, but toroidal coordinates are used. In the poloidal plane arbitrarily shaped convex domains are possible. Astron, Tokamak, and Levitron equilibria can be computed.
- MINIMUM-B EQUILIBRIA (D. V. Anderson, J. Killeen, C. G. Tull). This is a three-dimensional code that solves for plasma equilibria in open field geometries. The model consists of one scalar, elliptic partial differential equation involving a tensor pressure. A generalization of the ADI technique is used on a variable cylindrical mesh.
- VEPEC (D. V. Anderson, J. Breazeal). Program VEPEC computes open confinement equilibria by solving equations for the vector potential. Ampere's law is solved with the current density as a nonlinear function of the vector potential.

Vlasov and Particle Codes — The codes below are the most fundamental in that they follow in detail the motion of particles (or particle distribution functions) under the influence of their self-consistent electric and magnetic fields. They give the most detailed results, such as phase space distribution functions and orbits of individual particles.

- VLASOV (A. A. Mirin, K. D. Marx, M. G. McCoy). The VLASOV code is designed to study plasma sheath problems by solving the Vlasov equation. The model is one-dimensional (two-dimensional in phase space) and assumes a self-consistent electrostatic field. A variety of second-order difference methods is used.
- SUPERLAYER I (A. A. Mirin, J. A. Byers, J. Killeen). SUPERLAYER I is a particle code that simulates the formulations of a relativistic electron layer in ASTRON through pulse trapping and pulse stacking. It is an R-Z code in which azimuthal symmetry and a constant canonical angular momentum are assumed. Both the Lorentz and Coulomb gauges have been modeled. The equations for the vector and scalar potentials are integrated using an ADI algorithm, and the particle phase space coordinates are advanced using a time-centered algorithm.
- SUPERLAYER II (A. A. Mirin, J. A. Byers, D. Schnabel, S. L. Rompel). This code is an outgrowth of SUPERLAYER I designed to compute self-consistent magnetic fields for a high-beta mirror reactor. It differs from its predecessor in that it is a nonrelativistic Darwin model and the canonical angular momentum is not assumed to be constant, thereby requiring the solution of a separate particle equation for the azimuthal velocity.
- NOVA (B. McNamara, A. B. Landon). This is a highly modularized, very general simulation code, containing individual buffering, plotting, particle pushing, and field solving routines.
- MIRPLA (D. Fuss, B. McNamara). This is a 2 1/2-dimensional (2 spatial coordinates and 3 velocities) particle code for the investigation of electrostatic mirror instabilities. The ion equations of motion conserve energy and magnetic moment for zero electric field. A fast Poisson solver is used to compute the electromagnetic fields.
- SUPERADIABATICITY (J. A. Byers). This single particle program is designed to study superadiabaticity and confinement properties of particles moving in magnetic mirror fields and responding to fluctuating electric fields. The particles move in three dimensions.
- DCS (R. P. Freis, J. A. Byers). The DCS code is a two-dimensional simulation code that follows charged particles in self-consistent electrostatic fields with an arbitrary potential on the boundary. An iterative procedure is used to solve for steady state solutions.

- TIBRO (J. H. Foote, B. C. Howard, C. H. Finan III). This program calculates three-dimensional trajectories of charged particles in static magnetic fields. The computer code MAFCO is used to calculate the magnetic field at each orbit point based on an arbitrary set of current elements. The GEAR package is employed to advance the particle trajectories.

Fokker-Planck Codes — For thermonuclear plasmas it is generally not a good approximation to assume Maxwellian particle distributions. Furthermore, many plasmas are heated by injecting energetic particles that require a long time to slow down. To determine the actual distribution functions we require a kinetic equation such as the Fokker-Planck equation. The following codes are available at LLL.

- ISOTIONS (A. A. Mirin, A. H. Futch Jr., J. Killeen). This is a one-dimensional multispecies code that assumes uniformity in physical space and azimuthal symmetry in velocity space. The independent variable is velocity magnitude and the pitch angle distribution is that of a normal mode. A second-order, implicit difference method is employed. The code has been used to study plasma kinetics in both mirror and toroidal systems.
- HYBRID II (A. A. Mirin, J. Killeen, K. D. Marx, M. E. Rensink, M. G. McCoy, T. Cutler, L. LoDestro). Program Hybrid II is a two-dimensional multispecies code that assumes uniformity in physical space and azimuthal symmetry in velocity space. The independent variables are velocity magnitude and pitch angle. The electrons are represented by a one-dimensional distribution function. A split semi-implicit difference algorithm is employed. The code has been used to study plasma kinetics in both mirror and toroidal systems.
- TDMFP (A. A. Mirin, K. D. Marx, C. E. McDowell). Program TDMFP is similar to Hybrid II, except that the electrons are also treated as two-dimensional. The code is used to calculate electron loss rates for the direct converter.
- RWALK (K. D. Marx, C. E. McDowell, R. W. Moir, W. L. Barr). RWALK is a Monte Carlo code designed to calculate the small-angle collisional effects in a plasma. Random walks are carried out for both ions and electrons. The code is used to compute electron energy distributions at direct converter grids and to determine the ambipolar potential in mirror devices.

- HYBRID I-Z (A. A. Mirin, K. D. Marx, T. Cutler). Program Hybrid I-Z is a three-dimensional Fokker-Planck code in which an arbitrarily|spatially (Z) dependent magnetic field and plasma potential for a magnetic mirror configuration are assumed. The ion and electron velocity space distribution functions are advanced by integrating the collision operator over guiding center orbits in velocity space. An ADI method is used on a fixed two-dimensional velocity mesh.
- RFP (A. A. Mirin, A. H. Futch, Jr., D. Freeman). RFP is a radial generalization of the IOSTIONS Fokker-Planck code that takes into account finite Larmor radius effects for mirror machines. An arbitrary number of neutral beams and neutral gas species are considered.
- RUNAWAY (A. A. Mirin, J. Killeen). This is a multispecies Fokker-Planck code in which the distribution functions are expanded in a Legendre series. An electric field term is included, enabling one to treat the problem of runaway electrons and ions in a Tokamak.

Hybrid Codes — We classify as hybrid codes those that combine two basically different computational models. Two such codes are given below.

- FPT (A. A. Mirin, J. Killeen, K. D. Marx, M. R. Rensink, M. G. McCoy). The Fokker-Planck Transport code is a radial transport code in which energetic species are modeled using Fokker-Planck equations. Radial profiles for an arbitrary number of background ion species are represented as functions of time, and the hot species are represented as distribution functions in two-dimensional velocity space for each radial position. Iterative, implicit-difference algorithms on a fixed Eulerian mesh are used.
- GUIDON (C. G. Tull, T. H. Johnson, J. Killeen, M. E. Rensink). The GUIDON code is a combination of two separate physical models for axisymmetric confinement systems — a single fluid MHD representation of a background plasma and a guiding center particle simulation of beam-injected particles. The calculation is magnetically self-consistent. Relatively long time scales may be run, since the particles are advanced with guiding center formalism.

Discussion

A fundamental question concerning MHD and transport codes is the type of coordinate system to use. Flux coordinates tend to represent the physical phenomena fairly well if the problem of singularities and rezoning is handled adequately. Alternatively fixed standard (Cartesian, cylindrical) coordinate systems do not possess the rezoning problem but are inadequate in representing anisotropic transport when the perpendicular and parallel transport coefficients differ by several orders of magnitude.

Most of the aforementioned codes are two-dimensional. To adequately describe plasma phenomena, three-, four- and possibly five-dimensional codes will be needed. This will require, in addition to larger computers, more sophisticated programming techniques and numerical methods. Also because of the complexity of the higher dimensional equations, symbolic programming may be not only helpful, but indispensable.

Future Research

As indicated above, codes of dimension greater than two are required to describe plasma phenomena adequately. Work on three-dimension codes is already in progress.

The three-dimensional MHD code of Finan and Killeen is intended to be an all-purpose MHD code. It is written in general orthogonal coordinates and includes a complete MHD description of the plasma. Problems of long duration with a wide spectrum of time scales will be challenging.

A variety of numerical techniques will be investigated to compute plasma equilibria in three dimensions. The program of Anderson and Breazeal uses the ADI technique to solve the elliptic system, whereas the code of McNamara and Boyd (under development) uses Fourier transforms. Cyclic reduction will soon be investigated.

Much research is needed to construct higher-dimensional Fokker-Planck codes. Program HYBRID I-Z of Mirin and Marx (rewritten by Cutler) will be generalized to include an arbitrary number of ion species. To describe mirror systems more fully, radial dependence must be added to this code — a formidable task.

The GUIDON code of Tull, *et al.* will undergo a number of changes, the most important being the inclusion of a time-dependent MHD model rather than the existing equilibrium solver. The transport model in the FPT code of Mirin *et al.* will be generalized for arbitrary magnetic flux surfaces. This will require coupling in a cylindrical equilibria model such as the one currently used in GUIDON.

Information Processing

The applied mathematical research described in this section deals essentially with computational techniques to improve the Laboratory's ability to handle experimental data. Research areas include applied estimation theory, integral equations, mathematical statistics, pattern recognition, computational mathematics, and information theory.

Most of the research is associated with developing tools to process two-dimensional data sets. This reflects LLL needs and capabilities. These programmatic needs stem from the extensive use of image media for information recording and storage in experimental physics. Many of these applications involve diagnostic radiography. While computational signal processing has been used considerably in time-series analysis and filtering, the extension of these methods to two-dimensional data has been limited by computational and mathematical difficulties. The availability of our large-scale scientific computers has allowed us to study these problems, and motivated the development of relatively sophisticated and complex processing techniques.

Signal processing research will be divided into four main categories. The first is modeling to achieve a well-defined mathematical description that agrees with real-world phenomena. Development of the processing algorithms to solve problems is the second category. This development is dependent upon the construction models. In the third, computation issues related to the feasibility of the processing algorithms are studied. The fourth category contains more general research that extends two-dimensional theory to high-dimensional parameter spaces (Fig. 1).

Modeling

Modeling constructs appropriate mathematical systems, interpreted here in a signal processing context, to correspond with real-world phenomena. Subsequently these mathematical systems are analyzed to achieve a better understanding of the modeled phenomena. Under this broad research topic are three areas; sampling expansions, spectral estimation, and nonlinear models (Fig. 2). Each of these areas will be elucidated. Sampling theory is often the key element relating the discrete mathematics of computation to continuous space and/or time measurements. This theory has application to the solution of ordinary differential equations (ODE) and partial differential equations (PDE) by computer. The second area, two-dimensional spectral estimation, can be

Fig. 1

Fig. 2

viewed as the problem of determining finite-parameter system models for measured data by approximation in the wave number domain. Such finite-parameter models are used in characterizing the signal and noise in filtering problems. The third area, nonlinear modeling, contains models for the photographic process as well as for the response of the eye to visual stimuli.

Major Results — Optimum linear formulas have been developed for estimating continuous data from samples. Also the least upper bound on the error has been derived for an arbitrary linear reconstruction scheme^{25,26} for large classes of signals. The maximum entropy spectral estimation procedure has been extended to two dimensions²⁷ using the Markov field concept.²⁸

Future Plans — We will extend our sampling results to the two-dimensional case and apply them to imaging problems in an effort to reduce sampling rates and hence computational load. We will explore two-dimensional spectral estimation using explicit rather than implicit schemes. We will do picture coding using our newly developed two-dimensional recursive filtering results as well as investigate data compression for digital secure voice encoding and speaker verification. A major effort will be devoted to extending our optimum linear processing schemes to nonlinear and/or space-variant models.

Processing Algorithms

Processing algorithms are the mathematical formalisms by which the models are analysed. The processors may be divided into two sets depending on whether the problem is deterministic or stochastic (Fig. 3). The study of deterministic processors focuses on both recursive and nonrecursive filter design utilizing both a homomorphic method, involving a joint, nonlinear optimization, and a new version of the complex differential-correction algorithm. These filters can be used in many signal processing problems arising from two-dimensional experimental physical measurement, e.g., flash x rays and multiwire proportional counters.

For stochastic problems we have investigated the problem of two-dimensional Kalman discrete filters. This has been done for both scalar and vector scanning of two-dimensional data. These filters have application as recursive estimators for the random signal in noise problem.

A special class of the stochastic processors, namely those resulting from inverse problems, deserves special attention both because of its practical

Fig. 3

importance and difficulty of solution. The turbulent imaging problem is in this class.

Major Results — A stability test for two-dimensional recursive filters has been developed.²⁹ A general theory of two-dimensional spectral factorization³⁰ has led to a new design method³¹ for deterministic recursive filters. In the stochastic area, algorithms have been derived to allow near optimal Kalman filtering of images both in a vector and a scalar mode.^{32,33}

Future Plans — We will develop the method of Ekstrom *et al.*³¹ into a general design tool for producing high quality, L^P -approximate, half-plane recursive filters. The Kalman filtering routines will be applied to space-variant models and nonlinear processing methods, i.e., extended Kalman filter.

Under the heading of stochastic processing we will continue our study of two-dimensional Kalman filtering formalisms (both a scalar processor termed the reduced update Kalman filter and a vector processor termed the Kalman strip filter). We will also investigate the two-dimensional Wiener and constrained least-squares approaches. These stochastic processors are useful for performing image restoration when noise and signal can be usefully characterized by their second-order properties, e.g., imaging through the turbulent atmosphere using a short exposure time.

Computational Procedures

Computational procedures are the means of implementing the processing algorithms for computation on digital machines. This area deserves special attention in two-dimensional applications because of the often severe data management problems. We study digital implementation with large vector machines and special purpose configurations. The study is further divided into the equally important aspects of computations organization and memory management. The particular algorithms chosen for this study concern two-dimensional recursive filtering and two-dimensional Kalman filtering, of both the vector and scalar variety (Fig. 4).

Major Results — The merits of recursive vs nonrecursive filtering have been evaluated *vis-a-vis* the speed and memory size of the machine.³⁴ Also very efficient procedures for transposing large matrices that cannot be stored

Fig. 4

completely in core have been developed.³⁵ This has application to the two-dimensional fast Fourier transform programs, which are very useful in wave number filtering as well as in implementing large nonrecursive filters. Further, moderately sophisticated implementations of our two-dimensional Kalman filtering algorithms have been achieved.

Future Plans — We will study in more detail the specific problems of computation organization and memory management for both recursive and Kalman filtering of images, for both large vector machines and special purpose minicomputer type machines.

General Theory

This area is concerned with the extension of present two-dimensional theory in the realm of recursive procedures for estimation and detection in the stochastic case.³⁶ In both deterministic and stochastic areas, we are concerned with multidimensional extensions of two-dimensional signal processing theory and methods.³⁷ Multidimensional theory is studied to develop first a general theory of spectral factorization that will subsequently be applied to develop stable recursive operators or filters.

Also under the broad topic of general theory, we will investigate the pattern recognition approach to image analysis. This area has application in the biomedical area as well as in nuclear physics. We will be particularly concerned with the overlap between pattern recognition and signal processing, where the possibility of cross-fertilization is greatest (Fig. 5).

Major Results — A general likelihood ratio formula has been developed for the two-dimensional case.³⁶ This recursive formula leads to efficient implementation of optimal detectors for a large class of image fields. We are presently formulating a general theory of spectral factorization in N dimensions.³⁷ Results to date indicate a reasonably straightforward extension of the two-dimensional results.

Future Plans — We will implement optimal detection via likelihood ratios in combination with two-dimensional Kalman filters (reduced update and strip filter) which provide the required casual estimate. We will extend two-dimensional methods of design for recursive filters to the multidimensional case. We will investigate the pattern recognition approach from a signal processing viewpoint.

Fig. 5

Chemistry

The development of improved and more efficient mathematical techniques is crucial to the continued progress and success of computational chemistry because of the complexity of problems and the extent of data sets with which the modern chemist is involved. The following list is illustrative of the mathematical tools underlying broad areas of computational chemistry at LLL with respect to present research and future requirements. Much of the previously described work on theoretical atomic and molecular physics is also applicable to computational chemistry.

Crystallography.

Current procedures at LLL have used brute force matrix diagonalization methods for x-ray data refinement in crystalline structure determinations. Computational work has focused on intermetallic compounds, especially those containing plutonium, organic compounds relevant to high-explosives work, and inorganic compounds, especially those with appropriate high-temperature characteristics.

Future Direction and Needs — Fast Fourier transforms are needed to increase the speed of least-squares refinement of atomic coordinates, since one goes through a phase-minimization process by proceeding through convolution to fast Fourier transformation to derive the structural model. In addition, when dealing with powders rather than crystals, the automatic computer indexing of the powder pattern of a material whose unit-cell dimensions and crystal symmetry are not known in advance has long been a goal.

Improvements in fast Fourier transform techniques and convolution algorithms should be high priority projects during the next two to five year period. The library of codes used in the crystallographic work at LLL must be examined and optimized, perhaps for conversion to the CDC STAR-100 system. These codes include the STRUCTURE³⁸ and QTEST³⁹ computer codes. Improvements in graphical display procedures are being given attention,⁴⁰ and much additional work is needed in this area.

Statistics and Pattern Recognition

Pattern recognition is the mathematical process of determining one class of information from a data set containing information of much greater dimensions.⁴¹ It is a more general case of dimension reduction and is also one

of the branches of the science of artificial intelligence. It combines computer science and applied mathematics and has shown great promise in providing a general approach to solutions of widely different problems of data analysis.⁴²

A general statement of the type of problem that pattern recognition attempts to solve is as follows: given a set of objects and a list of measurements made on these objects, is it possible to find or predict a property of the objects that is not directly measurable but is known to be related in some unknown manner? In a simple example it would determine the concentration of component A from a set of analyses of a mixture containing component A in a situation where a simple analysis is not available. For simple analyses the process is relatively straightforward, but becomes difficult when the input data is inherently multidimensional, i.e., where the variables are interdependent. This is the case, for example, for an analysis that must contend with coordination reactions, matrix effects, nonlinear detectors, and nonlinear excitation. The problem also occurs for linear multidimensional data such as that obtained from photomicrographs or scanning electron micrographs.

During the past ten years researchers at LLL have applied various statistical and pattern-learning techniques to chemical data. From this work it was shown that reliable results can be obtained from data sets not believed to contain such information. Pattern recognition analyses are carried out on large general-purpose computers using PATTERN, the LLL interactive pattern recognition program.⁴³ Recent or current studies include modeling economic processes, chemical spectral analysis, modeling analytical chemistry processes,⁴⁴ improved uranium exploration, studying the connection between air pollution and health, the aging of multicomponent systems, compound (chemical) design, studying production related materials problems,⁴⁵ and relating chemical structure to biological activity.⁴⁶

Future Directions and Needs -- In certain cases, one can directly determine a molecular configuration from mass spectrograph, mass intensity data. One can train a program to discriminate between acceptable and nonacceptable performance for routine analyses using a training set. This area needs further development to improve available techniques, to develop new methods and techniques, and to define levels of confidence for the perceived pattern.

Future plans in using pattern recognition also include method/code development and improvement of machine-analyst interactions. The possible

uses of mini- or microcomputers for interactive graphics will be investigated. Application will be expanded in studying biological activity, materials science information, and crime analysis.

Reaction Dynamics and Scattering

Reaction dynamics and scattering theory involve the use of potential energy curves and multidimensional energy surfaces. For the dynamics these multidimensional hypersurfaces are fitted by an analytical function requiring complicated nonlinear fitting procedures and pattern-search techniques.⁴⁷ Scattering events include not only reactive and nonreactive chemical interactions, but also electron scattering and photoionization. The latter involve solving for numerical wavefunctions in one dimension,¹⁸ diagonalization of complex (imaginary) Hamiltonian matrices,¹⁹ and extensive use of expansion techniques for accurate descriptions of function.^{20,21}

Future Directions and Needs — Improvements in the pattern-search techniques used in the fitting of the multidimensional hypersurfaces must be devised and exploited so that the nonlinear analytical representations of the multidimensional data can be obtained.

In electron scattering and photoionization, much development of the underlying mathematical techniques in these very active areas can be expected in the next two to five years.

Numerical Mathematics and Statistics

This section contains a description of general efforts in numerical mathematics and statistics at LLL. In contrast to most of the previous sections, this work tends to be oriented toward broad coverage of mathematical problems in programs at the Laboratory, rather than being concentrated in a particular area of application.

Statistics

Statistics is a methodology for planning and designing experiments, summarizing experimental data, and drawing inferences or conclusions from the data. It is clear that there is need for much work in this area at LLL, and applications occur in essentially all departments and divisions of the Laboratory.

The activities of LLL's small statistical staff have primarily been direct consulting and problem solving, very little time (less than 10%) left for basic research. This should not be taken to imply that there is no need for statistical research at LLL. To the contrary, because of the size and complexity of Laboratory problems that are presented, it is continually necessary to extend existing statistical methods or develop entirely new techniques. The following is a partial list of problems addressed by LLL statisticians in recent years.

- Design and analysis of experiments (e.g., Ref. 48).
- Specifications for device components.
- Stochastic modeling applications.
- Application of queuing theory to the analysis of the drum input/output queue.⁴⁹
- Computation of percentile curves for salary guideline determination.
- Development and analysis of a failure rate model for Shiva.⁵⁰
- Linear and nonlinear regression analyses (many).
- Exploration of source data to find causes of unreliability in LLL computer systems.⁵¹
- Proposal of ways to use statistics to fine tune computer operating systems.⁵²
- Development of methods for measuring system performance.⁵³
- Formulation and analysis of a game theoretical model for missile vs missile strategy.

Future Needs — The Laboratory needs in statistics and probability theory are constantly expanding. For example, statistical studies in the planning stages of all LLL's experimental programs would ensure that the resulting data provide the maximum amount of useful information for the resources expended. It would also be in the Laboratory's interest to conduct research in accelerated life testing and in curve fitting techniques other than least-squares fitting. Accelerated life testing is a very promising method for assessing the reliability of extremely reliable devices (since testing under actual operating conditions would take too long). Least-squares fitting (linear and nonlinear) is not always the proper method for curve fitting. There are many other alternatives that must be explored, ranging from selecting a different minimization criterion (i.e., not minimizing the sum of squares of the residuals) to using approaches similar to those in pattern recognition.

Numerical Mathematics

To provide a setting for LLL work in numerical mathematics, we quote from COSERS.⁵⁴ "The output of research in numerical computation can be roughly divided into three categories: theory, methods and algorithms. ... By methods we mean general techniques and approaches that can be applied to a particular kind of problem. ... When a computational procedure is completely specified by a computer program we speak of it as an algorithm." According to this definition, approximately 60% of the LLL effort in numerical mathematics can be categorized as research in numerical computation. (Note that this differs somewhat from the definition of research given in Chapter 3 of this report.) Most of this work is in the development of numerical methods and algorithms, with some related theoretical work in the analysis of algorithms. The resulting general methods and software are used in many of the application areas described in other sections of this report.

Mathematical Software — To quote again from COSERS, "...if [an algorithm] has further attributes such as convenience of use, good documentation, detection and diagnosis of failure, and the like, we describe it as mathematical software. Even relatively specific methods ... have a wide variety of possible implementations. The difference in quality can be enormous. Mathematical software makes methods efficiently and widely available." A large fraction (50%) of the total numerical mathematics effort is devoted to mathematical software production and dissemination. This includes the development of software for library access and maintenance as well as the construction and testing of the mathematical software itself. Much of the latter also involves preliminary analysis of methods for accuracy and stability, and numerical comparison of methods, before actual commitment to software. This work on software development is designed to provide a collection of accurate and robust tools for the solution of numerical problems that frequently occur in the Laboratory's programmatic areas.

Mathematical Software Library — As a general laboratory service, a Mathematical Software Library (MSL) is maintained on the photostore.⁵⁵ In addition to software developed at LLL, MSL contains the best mathematical software available from external sources.

Ordinary Differential Equations — Laboratory needs (e.g., in chemical kinetics and atmospheric simulation problems) for the solution of the initial

value problem for large systems of stiff ODE's led to development of the GEAR package.⁵⁶ This package contains sophisticated algorithms for changing step size and integration method in an attempt to achieve optimal error control. As more and more applications have been found for GEAR, variants have been developed to take advantage of the special structure of the problem:

GEARB — banded Jacobian matrix.

GEARBIL — banded Jacobian, block-iterative solution for matrix in LCM.

GEARIB — implicit ODE's, banded Jacobian.

GEARS — general sparse Jacobian.

GEARV — vectorized.

Certain diurnal problems (in the atmospheric simulation model) could not be handled efficiently by GEAR. This led to the development of a new code, called EPISODE,⁴ which is based on truly variable step formulas. The variant EPISODEB, comparable to GEARB, is in the final documentation stage. This work represents years of analysis and performance testing to determine the best strategies to use of various classes of problems. Several Laboratory codes for solving chemical kinetics and atmospheric simulation problems (see section on Chemical Kinetics and Transport Phenomena) are based on variants of GEAR or EPISODE.

Partial Differential Equations — Use of the numerical method of lines coupled with the robust stiff ODE solvers described above has led to the development of PDESOL,⁵⁷ a very flexible package for the solution of a large class of nonlinear PDE's. While PDESOL is currently restricted to one(space)-dimensional parabolic PDE's, it can handle certain elliptic and hyperbolic problems, and plans have been made for extensions to two-dimensional problems. Currently under development is a new package, PDECOL, which uses collocation rather than finite difference methods for discretization of the spatial variable. It promises to be a significant improvement over PDESOL in terms of computational effort required for a specific accuracy for many types of problems. The major advantage of these general packages is that they enable the scientist to try a large number of mathematical models and solution techniques with relatively small investment in code development.

Linear Algebra — To support the software for solution of ODE and PDE systems, it has been necessary to develop software for the efficient solution of linear algebraic systems. Most of this software performs direct

solution of full or banded systems, but iterative methods have also been employed. A recent introduction has been the package YSMP for solution of sparse systems with arbitrary structure. An efficient routine for block tridiagonal systems has been developed, resulting from a need in the ANIMAL code (see section on Hydrodynamics). Software for the least-squares solution of overdetermined linear systems is in heavy use in data fitting applications through the Laboratory. Recently installed software for singular value decomposition promises satisfactory solutions to arbitrary linear system problems. As indicated in the section on Algorithms for new Computer Architectures below, work is in progress on the development of linear system software for the STAR-100.

While most matrix eigenvalue problems are adequately handled by the NSF-funded package EISPACK, much work is still needed in the treatment of large sparse matrices. In fact, the heart of the recently developed LLSMC (Livermore Lanczos Shell Model Code)⁵⁸ for the solution of a certain form of the Schroedinger equation is a vectorized implementation of a modified Lanczos algorithm for iteratively estimating eigenvalues of very large, sparse, symmetric matrices. Also under investigation are iterative refinement techniques for improving the accuracy of calculated eigensystems.⁵⁹

Interpolation and Surface Fitting — Motivated by the need for a more accurate representation of equation-of-state surfaces, work is well under way on the development of a collection of routine for one- and two-dimensional interpolation and least-squares fitting by piecewise polynominal functions (mostly cubic splines).⁶⁰ A large collection of software for solving non-linear least-squares and more general optimization problems has also been gathered. These are in the process of evaluation for applicability to Laboratory problems.

Miscellaneous — Other mathematical software is continually undergoing development and/or evaluation. Routines for accurate evaluation of many of the special functions of mathematical physics are made available as they are implemented and tested. A large number of routines for automatic evaluation of definite integrals is now available. Recent additions include routines to handle singular or highly oscillatory integrands. There is also continuing research on algorithms for evaluating multiple integrals.

Plans and Future Needs — Future efforts in mathematical software will include further development of all the above packages as needed to enhance the Laboratory's problem-solving ability. This will include the comparison of finite difference and finite element methods on Laboratory-related problems and the extension of the PDE packages to handle two-dimensional problems. There is a need for some fairly general packages with interactive graphics capabilities for fitting curves and surfaces to experimental data.

On a more general level, design of adequate test codes is of great importance, so that users can be assured of the quality of the software employed in the solution of their problems. In fact, basic research is needed on criteria for correctness of numerical software.

Algorithms for New Computer Architectures — Because LLL traditionally obtains the first of a new line of computing hardware, it is appropriate that some research on numerical algorithms for new computer architectures be supported by the Laboratory. In the past year about 25% of the numerical mathematics effort has been devoted to the development and testing of modules for the evaluation of vector elementary function for the STAR-100,⁶¹ the implementation and comparison of various algorithms for the solution of tridiagonal linear systems,⁶² and the development and analysis of a class of new methods for multiplication of banded matrices and solution of banded systems on vector processors.⁶³ Investigations are in progress on the linear algebra employed by two large hydrocodes (ANIMAL and LASNEX) to improve their efficiency on the STAR-100. Extensive investigation of the solution of PDE's on vector processors is contemplated.

Future Needs — The increasingly complex nature of current and planned new computer architectures demands a much more vigorous research and development program to make effective use of the potential of these new computers for numerical problem solving.

Other Applications

In this section, a number of more specialized studies are described that are generally outside the scope of research and development presented in earlier sections.

Solid and Structural Mechanics

The mechanics of solids treats continua having strength, as distinguished from fluids and gases. Here, the dimensions of the field are the same as that of the geometry. The mechanics of the structures deals with topologies of lines or surfaces embedded in a higher dimension. Thus, the governing equations of continuity for rods, beams, plates, shells, and solids involve distinct differential operators. The addition of constitutive relations such as plasticity and viscoelasticity, as well as elasticity, complete the governing system of equations, but form a more general problem than simply a set of PDE's. Mechanics treats the dynamic case containing second time derivatives and the quasi-static case where these terms are ignored. For linear elastic solids, the dynamic system is hyperbolic and for the static it is elliptic. The finite-element method (applying the Galerkin concept) is a powerful and versatile method of spatial discretization for all the classes of structures and solids, and especially for problems combining classes. Finally, implicit as well as explicit time integration methods are exploited, the former especially for stiff problems in dynamics. The static or equilibrium problem becomes a degenerate form of the implicit transient algorithm.

This work involves direct interaction with national technology development, implementing and extending outside codes, as well as original development. Key current and projected computational research follows.

Three-Dimensional Analysis — The use of higher order, finite element expansions within the eight node brick permits good bending behavior with coarse grids modeling linear elastic solids. Thermal gradients (source terms) can be captured as well.

The large capacity, block equation solver used in general three-dimensional structure computation is being optimized for improving data management and bandwidth minimization. Also, out-of-core profile solvers are being explored. These solvers can be vectorized for STAR application.

The lateral response of solids having axisymmetric geometry but non-symmetric loading is a three-dimensional problem. Expansion of the solution in a Fourier series about the axis of symmetry offers a compact description for problems of moderate transverse behavior. In fact the linear problem decouples into a superposition of two-dimensional problems. A code is under development to utilize this Fourier series in the angular variable with finite-element discretization in the (r, z) plane. Nonlinear behavior couples the

modes, but still results in an order of magnitude less computation than brute force three-dimensional brick discretization.

A three-dimensional, finite-deformation, explicit, finite element code is being developed to permit the dynamic analysis (including shock waves) of structures that cannot be characterized as axisymmetric. Thus far, elastic-plastic, soil, crushable foam, and hyperelastic (rubber) constitutive properties are implemented. Additional material types considered include compressible fluids and viscoelastic solids. The capability of the code at present permits over 2000 nodal points and brick elements. Automatic substructuring techniques are under consideration to enlarge this capacity by an order of magnitude.

Slide Lines and Voids — Often slip surfaces are required to model the behavior of physical systems properly. Available finite element codes do not provide this capability and, as a consequence, their usefulness may be restricted. To eliminate this shortcoming, a finite deformation, elastic-plastic, explicit, finite element code for slip surfaces has been developed and verified.⁶⁴

The formulation is based on a time-dependent transformation matrix that imposes constraints upon the equations of motion. These constraints have the effect of constraining the nodal points along a material interface to slide along the interface without penetration. A generalization permits voids to open whenever tensile stresses appear. Closure of voids poses a much more formidable problem since shock interface conditions must be imposed to properly set the interface velocities. Tied sliding, which is a special case, permits variable zoning at the material interface but does not permit sliding to occur. In this case the transformation matrix is independent of time and the formulation is exact.

Astrophysics

In addition to the previously mentioned hydrodynamic codes, there are several astrophysical codes:

- PER ASPRA: This is an axially symmetric hydrodynamics code with magnetic and gravitational fields, and neutrino transport by one group diffusion. It is used to calculate the collapse of old magnetic rotation stars. A version of the code exists with post-Newtonian approximation.

- ADASTRA: This program is a spherically symmetric hydrodynamics code with neutrino transport by multigroup discrete ordinates. Equations are general relativistic. The ADASTRA code is used to investigate supernova models and stellar collapse.
- SN: This program is used for the investigation of supernova models. It is a spherically symmetric hydrodynamics code with nonlocal thermodynamic equilibrium neutrino transport in multigroup diffusion. It uses an approximate form for general relativity, and includes neutral current effects in neutrino calculations, very detailed neutrino - material interactions, and equations of state.
- COKU: This program is an axially symmetric general relativistic hydrodynamics code with magnetic fields. The metric is assumed to be an explicit function of all variables with the exception of time. COKU is used to calculate the collapse of super massive stars. NOKU is a special version for use in the calculation of neutron stars.
- ROKU: This is an axially symmetric general relativistic hydrodynamics code with magnetic fields and a Kerr metric. It is used to calculate the flow of magnetized gas near a rotating charged black hole.
- TOKU: This is a three-dimensional Newtonian hydrodynamics code with gravitational field in a rotation coordinate system. It is used to investigate the stability of rotation stars, and material accretion in binary star systems.

Monte Carlo Methods

Monte Carlo methods may be loosely defined as those using random numbers and probability theory to get approximate answers (estimates) to mathematical and physical problems. These methods are usually reserved for problems whose treatment by more traditional methods is too difficult and/or time consuming.

Most of the Monte Carlo effort at LLL is in the field of neutron and radiation transport. Codes such as TART, MORSE, and others use more or less direct simulation of the individual particle transport processes to obtain results. More sophisticated variance reducing techniques are employed sparingly; these are potentially powerful but very hard to incorporate into these general purpose codes. (MORSE does have an adjoint option that is beginning to be used in shielding and deep penetration problems.)

In the T-Division four-dimensional laser code, Monte Carlo methods generate random phase screens to account for air turbulence. Current or recent LLL usage of Monte Carlo includes vulnerability studies and migration of faults in crystal lattices.

Monte Carlo methods are not readily adaptable to a vector mode of operation; most problems are essentially serial in nature. On the other hand, round off and truncation are seldom problems in Monte Carlo work. There might be some benefits in STAR operations with the two 32-bit work arithmetic option (rather than one 64-bit word).

Chapter 3

CONCLUSIONS AND RECOMMENDATIONS

Conclusion/Summary

As indicated in the Introduction, there is considerable R/D activity in applied and computational mathematics at LLL, despite the absence of a formal research program. Estimates of the distribution of this effort associated with the major application areas are given in Table 2. These figures represent composite FTE's rather than the number of specific individuals. The work is divided into the following categories:

- Research — Efforts or studies involving the development of new formalisms and methods (algorithms).
- Code Development — Computational implementation of specific methods.
- Applications — Use of computer codes and/or analysis for specific problems.

These numbers should be considered as best estimates of manpower directly involved in each area. The majority of R/D is generally oriented toward specific programmatic needs. As indicated in the table, this work is principally associated with the more development-related activities of code development and applications. Fundamental research involves only approximately 7% of the total effort of 365 FTE's. Based on the current research and development activity, certain categories of future needs of the Laboratory can be identified. Table 3 presents a summary of future research areas based on these needs. This table is a synthesis of the material described in Chapter 2. The three generic categories serve as a basic framework for broadly associating the applied and computational mathematics research essential to various Laboratory programs.

Table 2. Estimated distribution of applied mathematics efforts at LLL.

Application area	Expended Effort (FTE)			Total
	Research	Code development	Application	
Hydrodynamics	10	100	130	240
Chemical kinetics/ transport phenomena	3	10	15	28
Laser optics and related problems	4	9	12	25
Magnetic fusion energy research	2	9	13	24
Information processing	5	3	7	15
Chemistry	—	4	10	14
Numerical mathematics and statistics	2	5	7	14
Other applications	<u>1</u>	<u>2</u>	<u>2</u>	<u>5</u>
	27	142	196	365

There are a number of important conclusions that can be drawn from the preceding chapter and these two tables:

- There is a very broad spectrum of applied and computational mathematics R/D at LLL. The Laboratory has competent and well-informed research in most mathematical areas of programmatic interest.
- Only a small percentage of the total R/D effort is directly involved with fundamental research. It is the general consensus of those associated with this survey that all Laboratory programs would benefit from more basic research in applied and computational mathematics.
- It is evident that the people performing this R/D function are scattered throughout the Laboratory. As a consequence, there is considerable difficulty in coordinating related efforts. This has resulted in limited communication among researchers and some duplication of effort.
- There is an apparent time lag in incorporating new computational schemes into programmatic applications. Most of the heavily used application codes employ numerical methods that are at least ten years old despite important algorithmic advances during this period.

Table 3. Future research areas.

Generic category	Description of research areas and potential application
Improved numerical modeling capability	<p data-bbox="576 378 1312 438">Hydrodynamics — multifluid, multiphase, multi-dimensional.</p> <p data-bbox="576 459 1390 520">Chemical kinetics — porous flow, coupling to transport, reactive turbulence, kinetics theory.</p> <p data-bbox="576 541 1390 632">MFE — multidimensional MHD, multidimensional and multispecies Fokker-Planck, nonequilibrium plasma simulation.</p> <p data-bbox="576 653 1344 714">Equation of state — mathematical formulation and implementation.</p> <p data-bbox="576 735 1438 825">Lasers — atomic and molecular theory, multidimensional nonlinear wave propagation, laser material interaction.</p>
Improved ability to handle experimental data	<p data-bbox="576 842 1451 903">Information modeling — multidimensional sampling theory, spectral estimation, function representation.</p> <p data-bbox="576 924 1386 984">Processing — multidimensional nonlinear processors, stochastic and deterministic formalisms.</p> <p data-bbox="576 1005 1438 1066">General — optimal detection and classification, multi-dimensional spectral factorization.</p> <p data-bbox="576 1087 1101 1117">Implementation — fast transforms.</p>
Enhanced numerical techniques for general application	<p data-bbox="576 1129 1438 1251">Partial differential equations — implicit vs explicit methods, finite element vs finite difference methods, interface and discontinuity representation, higher order methods.</p> <p data-bbox="576 1272 1341 1333">Ordinary differential equations — stiff systems, general solution package.</p> <p data-bbox="576 1354 1406 1415">Matrix operations — sparse matrices, diagonalization techniques for large matrices, eigensystems.</p> <p data-bbox="576 1436 1373 1497">Interpolation — multidimensional, nonlinear least-squares.</p> <p data-bbox="576 1518 1406 1579">Statistics — accelerated life testing, general curve fitting techniques, advanced Monte Carlo methods.</p> <p data-bbox="576 1600 1373 1661">Vectorization — restructuring numerical algorithms to utilize new computer architectures.</p>

- Despite the Laboratory's tradition of acquiring Model 1 of new high-performance scientific computers, there is virtually no research pursued on the compatibility of numerical algorithms and advanced computer architectures. One result of this is the lack of proper projection of future programmatic computer requirements for utilizing advanced algorithms and architectures.

Recommendations

To address the issues raised above, we recommend the following. As a necessary first step we recommend that *the Laboratory adopt a formal policy to establish and support a research program in applied and computational mathematics*. This program should take advantage of existing expertise that is distributed throughout the Laboratory. This would allow utilization of the unique opportunity that exists here to carry out fundamental mathematical research within the context of physical applications. Proper sources (both internal and external) of financial support for this program should be identified and developed.

While the precise scope of this program must depend (in both direction and extent) on these sources of support, we recommend the inclusion of:

- The formation of a Laboratory-wide coordinating committee for applied and computational mathematics (A/C Math). It is proposed that this committee would serve two functions.
 - Coordinate and review internally and externally funded basic research in A/C Math.
 - Serve in an advisory capacity to programmatic developments in A/C Math.

This committee should be comprised of knowledgeable representatives from various divisions and programs of the Laboratory. As such it would serve as the focal point of communications between individual researchers and programs.

- The re-institution and support of a Visiting Scientist and Post-doctoral Program. This would broaden the Laboratory's expertise and is in direct support of the established objective of ERDA in technology transfer. Furthermore, other means of enhancing interactions with the outside community should be explored, such as sponsoring and organizing appropriate symposia and conferences at LLL. By encouraging programmatic participation in these activities,

timely implementation of new advances in computational mathematics could be achieved.

- The study of the interactions between mathematical methods and computer architectures. This study is necessitated by the Laboratory's ever-increasing requirement for computational capability. Development of methods tailored for current hardware should be a part of this study. However, its major objective should be the analysis of the compatibility of advanced numerical algorithms and computer architectures.

REFERENCES

1. R. P. Dickinson and R. J. Gelinas, *SETKIN: Chemical Kinetics Preprocessor Code*, Lawrence Livermore Laboratory, Preprint UCRL-77001 (1975).
2. R. P. Dickinson and R. J. Gelinas, *Sensitivity Analysis of Ordinary Differential Equation System - A Direct Variation Method*, Lawrence Livermore Laboratory, Preprint UCRL-76811 (1975); *J. Comp. Phys.*, in press.
3. R. J. Gelinas and R. P. Dickinson, *GENKIN-1, A General Kinetics Code for Atmospheric Application*, Lawrence Livermore Laboratory, Rept. UCID-16577 (1974).
4. G. D. Byrne and A. C. Hindmarsh, "A Polyalgorithm for the Numerical Solution of Ordinary Differential Equations," *ACM Trans. Math. Software*, 1, 71 (1975); Lawrence Livermore Laboratory, Preprint, UCRL-75652 (1975).
5. J. S. Chang, A. C. Hindmarsh and N. K. Madsen, "Simulation of Chemical Kinetics Transport in the Stratosphere," in *Stiff Differential Systems*, R. A. Willoughby, Ed. (Plenum Publishing Co., New York, 1974), p. 51.
6. M. C. MacCracken, D. J. Wuebbles, J. J. Walton, W. H. Duewer, and K. E. Grant, *The Livermore Regional Air Quality Model: I. Concept and Development*, Lawrence Livermore Laboratory, Preprint UCRL-77475, Part 1 (1975).
7. J. S. Chang, "Simulations, Perturbations and Interpretations," in *Proc. 3rd Conf. Climatic Impact Asses. Prog.*, Cambridge, Mass., 1974 (U. S. Dept. Transportation, Cambridge, 1974). p. 330.
8. M. C. MacCracken and J. S. Chang, *A Preliminary Study of the Potential Chemical and Climatic Effects of Atmospheric Nuclear Explosions*, Lawrence Livermore Laboratory, Rept. UCRL-51653 (1975).
9. J. S. Chang, D. J. Wuebbles and W. H. Duewer, *Sensitivity to Parameter Uncertainties for Ozone Reduction from Chlorofluoromethanes*, Lawrence Livermore Laboratory, Preprint UCRL-77432 (1976).
10. A. M. Winslow, *Numerical Model of Packed Bed Coal Gasification*, Lawrence Livermore Laboratory, Preprint UCRL-77627 (1976); to be presented at the 16th Int. Symp. Combustion, Aug. 15-21, 1976, Cambridge, Mass.
11. C. K. Westbrook, *Three-Dimensional Numerical Modeling of Liquid Fuel Sprays*, Lawrence Livermore Laboratory, Preprint UCRL-77621 (1976); to be presented at the 16th Int. Symp. Combustion, Aug. 15-21, 1976, Cambridge, Mass.

12. C. K. Westbrook, H. C. Gupta, and F. V. Bracco, "Mathematical Modeling of Two-Phase, Unsteady Two-Dimensional Flows," *Proc. 5th Intern. Colloq. Gasdynam. Explosions React. Syst., Bourges, France 1975*, in preparation.
13. C. K. Westbrook, *The CRIME Code: Chemically Reactive Implicit Multiphase Engine Model*, in preparation.
14. C. W. Gear, "The Automatic Integration of Ordinal Differential Equations," *Comm. ACM* 14 (3), 176 (1971).
15. H. F. Schaefer, *The Electronic Structure of Atoms and Molecules. A Survey of Rigorous Quantum Mechanical Results* (Addison-Wesley, Reading, Mass. 1971).
16. I. Shavitt, C. F. Bender, A. Papano, R. P. Hosterig, *J. Comp. Phys.* 11 90 (1973).
17. R. H. Hausman, Jr., S. D. Bloom, and C. F. Bender, *Chem. Phys. Letts.* 32, 483 (1975).
18. A. W. Fliflet, R. L. Chase, and H. P. Kelley, *J. Phys. B* 7, L443 (1974).
19. T. N. Rescigno and W. P. Reinhardt, *Phys. Rev. A* 8, 2828 (1973).
20. T. N. Rescigno and V. McKoy, *Phys. Rev. A* 12, 522 (1975).
21. B. W. Shore, *J. Phys. B* 7, 2502 (1974).
22. The first detailed atmospheric time-independent laser propagation codes to be developed are described in A. H. Aitken, J. H. Hayes, and P. B. Ulrich, *Propagation of High Energy 10.6 Micron Laser Beams Through the Atmosphere*, U. S. Naval Research Laboratory, Washington, D.C., Rept. 7293 (1971), and J. Hermann and L. C. Bradley, *Numerical Calculations of Light Propagation*, MIT Lincoln Laboratory, Lexington, Mass., Rept. LTP-10 (1971).
23. J. A. Fleck, Jr., J. R. Morris, and M. D. Feit, *Time-Dependent Propagation of High Energy Laser Beams Through the Atmosphere*, Lawrence Livermore Laboratory, Rept. UCRL-51826 (1976); *J. Appl. Phys.*, in press.
24. A. Edward, N. Ferriter, J. A. Fleck, and A. M. Winslow, *A Theoretical Description of the Interaction of a Pulsed Laser and a Target in an Air Environment*. Lawrence Livermore Laboratory, Rept. UCRL-51489 (1973).
25. E. Mendelovicz and J. W. Sherman, "Truncation Error Bounds for Signal Sampling," *Proc. 9th Asilomar Conf. Circuits, Systems, Comput., Pacific Grove, Ca., 1975* (Western Periodicals, North Hollywood, 1976), p. 16.
26. E. Mendelovicz, J. W. Sherman and J. T. Murphy, "Signal Sampling Theorems and Truncation Error Bounds," submitted to *IEEE Trans. Inf. Theory*.

27. J. W. Woods, "Two-Dimensional Markov Spectral Estimation," *IEEE Trans. Inf. Theory*, in press.
28. J. W. Woods, "Two Dimensional Discrete Markov Random Fields," *IEEE Trans. Inf. Theory* IT-18, 232 (1972).
29. M. P. Ekstrom and J. W. Woods, "Stability of Two-Dimensional Recursive Filters," *8th Ann. Princeton Conf. Inf. Sci. Syst.*, Princeton, 1974, (Princeton University Press, Princeton, 1974), p. 120; Lawrence Livermore Laboratory, Preprint UCRL-75326 (1974).
30. M. P. Ekstrom and J. W. Woods, "Two-Dimensional Spectral Factorization with Applications in Recursive Digital Filtering," *IEEE Trans. Acoust., Speech Signal Process.* ASSP-24, 115 (1976); Lawrence Livermore Laboratory, Preprint UCRL-76542 (1975).
31. M. P. Ekstrom, S. K. Mitra and J. W. Woods, NSF Grant: "Efficient Design of Two-Dimensional Recursive Digital Filters."
32. J. W. Wood and C. H. Radewan, "The Kalman Strip Filter — A Two-Dimensional Recursive Vector Processor," *Proc. 9th Asilomar Conf. Circuits, Systems Comput.* Pacific Grove, Calif. 1975 (Western Periodicals, North Hollywood, 1975), p. 101; Lawrence Livermore Laboratory, Preprint UCRL-77447 (1975).
33. J. W. Woods and C. H. Radewan, "Kalman Filtering in Two-Dimensions," to be presented at *IEEE Int. Symp. Inf. Theory*, Ronneby, Sweden, 1976.
34. M. P. Ekstrom, R. E. Twogood, "Recursive and Non-Recursive Digital Filtering of Images: Some Computational Considerations," presented at the *7th Asilomar Conf. Circuits, Systems Comput.* Pacific Grove, Calif., 1973; Lawrence Livermore Laboratory, Preprint UCRL-74979 (1973).
35. R. E. Twogood, M. P. Ekstrom, "An Extension of Eklundh's Matrix Transposition Algorithm and its Application in Digital Image Processing," *IEEE Trans. Comput.* in press; Lawrence Livermore Laboratory, Preprint UCRL-75986 (1975).
36. J. W. Woods, *Estimator-Correlator in Two-Dimensions*, in preparation.
37. M. P. Ekstrom and J. W. Woods, "Spectral Factorization in N-Dimensions," in preparation.
38. Lawrence Livermore Laboratory Chemistry Department Technical Note No. 247 — 67.
39. Gordon S. Smith and E. Kahara, *J. Appl. Crystallog.* 8, 681 (1975).

40. D. L. Vickers, G. S. Smith, S. R. Levine, and L. G. Cross, *Two Unusual Three-Dimensional Displays*, Lawrence Livermore Laboratory, Preprint UCRL-77526 (1976); *Trans. Amer. Crystallog. Assoc.*, in press.
41. J. T. Tou and R. C. Gonzales, *Pattern Recognition Principles* (Addison-Wesley, Reading, Mass., 1974).
42. P. C. Juis and T. L. Ssenhour, *Chemical Applications of Pattern Recognition* (Wiley, New York, 1975).
43. L. A. Cox, Jr. and C. F. Bender, *PATTER: A Polyalgorithm for the Analysis of Generalized Data Sets. Principles and Practice*, Lawrence Livermore Laboratory, Rept. UCID-16915 (1975).
44. L. R. Carlson, C. F. Bender, and R. H. Pritchard, "Pattern Recognition Techniques for Modeling Analytical Systems," *Res. Develop.* 26, 34 (1974).
45. C. F. Bender, L. R. Carlson, and R. H. Pritchard, *Pattern Recognition for Understanding and Modeling Materials Problems*, Lawrence Livermore Laboratory, Preprint UCRL-76541 (1975).
46. B. R. Kowalski and C. F. Bender, *J. Amer. Chem. Soc.* 96, 916 (1974).
47. A. Wagner, A. C. Wahl, A. M. Karo, and R. H. Krejci, *Classical Inelastic Scattering in $Li + H_2$: A Comparison of Different Potential Energy Surfaces*, in preparation.
48. H. G. Hammon, J. P. Bell, and N. W. Hetherington, *Calculation of Distribution of Oligomers and Free Diisocyanate in Urethane Prepolymers*, Lawrence Livermore Laboratory, Preprint UCRL-76687 (1975); submitted to *J. Polym. Sci., Part B*.
49. J. I. Karush and N. G. Smiriga, *Analysis of the Input/Output Queue of a Paged Drum*, Lawrence Livermore Laboratory, Preprint UCRL-77594 (1975); submitted to *J. Assoc. Comput. Mach.*
50. N. G. Smiriga, *The Reliability of Shiva*, Lawrence Livermore Laboratory, Numerical Mathematics Group Tech. Memo, No. 76-1, (1976).
51. P. M. Gluckman, Solving Maintenance Problems, presented at *AESOP Conf. Operations Data Center Managers, San Francisco, 1976*.
52. T. Fallon and P. M. Gluckman, Using a Statistical Procedure to Fine Tune a Computer Operation System, *Proc. Computer Sci. Statistics 8th Ann. Symp. Interfacem UCLA 1975*, (Health Sciences Computing Facility, UCLA, Los Angeles, 1975), p. 494.
53. P. M. Gluckman, User Related Indices of Computer Performance, presented at *AESOP Conf. Chicago, 1975*.

54. Draft report, dated December 1975, of the NSF-funded COSERS (Computer Science and Engineering Research Study) Panel on Numerical Computation.
55. F. N. Fritsch and A. W. Hall, *Numerical Mathematics Group Mathematical Software Library Catalog*, Lawrence Livermore Laboratory, Rept. UCID-30136 (1976).
56. A. C. Hindmarsh, GEAR: *Ordinary Differential Equation System Solver*, Lawrence Livermore Laboratory, Rept. UCID-30001, Rev. 3 (1974).
57. R. F. Sincovec and N. K. Madsen "Software for Nonlinear Partial Differential Equations," *ACM Trans. Math. Software* 1 (3) 232, 261 (1975); Lawrence Livermore Laboratory, Preprint UCRL-75658 (1975).
58. R. F. Hausman, Jr., *A Vector Method for Large Scale Configuration Interaction Problems*, Ph.D. thesis, University of California, Davis, in preparation.
59. R. E. von Holdt, *Normalizable Matrix Eigensystem Refinement*, Lawrence Livermore Laboratory, Preprint UCRL-77675, Revision 1 (1976), submitted to *Linear Algebra Appl.*
60. R. E. Carlson and R. P. Dickinson, Jr., *A Comparison of Piecewise Cubic Interpolation Schemes*, Lawrence Livermore Laboratory, Preprint UCRL-77893, (1976); submitted to *SIAM Rev.*
61. R. E. von Holdt, *STAR "Basic" Mathematical Subroutines*, Lawrence Livermore Laboratory, Rept. UCID-30123 (1975).
62. N. K. Madsen and G. H. Rodrigue, *A Comparison of Direct Methods for Tridiagonal Systems on the CDC STAR-100*, Lawrence Livermore Laboratory, Preprint UCRL-76993 (1975); submitted to *ACM Trans. Math. Software*.
63. G. H. Rodrigue, N. K. Madsen, J. I. Karush, *Cyclic Reduction for Banded Linear Equations*, Lawrence Livermore Laboratory, Rept. UCRL, in preparation.
64. J. O. Halliquist, *A Procedure for the Solution of Large Deformation Contact-Impact Problems by the Finite Element Method*, Lawrence Livermore Laboratory, Rept. UCRL-52066, to be released.

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